

# Discrete Orthogonality Relations for the Multi-Indexed Orthogonal Polynomials in Discrete Quantum Mechanics with Pure Imaginary Shifts

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## Abstract

The discrete orthogonality relations for the multi-indexed orthogonal polynomials in discrete quantum mechanics with pure imaginary shifts are investigated. We show that the discrete orthogonality relations hold for the case-(1) multi-indexed orthogonal polynomials of continuous Hahn, Wilson and Askey-Wilson types, and for the Krein-Adler type multi-indexed orthogonal polynomials in discrete quantum mechanics with pure imaginary shifts, and conjecture their normalization constants. In appendix we revisit the discrete orthogonality relations for the multi-indexed orthogonal polynomials in ordinary quantum mechanics and conjecture their normalization constants.

## 1 Introduction

Ordinary orthogonal polynomials in one variable,  $P_n(\eta)$  ( $n \in \mathbb{Z}_{\geq 0}$ ), are characterized by the three term recurrence relations [1],

$$\eta P_n(\eta) = A_n P_{n+1}(\eta) + B_n P_n(\eta) + C_n P_{n-1}(\eta) \quad (n \in \mathbb{Z}_{\geq 0}), \quad (1.1)$$

where  $P_n(\eta)$  is a polynomial of degree  $n$  in  $\eta$  and  $P_{-1}(\eta) = 0$ . The hypergeometric orthogonal polynomials of the Askey scheme satisfy the second order differential or difference equations [2]. New types of orthogonal polynomials  $P_{\mathcal{D},n}(\eta)$  ( $n \in \mathbb{Z}_{\geq 0}$ ), exceptional or multi-indexed orthogonal polynomials [3]–[14], satisfy the second order differential or difference equations, but do not satisfy the three term recurrence relations because of the missing degrees. We distinguish the following two cases; the set of missing degrees  $\mathcal{I} = \mathbb{Z}_{\geq 0} \setminus \{\deg P_{\mathcal{D},n}(\eta) | n \in \mathbb{Z}_{\geq 0}\}$  is case-(1):  $\mathcal{I} = \{0, 1, \dots, \ell - 1\}$ , or case-(2):  $\mathcal{I} \neq \{0, 1, \dots, \ell - 1\}$ , where  $\ell$  is a positive integer. The situation of case-(1) is called stable in [5]. Our study of orthogonal polynomials

is based on the quantum mechanical formulation: ordinary quantum mechanics (oQM), discrete quantum mechanics with pure imaginary shifts (idQM) [15]–[18] and discrete quantum mechanics with real shifts (rdQM) [19]–[21]. The Schrödinger equation of oQM is a differential equation and that of dQM is a difference equation. We deform exactly solvable quantum mechanical systems by multi-step Darboux transformations and obtain multi-indexed polynomials as eigenfunctions of the deformed systems. They are polynomials in the sinusoidal coordinate  $\eta(x)$  [22, 23],  $P_{\mathcal{D},n}(\eta(x))$ , where  $x$  is the coordinate of the quantum system. The case-(1) multi-indexed polynomials are obtained by taking the virtual state wavefunctions as seed solutions of the Darboux transformations. When the eigenfunctions are taken as seed solutions [24, 25], the resulting multi-indexed polynomials are case-(2), and we call them Krein-Adler type multi-indexed polynomials.

Any ordinary orthogonal polynomials  $P_n(\eta)$  satisfy the discrete orthogonal relations. Let us fix a positive integer  $\mathcal{N}$  and denote the zeros of  $P_{\mathcal{N}}(\eta)$  as  $\eta_j$  ( $j = 1, 2, \dots, \mathcal{N}$ ). Then the following discrete orthogonal relations hold [1]:

$$\sum_{j=1}^{\mathcal{N}} \text{sgn}(C_{\mathcal{N}}) \frac{P'_{\mathcal{N}}(\eta_j)}{P_{\mathcal{N}-1}(\eta_j)} \cdot \frac{P_n(\eta_j)}{P'_{\mathcal{N}}(\eta_j)} \frac{P_m(\eta_j)}{P'_{\mathcal{N}}(\eta_j)} = |C_{\mathcal{N}}| \frac{h_n}{h_{\mathcal{N}}} \delta_{nm} \quad (0 \leq n, m < \mathcal{N}), \quad (1.2)$$

where  $f'(x) = \frac{df(x)}{dx}$ , and  $\text{sgn}(C_{\mathcal{N}})$  is inserted for the positivity of the weight factor. Since the multi-indexed orthogonal polynomials  $P_{\mathcal{D},n}(\eta)$  are deformations of the ordinary orthogonal polynomials  $P_n(\eta)$ , it is expected that the multi-indexed polynomials also satisfy the discrete orthogonal relations. We naively expected the following:

$$\sum_{j=1}^{\tilde{\mathcal{N}}} \frac{P'_{\mathcal{D},\mathcal{N}}(\eta_j)}{P_{\mathcal{D},\mathcal{N}-1}(\eta_j)} \cdot \frac{P_{\mathcal{D},n}(\eta_j)}{P'_{\mathcal{D},\mathcal{N}}(\eta_j)} \frac{P_{\mathcal{D},m}(\eta_j)}{P'_{\mathcal{D},\mathcal{N}}(\eta_j)} \stackrel{?}{=} 0 \quad (n \neq m, \ 0 \leq n, m < \mathcal{N}), \quad (1.3)$$

where  $\tilde{\mathcal{N}} = \deg P_{\mathcal{D},\mathcal{N}}(\eta)$ . At first, we approached this problem by numerical calculation for the case-(1) multi-indexed polynomials of Laguerre, Jacobi, Wilson and Askey-Wilson types. It suggested that the discrete orthogonal relations hold for the multi-indexed polynomials, but (1.3) does not hold, namely the weight is not given by  $P'_{\mathcal{D},\mathcal{N}}(\eta_j)/P_{\mathcal{D},\mathcal{N}-1}(\eta_j)$ . In a private communication (2017), Sasaki informed the author that the weights for the multi-indexed Laguerre (L) and Jacobi (J) (and Hermite (H)) polynomials are given by  $1/c_2(\eta_j)$ , based on the perturbations around the zeros of orthogonal polynomials [26]. Here  $c_2(\eta)$  is given by

(2.132) of [18]

$$c_2(\eta) = \begin{cases} \frac{1}{4} & : \text{H} \\ \eta & : \text{L} \\ 1 - \eta^2 & : \text{J} \end{cases} . \quad (1.4)$$

In fact,  $P_n(\eta) = H_n(\eta), L_n^{(g-\frac{1}{2})}(\eta), P_n^{(g-\frac{1}{2}, h-\frac{1}{2})}(\eta)$  for H, L, J cases satisfy

$$\text{H} : P'_n(\eta) - 2nP_{n-1}(\eta) = 0,$$

$$\text{L} : \eta P'_n(\eta) + (n + g - \frac{1}{2})P_{n-1}(\eta) = nP_n(\eta),$$

$$\begin{aligned} \text{J} : & (2n + g + h - 1)(1 - \eta^2)P'_n(\eta) - 2(n + g - \frac{1}{2})(n + h - \frac{1}{2})P_{n-1}(\eta) \\ & = -n(h - g + (2n + g + h - 1)\eta)P_n(\eta), \end{aligned}$$

and these imply

$$\frac{P'_{\mathcal{N}}(\eta_j)}{P_{\mathcal{N}-1}(\eta_j)} = \begin{cases} \frac{1}{4} \times 8\mathcal{N} & : \text{H} \\ \frac{1}{\eta_j} \times (-1)(\mathcal{N} + g - \frac{1}{2}) & : \text{L} \\ \frac{1}{1 - \eta_j^2} \times \frac{2(\mathcal{N} + g - \frac{1}{2})(\mathcal{N} + h - \frac{1}{2})}{2\mathcal{N} + g + h - 1} & : \text{J} \end{cases} .$$

We verified this weight  $1/c_2(\eta_j)$  gives the discrete orthogonality relations for the case-(1) multi-indexed Laguerre and Jacobi polynomials by numerical calculation. For the case-(1) multi-indexed Wilson and Askey-Wilson polynomials, however, we could not find analytical expression of the weight at that time.

Recently Ho and Sasaki showed that the discrete orthogonality relations with the weight  $1/c_2(\eta_j)$  hold for the multi-indexed orthogonal polynomials in oQM: the case-(1) multi-indexed Laguerre and Jacobi polynomials, and the Krein-Adler type multi-indexed polynomials based on the Hermite, Laguerre and Jacobi polynomials [27]. Motivated by the perturbations around the zeros of orthogonal polynomials [26], they consider a matrix  $\widetilde{\mathcal{M}}$  and its symmetric version  $\mathcal{M}$ . Orthogonality of the eigenvectors of this symmetric matrix  $\mathcal{M}$  implies the discrete orthogonality relations for the multi-indexed polynomials.

In this paper, we consider the discrete orthogonality relations for the multi-indexed orthogonal polynomials in idQM. The strategy is the same as Ho-Sasaki. By considering a matrix  $\widetilde{\mathcal{M}}$  and its symmetric version  $\mathcal{M}$ , we show that the discrete orthogonality relations hold for the case-(1) multi-indexed polynomials of continuous Hahn, Wilson and Askey-Wilson types, and the Krein-Adler type multi-indexed polynomials.

This paper is organized as follows. In section 2 we present a general theory of the discrete orthogonality relations for orthogonal polynomials satisfying differential or difference equations. In section 3 the discrete orthogonality relations for the case-(1) multi-indexed orthogonal polynomials of continuous Hahn, Wilson and Askey-Wilson types are presented. Those for the Krein-Adler type multi-indexed orthogonal polynomials are given in section 4. Section 5 is for a summary and comments. In Appendix A Proposition 3.1 is proved. In Appendix B we revisit the discrete orthogonality relations for the multi-indexed orthogonal polynomials in oQM.

## 2 Discrete Orthogonality Relations

In this section we present a general theory of the discrete orthogonality relations for orthogonal polynomials satisfying differential or difference equations. The basic idea is given in [27].

Let us consider  $\check{P}_n(x) = P_n(\eta(x))$  ( $n \in \mathbb{Z}_{\geq 0}$ ), where  $x$  is a coordinate of some quantum system (physical range:  $x_1 \leq x \leq x_2$ ),  $\eta(x)$  is the sinusoidal coordinate [22, 23], and  $P_n(\eta)$  is a polynomial in  $\eta$ . We assume that  $P_n(\eta)$ 's are orthogonal polynomials,

$$\int_{x_1}^{x_2} dx \psi(x)^2 \check{P}_n(x) \check{P}_m(x) = h_n \delta_{nm} \quad (n, m \in \mathbb{Z}_{\geq 0}), \quad (2.1)$$

and satisfy a differential or difference equation,

$$\tilde{\mathcal{H}} \check{P}_n(x) = \mathcal{E}_n \check{P}_n(x) \quad (n \in \mathbb{Z}_{\geq 0}). \quad (2.2)$$

Here  $\psi(x)^2$  is a weight function,  $h_n$ 's are normalization constants ( $h_n > 0$ ), a differential or difference operator  $\tilde{\mathcal{H}}$  is a transformed Hamiltonian ('true' Hamiltonian is  $\mathcal{H} = \psi(x) \circ \tilde{\mathcal{H}} \circ \psi(x)^{-1}$ ), and  $\mathcal{E}_n$ 's are its energy eigenvalues. We assume  $\deg P_n < \deg P_m$  and  $\mathcal{E}_n < \mathcal{E}_m$  for  $n < m$ . The degree of  $P_n$  is  $\deg P_n = n$  for ordinary orthogonal polynomials, but  $\deg P_n \geq n$  for multi-indexed orthogonal polynomials.

Let us fix a non-negative integer  $\mathcal{N}$  and set  $\tilde{\mathcal{N}} = \deg P_{\mathcal{N}}$ . We denote the zeros of  $P_{\mathcal{N}}(\eta)$  as  $\eta_j^{[\mathcal{N}]}$  ( $j = 1, 2, \dots, \tilde{\mathcal{N}}$ ), which may be complex, and assume that they are simple. The sinusoidal coordinates considered in this paper are  $\eta(x) = x, x^2$  and  $\cos x$  (or  $\cos 2x$ ). The sinusoidal coordinate  $\eta(x)$  and the coordinate  $x$  have a one-to-one correspondence for the physical value of  $x$ , but this may not be the case for unphysical value of  $x$ . We fix  $x_j^{[\mathcal{N}]}$  uniquely, which gives  $\eta_j^{[\mathcal{N}]} = \eta(x_j^{[\mathcal{N}]})$ , by requiring  $x_1 \leq \text{Re } x_j^{[\mathcal{N}]} \leq x_2$ .

Let us assume the existence of  $\check{\mathcal{P}}_a(x) = \mathcal{P}_a(\eta(x))$  ( $a = 1, 2, \dots, \tilde{\mathcal{N}}$ ) that satisfy the following conditions:

$$\begin{aligned}
\text{(i)} & : \mathcal{P}_a(\eta) : \text{a polynomial in } \eta, \\
\text{(ii)} & : \deg \mathcal{P}_a < \tilde{\mathcal{N}}, \\
\text{(iii)} & : \tilde{\mathcal{H}}\check{\mathcal{P}}_a(x)|_{x=x_j^{[\mathcal{N}]}] = \mathcal{E}_a^{\mathcal{P}} \mathcal{P}_a(\eta_j^{[\mathcal{N}]})}, \\
\text{(iv)} & : \mathcal{E}_a^{\mathcal{P}} \neq \mathcal{E}_b^{\mathcal{P}} \quad (a \neq b).
\end{aligned} \tag{2.3}$$

The condition  $\deg \mathcal{P}_a < \deg \mathcal{P}_b$  for  $a < b$  is not imposed. Note that  $P_n(\eta)$  ( $n = 0, 1, \dots, \mathcal{N}-1$ ) satisfy the conditions (2.3) with  $\mathcal{E}_a^{\mathcal{P}} = \mathcal{E}_n$ . Since  $\mathcal{P}_a$  is a polynomial of  $\deg \mathcal{P}_a < \tilde{\mathcal{N}}$ , it is expressed as

$$\mathcal{P}_a(\eta) = \sum_{j=1}^{\tilde{\mathcal{N}}} \frac{\prod_{\substack{l=1 \\ l \neq j}}^{\tilde{\mathcal{N}}} (\eta - \eta_l^{[\mathcal{N}]})}{\prod_{\substack{l=1 \\ l \neq j}}^{\tilde{\mathcal{N}}} (\eta_j^{[\mathcal{N}]} - \eta_l^{[\mathcal{N}]})} \mathcal{P}_a(\eta_j^{[\mathcal{N}]}), \tag{2.4}$$

because the both sides agree at  $\tilde{\mathcal{N}}$  points  $\eta = \eta_j^{[\mathcal{N}]}$ . Note that this can be rewritten as

$$\mathcal{P}_a(\eta) = \sum_{j=1}^{\tilde{\mathcal{N}}} \frac{c_{\mathcal{N}}^{\mathcal{P}} \prod_{l=1}^{\tilde{\mathcal{N}}} (\eta - \eta_l^{[\mathcal{N}]})}{(\eta - \eta_j^{[\mathcal{N}]}) c_{\mathcal{N}}^{\mathcal{P}} \prod_{\substack{l=1 \\ l \neq j}}^{\tilde{\mathcal{N}}} (\eta_j^{[\mathcal{N}]} - \eta_l^{[\mathcal{N}]})} \mathcal{P}_a(\eta_j^{[\mathcal{N}]}) = \sum_{j=1}^{\tilde{\mathcal{N}}} \frac{P_{\mathcal{N}}(\eta)}{\eta - \eta_j^{[\mathcal{N}]}} \frac{\mathcal{P}_a(\eta_j^{[\mathcal{N}]})}{P'_{\mathcal{N}}(\eta_j^{[\mathcal{N}]})}, \tag{2.5}$$

where  $P_{\mathcal{N}}(\eta) = c_{\mathcal{N}}^{\mathcal{P}} \eta^{\tilde{\mathcal{N}}} + (\text{lower degree terms})$  and  $P'_{\mathcal{N}}(\eta) = \frac{d}{d\eta} P_{\mathcal{N}}(\eta)$ . By replacing  $j$  with  $k$  in (2.4), the action of  $\tilde{\mathcal{H}}$  on  $\check{\mathcal{P}}_a(x)$  is

$$\tilde{\mathcal{H}}\check{\mathcal{P}}_a(x) = \sum_{k=1}^{\tilde{\mathcal{N}}} \tilde{\mathcal{H}} \prod_{\substack{l=1 \\ l \neq k}}^{\tilde{\mathcal{N}}} (\eta(x) - \eta_l^{[\mathcal{N}]}) \times \frac{\mathcal{P}_a(\eta_k^{[\mathcal{N}]})}{\prod_{\substack{l=1 \\ l \neq k}}^{\tilde{\mathcal{N}}} (\eta_k^{[\mathcal{N}]} - \eta_l^{[\mathcal{N}]})}. \tag{2.6}$$

Let us evaluate this equation at  $x = x_j^{[\mathcal{N}]}$ . By the condition (iii) in (2.3), we obtain

$$\mathcal{E}_a^{\mathcal{P}} \mathcal{P}_a(\eta_j^{[\mathcal{N}]}) = \sum_{k=1}^{\tilde{\mathcal{N}}} \tilde{\mathcal{M}}_{jk} \prod_{\substack{l=1 \\ l \neq j}}^{\tilde{\mathcal{N}}} (\eta_j^{[\mathcal{N}]} - \eta_l^{[\mathcal{N}]}) \times \frac{\mathcal{P}_a(\eta_k^{[\mathcal{N}]})}{\prod_{\substack{l=1 \\ l \neq k}}^{\tilde{\mathcal{N}}} (\eta_k^{[\mathcal{N}]} - \eta_l^{[\mathcal{N}]})}, \tag{2.7}$$

where  $\tilde{\mathcal{M}}_{jk}$  is defined by

$$\tilde{\mathcal{M}}_{jk} \stackrel{\text{def}}{=} \frac{\tilde{\mathcal{H}} \prod_{\substack{l=1 \\ l \neq k}}^{\tilde{\mathcal{N}}} (\eta(x) - \eta_l^{[\mathcal{N}]}) \Big|_{x=x_j^{[\mathcal{N}]}}}{\prod_{\substack{l=1 \\ l \neq j}}^{\tilde{\mathcal{N}}} (\eta_j^{[\mathcal{N}]} - \eta_l^{[\mathcal{N}]})} \quad (j, k = 1, 2, \dots, \tilde{\mathcal{N}}). \tag{2.8}$$

By dividing (2.7) by  $\prod_{\substack{l=1 \\ l \neq j}}^{\tilde{\mathcal{N}}} (\eta_j^{[\mathcal{N}]} - \eta_l^{[\mathcal{N}]})$ , it becomes

$$\widetilde{\mathcal{M}} \tilde{v}^{(a)} = \mathcal{E}_a^{\mathcal{P}} \tilde{v}^{(a)}, \quad (2.9)$$

where a  $\tilde{\mathcal{N}} \times \tilde{\mathcal{N}}$  matrix  $\widetilde{\mathcal{M}}$  and  $\tilde{\mathcal{N}}$ -dimensional column vectors  $\tilde{v}^{(a)}$  are defined by

$$\widetilde{\mathcal{M}} = (\widetilde{\mathcal{M}}_{jk}), \quad \tilde{v}^{(a)} = (\tilde{v}_j^{(a)}), \quad \tilde{v}_j^{(a)} \stackrel{\text{def}}{=} \frac{\mathcal{P}_a(\eta_j^{[\mathcal{N}]})}{\prod_{\substack{l=1 \\ l \neq j}}^{\tilde{\mathcal{N}}} (\eta_j^{[\mathcal{N}]} - \eta_l^{[\mathcal{N}]})} = c_{\mathcal{N}}^{\mathcal{P}} \frac{\mathcal{P}_a(\eta_j^{[\mathcal{N}]})}{P'_{\mathcal{N}}(\eta_j^{[\mathcal{N}]})}. \quad (2.10)$$

By a similarity transformation in terms of a diagonal matrix  $G = \text{diag}(g_1, \dots, g_{\tilde{\mathcal{N}}})$ , we define a matrix  $\mathcal{M}$  and vectors  $v^{(a)}$  as

$$\mathcal{M} \stackrel{\text{def}}{=} G^{-1} \widetilde{\mathcal{M}} G, \quad v^{(a)} \stackrel{\text{def}}{=} G^{-1} \tilde{v}^{(a)} \quad \left( \Rightarrow \mathcal{M}_{jk} = \frac{g_k}{g_j} \widetilde{\mathcal{M}}_{jk}, \quad v_j^{(a)} = \frac{1}{g_j} \tilde{v}_j^{(a)}, \quad \mathcal{M} v^{(a)} = \mathcal{E}_a^{\mathcal{P}} v^{(a)} \right). \quad (2.11)$$

We assume the existence of  $G$  such that  $\mathcal{M}$  is symmetric,

$$\mathcal{M}_{jk} = \mathcal{M}_{kj}. \quad (2.12)$$

Then we have the following theorem.

**Theorem 2.1** *For  $\check{P}_n(x)$  satisfying (2.2),  $\mathcal{P}_a(\eta)$  satisfying (2.3) and  $G$  giving (2.12), we have the discrete orthogonality relations:*

$$\sum_{j=1}^{\tilde{\mathcal{N}}} \frac{1}{g_j^2} \frac{\mathcal{P}_a(\eta_j^{[\mathcal{N}]})}{P'_{\mathcal{N}}(\eta_j^{[\mathcal{N}]})} \frac{\mathcal{P}_b(\eta_j^{[\mathcal{N}]})}{P'_{\mathcal{N}}(\eta_j^{[\mathcal{N}]})} = k_a^{[\mathcal{N}]} \delta_{ab} \quad (a, b = 1, 2, \dots, \tilde{\mathcal{N}}), \quad (2.13)$$

where  $k_a^{[\mathcal{N}]}$ 's are normalization constants.

Proof: Let us consider a vector space  $\mathbb{C}^{\tilde{\mathcal{N}}} \ni v = (v_j)$  and a bilinear form  $\langle \cdot, \cdot \rangle : \mathbb{C}^{\tilde{\mathcal{N}}} \times \mathbb{C}^{\tilde{\mathcal{N}}} \rightarrow \mathbb{C}$ ,

$$\langle v, w \rangle \stackrel{\text{def}}{=} \sum_{j=1}^{\tilde{\mathcal{N}}} v_j w_j \quad (v, w \in \mathbb{C}^{\tilde{\mathcal{N}}}).$$

Since  $\mathcal{M}$  is symmetric, we have  $\langle \mathcal{M}v, w \rangle = \langle v, \mathcal{M}w \rangle$ . For  $v^{(a)}$  and  $v^{(b)}$ , we have

$$\langle v^{(a)}, v^{(b)} \rangle = \sum_{j=1}^{\tilde{\mathcal{N}}} \frac{1}{g_j^2} \tilde{v}_j^{(a)} \tilde{v}_j^{(b)} = (c_{\mathcal{N}}^{\mathcal{P}})^2 \sum_{j=1}^{\tilde{\mathcal{N}}} \frac{1}{g_j^2} \frac{\mathcal{P}_a(\eta_j^{[\mathcal{N}]})}{P'_{\mathcal{N}}(\eta_j^{[\mathcal{N}]})} \frac{\mathcal{P}_b(\eta_j^{[\mathcal{N}]})}{P'_{\mathcal{N}}(\eta_j^{[\mathcal{N}]})},$$

and

$$\mathcal{E}_a^{\mathcal{P}} \langle v^{(a)}, v^{(b)} \rangle = \langle \mathcal{M} v^{(a)}, v^{(b)} \rangle = \langle v^{(a)}, \mathcal{M} v^{(b)} \rangle = \mathcal{E}_b^{\mathcal{P}} \langle v^{(a)}, v^{(b)} \rangle,$$

which implies  $\langle v^{(a)}, v^{(b)} \rangle = 0$  for  $a \neq b$ . By setting  $k_a^{[\mathcal{N}]}$  as  $k_a^{[\mathcal{N}]} = (c_{\mathcal{N}}^P)^{-2} \langle v^{(a)}, v^{(a)} \rangle$ , we obtain (2.13).  $\square$

**Remark 2.1** The weight  $1/g_j^2$  in (2.13) may not be positive and may be complex, and the normalization constant  $k_a^{[\mathcal{N}]}$  may not be positive.

**Remark 2.2** The proof uses (2.2) but not (2.1) explicitly, and the theorem states nothing about the properties of  $k_a^{[\mathcal{N}]}$ . The theorem states nothing for  $\tilde{\mathcal{N}} = 0, 1$  cases either. Let us consider  $\mathcal{P}_a = P_n$  case. By using (2.1) and (2.5), we have

$$\begin{aligned} & \int_{x_1}^{x_2} dx \psi(x)^2 \check{P}_n(x) \check{P}_m(x) = h_n \delta_{nm} \\ &= \sum_{j=1}^{\tilde{\mathcal{N}}} \sum_{k=1}^{\tilde{\mathcal{N}}} \frac{P_n(\eta_j^{[\mathcal{N}]})}{P'_n(\eta_j^{[\mathcal{N}]})} \frac{P_m(\eta_k^{[\mathcal{N}]})}{P'_m(\eta_k^{[\mathcal{N}]})} \int_{x_1}^{x_2} dx \psi(x)^2 \frac{\check{P}_n(x)}{\eta(x) - \eta_j^{[\mathcal{N}]}} \frac{\check{P}_m(x)}{\eta(x) - \eta_k^{[\mathcal{N}]}}. \end{aligned} \quad (2.14)$$

Since we know Theorem 2.1, we naively expect the following equation,

$$\int_{x_1}^{x_2} dx \psi(x)^2 \frac{\check{P}_n(x)}{\eta(x) - \eta_j^{[\mathcal{N}]}} \frac{\check{P}_m(x)}{\eta(x) - \eta_k^{[\mathcal{N}]}} \stackrel{?}{=} 0 \quad (j \neq k). \quad (2.15)$$

However, numerical calculation shows that this equation holds for ordinary orthogonal polynomials, but does not for the multi-indexed orthogonal polynomials.

**Remark 2.3** The Ho-Sasaki's matrices in [27],  $\tilde{\mathcal{M}}^{\text{HS}}$  and  $\mathcal{M}^{\text{HS}}$ , correspond to  $\tilde{\mathcal{M}} - \mathcal{E}_{\mathcal{N}} \mathbf{1}$  and  $-\mathcal{M} + \mathcal{E}_{\mathcal{N}} \mathbf{1}$ , respectively. Their matrices are motivated by the perturbation around the zeros of orthogonal polynomials [26] and the scalar matrix  $\mathcal{E}_{\mathcal{N}} \mathbf{1}$  is subtracted.

We present examples of Theorem 2.1 in the following sections.

### 3 Multi-Indexed Orthogonal Polynomials

In this section, after recapitulating the case-(1) multi-indexed orthogonal polynomials in discrete quantum mechanics with pure imaginary shifts, we show their discrete orthogonality relations and conjecture the normalization constants.

The notations  $P_n$  and  $\tilde{\mathcal{H}}$  in § 2 correspond to  $P_{\mathcal{D},n}$  and  $\tilde{\mathcal{H}}_{\mathcal{D}}$  in this section, respectively.

### 3.1 Discrete quantum mechanics with pure imaginary shifts

Let us recapitulate the discrete quantum mechanics with pure imaginary shifts (idQM) [15, 18]. The dynamical variables of idQM are the real coordinate  $x$  ( $x_1 \leq x \leq x_2$ ) and the conjugate momentum  $p = -i \frac{d}{dx}$ , which are governed by the following factorized positive semi-definite Hamiltonian:

$$\mathcal{H} \stackrel{\text{def}}{=} \sqrt{V(x)} e^{\gamma p} \sqrt{V^*(x)} + \sqrt{V^*(x)} e^{-\gamma p} \sqrt{V(x)} - V(x) - V^*(x) = \mathcal{A}^\dagger \mathcal{A}, \quad (3.1)$$

$$\mathcal{A} \stackrel{\text{def}}{=} i(e^{\frac{\gamma}{2}p} \sqrt{V^*(x)} - e^{-\frac{\gamma}{2}p} \sqrt{V(x)}), \quad \mathcal{A}^\dagger \stackrel{\text{def}}{=} -i(\sqrt{V(x)} e^{\frac{\gamma}{2}p} - \sqrt{V^*(x)} e^{-\frac{\gamma}{2}p}). \quad (3.2)$$

Here the potential function  $V(x)$  is an analytic function of  $x$  and  $\gamma$  is a real constant. The  $*$ -operation on an analytic function  $f(x) = \sum_n a_n x^n$  ( $a_n \in \mathbb{C}$ ) is defined by  $f^*(x) = \sum_n a_n^* x^n$ , in which  $a_n^*$  is the complex conjugation of  $a_n$ . Note that  $\sqrt{\phantom{x}}$  is a square root as a complex function. The Schrödinger equation

$$\mathcal{H}\phi_n(x) = \mathcal{E}_n \phi_n(x) \quad (n \in \mathbb{Z}_{\geq 0}), \quad (3.3)$$

is an analytic difference equation with pure imaginary shifts. The inner product of two functions  $f(x)$  and  $g(x)$  is given by  $(f, g) \stackrel{\text{def}}{=} \int_{x_1}^{x_2} dx f^*(x)g(x)$ . The hermiticity of  $\mathcal{H}$ ,  $(f, \mathcal{H}g) = (\mathcal{H}f, g)$ , depends on singularities of some functions in the rectangular domain  $D_\gamma$  [15, 23, 9],

$$D_\gamma \stackrel{\text{def}}{=} \{x \in \mathbb{C} \mid x_1 \leq \text{Re } x \leq x_2, |\text{Im } x| \leq \frac{1}{2}|\gamma|\}. \quad (3.4)$$

The eigenfunctions  $\phi_n(x)$  can be chosen ‘real’,  $\phi_n^*(x) = \phi_n(x)$ , and the orthogonality relations read

$$(\phi_n, \phi_m) = h_n \delta_{nm} \quad (n, m \in \mathbb{Z}_{\geq 0}), \quad 0 < h_n < \infty. \quad (3.5)$$

We consider the idQM systems whose eigenfunctions  $\phi_n(x)$  (3.3) have the following form:

$$\phi_n(x) = \phi_0(x) \check{P}_n(x), \quad \check{P}_n(x) \stackrel{\text{def}}{=} P_n(\eta(x)) \quad (n \in \mathbb{Z}_{\geq 0}), \quad (3.6)$$

where  $\eta(x)$  is a sinusoidal coordinate [22, 23] and  $P_n(\eta)$  is an orthogonal polynomial of degree  $n$  in  $\eta$  and satisfies  $\check{P}_n^*(x) = \check{P}_n(x)$ . The energy eigenvalues satisfy  $0 = \mathcal{E}_0 < \mathcal{E}_1 < \mathcal{E}_2 < \dots$ . As a polynomial  $P_n(\eta)$ , we consider the continuous Hahn (cH), Wilson (W) and Askey-Wilson (AW) polynomials etc., which are members of the Askey-scheme of hypergeometric orthogonal polynomials [2]. We call the idQM system by the name of the orthogonal polynomial: continuous Hahn system, Wilson system, Askey-Wilson system etc. The similarity



transformation in terms of the ground state wavefunction gives the difference operator  $\tilde{\mathcal{H}}$ , which acts on the polynomial eigenfunctions and is square root free,

$$\tilde{\mathcal{H}} \stackrel{\text{def}}{=} \phi_0(x)^{-1} \circ \mathcal{H} \circ \phi_0(x) = V(x)(e^{\gamma p} - 1) + V^*(x)(e^{-\gamma p} - 1), \quad (3.7)$$

$$\tilde{\mathcal{H}}\check{P}_n(x) = \mathcal{E}_n\check{P}_n(x) \quad (n \in \mathbb{Z}_{\geq 0}). \quad (3.8)$$

Concrete idQM systems have a set of parameters  $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \dots)$  and various quantities depend on them. If necessary, their dependence is expressed like,  $f = f(\boldsymbol{\lambda})$ ,  $f(x) = f(x; \boldsymbol{\lambda})$ . For cH, W and AW systems, the parameters are  $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \lambda_3, \lambda_4)$  ( $\lambda_i \in \mathbb{C}$ ,  $\text{Re } \lambda_i > 0$ ) and satisfy

$$\text{cH} : \lambda_3 = \lambda_1^*, \quad \lambda_4 = \lambda_2^*, \quad (3.9)$$

$$\text{W, AW} : \{\lambda_1^*, \lambda_2^*, \lambda_3^*, \lambda_4^*\} = \{\lambda_1, \lambda_2, \lambda_3, \lambda_4\} \quad (\text{as a set}), \quad (3.10)$$

We remark that  $\boldsymbol{\lambda}$  for cH is taken as  $\boldsymbol{\lambda} = (\lambda_1, \lambda_2)$  in [14] because of (3.9). The AW system contains the parameter  $q$  ( $0 < q < 1$ ).

The data for  $V(x)$ ,  $\mathcal{E}_n$ ,  $\phi_0(x)$ ,  $P_n(\eta)$ ,  $\eta(x)$ ,  $h_n$  are given in § 2.2 of [14] and (2.25)–(2.26) of [28]. The parameters are  $\boldsymbol{\lambda} = (a_1, a_2, a_3, a_4)$  for cH and W ( $b_1 = a_1 + a_2 + a_3 + a_4$ ), and  $q^\lambda = (a_1, a_2, a_3, a_4)$  for AW ( $b_4 = a_1 a_2 a_3 a_4$ ).

## 3.2 Darboux transformations

The exactly solvable idQM systems in § 3.1 can be deformed by the multi-step Darboux transformations. We consider the Darboux transformations with virtual state wavefunctions as seed solutions. The  $M$ -step Darboux transformations are as follows. Take  $M$  virtual state wave functions,  $\tilde{\phi}_{d_1}(x), \tilde{\phi}_{d_2}(x), \dots, \tilde{\phi}_{d_M}(x)$  ( $d_j$  : mutually distinct), which are solutions of the Schrödinger equation,

$$\mathcal{H}\tilde{\phi}_v(x) = \tilde{\mathcal{E}}_v\tilde{\phi}_v(x), \quad \tilde{\mathcal{E}}_v < 0. \quad (3.11)$$

Note that  $\tilde{\phi}_v^*(x) = \tilde{\phi}_v(x)$ . In the  $s$ -step ( $1 \leq s \leq M$ ), we have [9] ( $s = 0$  :  $\mathcal{H} = \hat{\mathcal{A}}_{d_1}^\dagger \hat{\mathcal{A}}_{d_1} + \tilde{\mathcal{E}}_{d_1}$ )

$$\mathcal{H}_{d_1 \dots d_s} \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1 \dots d_s} \hat{\mathcal{A}}_{d_1 \dots d_s}^\dagger + \tilde{\mathcal{E}}_{d_s} = \hat{\mathcal{A}}_{d_1 \dots d_s d_{s+1}}^\dagger \hat{\mathcal{A}}_{d_1 \dots d_s d_{s+1}} + \tilde{\mathcal{E}}_{d_{s+1}}, \quad (3.12)$$

$$\begin{aligned} \hat{\mathcal{A}}_{d_1 \dots d_s} &\stackrel{\text{def}}{=} i \left( e^{\frac{\gamma}{2} p} \sqrt{\hat{V}_{d_1 \dots d_s}^*(x)} - e^{-\frac{\gamma}{2} p} \sqrt{\hat{V}_{d_1 \dots d_s}(x)} \right), \\ \hat{\mathcal{A}}_{d_1 \dots d_s}^\dagger &\stackrel{\text{def}}{=} -i \left( \sqrt{\hat{V}_{d_1 \dots d_s}(x)} e^{\frac{\gamma}{2} p} - \sqrt{\hat{V}_{d_1 \dots d_s}^*(x)} e^{-\frac{\gamma}{2} p} \right), \\ \hat{V}_{d_1 \dots d_s}(x) &\stackrel{\text{def}}{=} \sqrt{V(x - i \frac{s-1}{2} \gamma) V^*(x - i \frac{s+1}{2} \gamma)} \end{aligned} \quad (3.13)$$

$$\times \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_{s-1}}](x + i\frac{\gamma}{2})}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_{s-1}}](x - i\frac{\gamma}{2})} \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x - i\gamma)}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x)}, \quad (3.14)$$

$$\begin{aligned} \phi_{d_1 \dots d_s n}(x) &\stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1 \dots d_s} \phi_{d_1 \dots d_{s-1} n}(x) = \phi_{d_1 \dots d_s n}^*(x) \quad (n \in \mathbb{Z}_{\geq 0}) \\ &= A(x) W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \phi_n](x), \end{aligned} \quad (3.15)$$

$$A(x) = \left( \frac{\sqrt{\prod_{j=0}^{s-1} V(x + i(\frac{s}{2} - j)\gamma) V^*(x - i(\frac{s}{2} - j)\gamma)}}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x - i\frac{\gamma}{2}) W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x + i\frac{\gamma}{2})} \right)^{\frac{1}{2}}, \quad (3.16)$$

$$\begin{aligned} \tilde{\phi}_{d_1 \dots d_s v}(x) &\stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1 \dots d_s} \tilde{\phi}_{d_1 \dots d_{s-1} v}(x) = \tilde{\phi}_{d_1 \dots d_s v}^*(x) \quad (v \in \{d_1, \dots, d_M\} \setminus \{d_1, \dots, d_s\}) \\ &= A(x) W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \tilde{\phi}_v](x), \end{aligned} \quad (3.17)$$

$$\mathcal{H}_{d_1 \dots d_s} \phi_{d_1 \dots d_s n}(x) = \mathcal{E}_n \phi_{d_1 \dots d_s n}(x) \quad (n \in \mathbb{Z}_{\geq 0}), \quad (3.18)$$

$$\mathcal{H}_{d_1 \dots d_s} \tilde{\phi}_{d_1 \dots d_s v}(x) = \tilde{\mathcal{E}}_v \tilde{\phi}_{d_1 \dots d_s v}(x) \quad (v \in \{d_1, \dots, d_M\} \setminus \{d_1, \dots, d_s\}), \quad (3.19)$$

$$(\phi_{d_1 \dots d_s n}, \phi_{d_1 \dots d_s m}) = \prod_{j=1}^s (\mathcal{E}_n - \tilde{\mathcal{E}}_{d_j}) \cdot h_n \delta_{nm} \quad (n, m \in \mathbb{Z}_{\geq 0}), \quad (3.20)$$

where  $W_\gamma[f_1, \dots, f_n]$  is the Casorati determinant of a set of  $n$  functions  $\{f_j(x)\}$ ,

$$W_\gamma[f_1, \dots, f_n](x) \stackrel{\text{def}}{=} i^{\frac{1}{2}n(n-1)} \det \left( f_k(x_j^{(n)}) \right)_{1 \leq j, k \leq n}, \quad x_j^{(n)} \stackrel{\text{def}}{=} x + i(\frac{n+1}{2} - j)\gamma, \quad (3.21)$$

(for  $n = 0$ , we set  $W_\gamma[\cdot](x) = 1$ ). The operators  $\hat{\mathcal{A}}_{d_1 \dots d_s}$  and  $\hat{\mathcal{A}}_{d_1 \dots d_s}^\dagger$  have no zero modes, which is the characterization of virtual state wavefunctions (For cH case, we relax this condition because these operators may be singular in the intermediate steps.). Therefore the deformed systems are isospectral to the original system. The deformed Hamiltonian  $\mathcal{H}_{d_1 \dots d_s}$  can be rewritten in the standard form:

$$\mathcal{H}_{d_1 \dots d_s} = \mathcal{A}_{d_1 \dots d_s}^\dagger \mathcal{A}_{d_1 \dots d_s}, \quad (3.22)$$

$$\begin{aligned} \mathcal{A}_{d_1 \dots d_s} &\stackrel{\text{def}}{=} i \left( e^{\frac{\gamma}{2}p} \sqrt{V_{d_1 \dots d_s}^*}(x) - e^{-\frac{\gamma}{2}p} \sqrt{V_{d_1 \dots d_s}}(x) \right), \\ \mathcal{A}_{d_1 \dots d_s}^\dagger &\stackrel{\text{def}}{=} -i \left( \sqrt{V_{d_1 \dots d_s}}(x) e^{\frac{\gamma}{2}p} - \sqrt{V_{d_1 \dots d_s}^*}(x) e^{-\frac{\gamma}{2}p} \right), \end{aligned} \quad (3.23)$$

$$\begin{aligned} V_{d_1 \dots d_s}(x) &\stackrel{\text{def}}{=} \sqrt{V(x - i\frac{s}{2}\gamma) V^*(x - i\frac{s+2}{2}\gamma)} \\ &\times \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x + i\frac{\gamma}{2})}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x - i\frac{\gamma}{2})} \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \phi_0](x - i\gamma)}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \phi_0](x)}. \end{aligned} \quad (3.24)$$

These formulas (3.12)–(3.24) (except for (3.20)) are derived algebraically ((3.20) is derived only formally unless  $\mathcal{H}_{d_1 \dots d_{s'}}$  ( $s' \leq s$ ) are hermite). The hermiticity of  $\mathcal{H}_{d_1 \dots d_s}$  etc. should be considered in each case.

### 3.3 Multi-indexed orthogonal polynomials

We recapitulate the case-(1) multi-indexed orthogonal polynomials of cH, W and AW types.

There are two types of the virtual state wavefunctions, type I  $\tilde{\phi}_v^I(x)$  and type II  $\tilde{\phi}_v^{II}(x)$  for cH, W and AW idQM systems. The deformed systems are labeled by the index set  $\mathcal{D}$ ,

$$\begin{aligned}\mathcal{D} &= \{d_1, \dots, d_M\} \quad (d_j \in \mathbb{Z}_{\geq 0}), \quad \mathcal{D} = \mathcal{D}^I \cup \mathcal{D}^{II}, \quad M = M_I + M_{II}, \\ \mathcal{D}^I &\stackrel{\text{def}}{=} \{d \in \mathcal{D} \mid d : \text{type I}\} = \{d_1^I, \dots, d_{M_I}^I\} \quad (d_j^I : \text{mutually distinct}), \\ \mathcal{D}^{II} &\stackrel{\text{def}}{=} \{d \in \mathcal{D} \mid d : \text{type II}\} = \{d_1^{II}, \dots, d_{M_{II}}^{II}\} \quad (d_j^{II} : \text{mutually distinct}),\end{aligned}\tag{3.25}$$

which are the degrees and types of the virtual state wavefunctions used in  $M$ -step Darboux transformations. The Hamiltonian is deformed as  $\mathcal{H} \rightarrow \mathcal{H}_{d_1} \rightarrow \mathcal{H}_{d_1 d_2} \rightarrow \dots \rightarrow \mathcal{H}_{d_1 \dots d_s} \rightarrow \dots \rightarrow \mathcal{H}_{d_1 \dots d_M} = \mathcal{H}_{\mathcal{D}}$  by  $M$ -step Darboux transformations. Various quantities of the deformed systems are denoted as  $\mathcal{H}_{\mathcal{D}}$ ,  $\phi_{\mathcal{D},n}$ ,  $\mathcal{A}_{\mathcal{D}}$ , etc. Exactly speaking,  $\mathcal{D}$  is an ordered set. When the ordered set  $\mathcal{D}$  is  $\mathcal{D} = \{d_1^I, \dots, d_{M_I}^I, d_1^{II}, \dots, d_{M_{II}}^{II}\}$  with  $0 \leq d_1^I < \dots < d_{M_I}^I$  and  $0 \leq d_1^{II} < \dots < d_{M_{II}}^{II}$ , we call it the standard order. Under the permutation of  $d_j$ 's, the deformed Hamiltonian  $\mathcal{H}_{\mathcal{D}}$  is invariant, but the denominator polynomial  $\check{\Xi}_{\mathcal{D}}(x)$  and the multi-indexed polynomials  $\check{P}_{\mathcal{D},n}(x)$  may change their signs. Unless otherwise mentioned, we do not care much about the order of  $\mathcal{D}$ .

The denominator polynomial  $\Xi_{\mathcal{D}}$  and the multi-indexed polynomials  $P_{\mathcal{D},n}$  are constructed as polynomial parts of the Casoratians  $W_{\gamma}[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}](x)$  and  $W_{\gamma}[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \phi_n](x)$ , respectively,

$$W_{\gamma}[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}](x) = g_{\mathcal{D}}(x) \check{\Xi}_{\mathcal{D}}(x), \quad \check{\Xi}_{\mathcal{D}}(x) \stackrel{\text{def}}{=} \Xi_{\mathcal{D}}(\eta(x)),\tag{3.26}$$

$$W_{\gamma}[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \phi_n](x) = g_{\mathcal{D}}^P(x) \check{P}_{\mathcal{D},n}(x), \quad \check{P}_{\mathcal{D},n}(x) \stackrel{\text{def}}{=} P_{\mathcal{D},n}(\eta(x)),\tag{3.27}$$

whose concrete definitions are given by (3.18)–(3.19) of [14] and (3.37)–(3.38) of [9], and  $g_{\mathcal{D}}(x)$  and  $g_{\mathcal{D}}^P(x)$  can be read from (3.25)–(3.26) of [14] and (3.50)–(3.51) of [29] with  $W_{\gamma}[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}](x) = \prod_{j=1}^M \phi_0(x_j^{(M)}) \cdot W_{\gamma}[\nu^{-1} \check{\xi}_{d_1}, \dots, \nu^{-1} \check{\xi}_{d_M}](x)$  and  $W_{\gamma}[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \phi_n](x) = \prod_{j=1}^{M+1} \phi_0(x_j^{(M+1)}) \cdot W_{\gamma}[\nu^{-1} \check{\xi}_{d_1}, \dots, \nu^{-1} \check{\xi}_{d_M}, \check{P}_n](x)$ . We remark that  $g_{\mathcal{D}}(x)$  and  $g_{\mathcal{D}}^P(x)$  depend on  $M_I$  and  $M_{II}$ , but not on the specific values of  $d_j$  and  $n$ . Note that  $\check{\Xi}_{\mathcal{D}}^*(x) = \check{\Xi}_{\mathcal{D}}(x)$  and  $\check{P}_{\mathcal{D},n}^*(x) = \check{P}_{\mathcal{D},n}(x)$ . The denominator polynomial  $\Xi_{\mathcal{D}}(\eta)$  and the multi-indexed polynomials  $P_{\mathcal{D},n}(\eta)$  are polynomials in  $\eta$  and their degrees are  $\ell_{\mathcal{D}}$  and  $\ell_{\mathcal{D}} + n$ , respectively (we

assume  $c_{\mathcal{D}}^{\Xi} \neq 0$  and  $c_{\mathcal{D},n}^P \neq 0$ , see (A.1)–(A.2) of [14] and (A.40)–(A.41) of [30]). Here  $\ell_{\mathcal{D}}$  is

$$\ell_{\mathcal{D}} \stackrel{\text{def}}{=} \sum_{j=1}^M d_j - \frac{1}{2}M(M-1) + 2M_{\text{I}}M_{\text{II}}. \quad (3.28)$$

We remark that  $P_{\mathcal{D},0}$  and  $\Xi_{\mathcal{D}}$  are proportional,  $\check{P}_{\mathcal{D},0}(x; \boldsymbol{\lambda}) \propto \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})$ , (A.3) of [14], (3.44) of [9], which is a consequence of the shape invariance.

The eigenfunctions of the deformed system (3.15) are expressed in terms of the ground state wavefunction  $\phi_0(x)$  with shifted parameters, the denominator polynomials  $\check{\Xi}_{\mathcal{D}}(x)$  and the multi-indexed polynomial  $\check{P}_{\mathcal{D},n}(x)$  as

$$\phi_{\mathcal{D}n}(x) = c_{\mathcal{D}}^{\phi} \psi_{\mathcal{D}}(x) \check{P}_{\mathcal{D},n}(x) \quad (n \in \mathbb{Z}_{\geq 0}), \quad (3.29)$$

$$\psi_{\mathcal{D}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{\phi_0(x; \boldsymbol{\lambda}_{\mathcal{D}})}{\sqrt{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}}, \quad (3.30)$$

where  $c_{\mathcal{D}}^{\phi}$  and  $\boldsymbol{\lambda}_{\mathcal{D}}$  (which is denoted as  $\boldsymbol{\lambda}^{[M_{\text{I}}, M_{\text{II}}]}$  in previous papers) are

$$c_{\mathcal{D}}^{\phi} = \alpha^{\text{I}}(\boldsymbol{\lambda})^{\frac{1}{2}M_{\text{I}}} \alpha^{\text{II}}(\boldsymbol{\lambda})^{\frac{1}{2}M_{\text{II}}} \kappa^{\frac{1}{4}M(M-1) + M_{\text{I}}M_{\text{II}}}, \quad (3.31)$$

$$\boldsymbol{\lambda}_{\mathcal{D}} \stackrel{\text{def}}{=} \boldsymbol{\lambda} + M_{\text{I}}\tilde{\boldsymbol{\delta}}^{\text{I}} + M_{\text{II}}\tilde{\boldsymbol{\delta}}^{\text{II}}. \quad (3.32)$$

Here explicit forms of  $\alpha(\boldsymbol{\lambda})$  and  $\tilde{\boldsymbol{\delta}}$  are given by (3.1), (3.3) of [14] and (3.25), (3.27) of [9].

The deformed Hamiltonian  $\mathcal{H}_{\mathcal{D}}$  in the standard form (3.22) is specified by the potential function  $V_{\mathcal{D}}$  (3.24) and it is expressed in terms of the potential function  $V(x)$  with shifted parameters and the denominator polynomial  $\check{\Xi}_{\mathcal{D}}(x)$  (with shifted parameters),

$$V_{\mathcal{D}}(x; \boldsymbol{\lambda}) = V(x; \boldsymbol{\lambda}_{\mathcal{D}}) \frac{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})} \frac{\check{\Xi}_{\mathcal{D}}(x - i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})}. \quad (3.33)$$

In order for the deformed Hamiltonian  $\mathcal{H}_{\mathcal{D}}$  to be hermitian, the parameters  $\boldsymbol{\lambda}$  are restricted. As a sufficient condition for the hermiticity, we have the following [9, 14]:

$$\text{The denominator polynomial } \check{\Xi}_{\mathcal{D}}(x) \text{ has no zero in } D_{\gamma} \text{ (3.4)}. \quad (3.34)$$

For cH case, the degree of  $\Xi_{\mathcal{D}}(\eta)$ ,  $\ell_{\mathcal{D}}$ , should be even. In the following, we assume that the range of parameters is chosen so that the deformed Hamiltonian  $\mathcal{H}_{\mathcal{D}}$  is hermitian.

The orthogonality of the eigenfunctions (3.20), namely, those of the multi-indexed polynomials  $\check{P}_{\mathcal{D},n}(x)$  are

$$\int_{x_1}^{x_2} dx \psi_{\mathcal{D}}(x)^2 \check{P}_{\mathcal{D},n}(x) \check{P}_{\mathcal{D},m}(x) = h_{\mathcal{D},n} \delta_{nm} \quad (n, m \in \mathbb{Z}_{\geq 0}), \quad (3.35)$$

$$h_{\mathcal{D},n} = (c_{\mathcal{D}}^{\phi})^{-2} h_n \prod_{j=1}^{M_I} (\mathcal{E}_n - \tilde{\mathcal{E}}_{d_j^I}^I) \cdot \prod_{j=1}^{M_{II}} (\mathcal{E}_n - \tilde{\mathcal{E}}_{d_j^{II}}^{II}), \quad (3.36)$$

where explicit forms of  $\tilde{\mathcal{E}}_v$  are given by (3.7) of [14] and (3.29) of [9]. The multi-indexed orthogonal polynomial  $P_{\mathcal{D},n}(\eta)$  has  $n$  zeros in the physical region  $\eta_{\min} < \eta < \eta_{\max}$  ( $\eta_{\min} \stackrel{\text{def}}{=} \min(\eta(x_1), \eta(x_2))$ ,  $\eta_{\max} \stackrel{\text{def}}{=} \max(\eta(x_1), \eta(x_2))$ ), which interlace the  $n+1$  zeros of  $P_{\mathcal{D},n+1}(\eta)$  in the physical region, and  $\ell_{\mathcal{D}}$  zeros in the unphysical region  $\eta \in \mathbb{C} \setminus (\eta_{\min}, \eta_{\max})$ .

The similarity transformed Hamiltonian in terms of  $\psi_{\mathcal{D}}(x)$  is square root free,

$$\begin{aligned} \tilde{\mathcal{H}}_{\mathcal{D}} &\stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x)^{-1} \circ \mathcal{H}_{\mathcal{D}} \circ \psi_{\mathcal{D}}(x) \\ &= V(x; \boldsymbol{\lambda}_{\mathcal{D}}) \frac{\tilde{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\tilde{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})} \left( e^{\gamma p} - \frac{\tilde{\Xi}_{\mathcal{D}}(x - i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\tilde{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \right) \\ &\quad + V^*(x; \boldsymbol{\lambda}_{\mathcal{D}}) \frac{\tilde{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\tilde{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})} \left( e^{-\gamma p} - \frac{\tilde{\Xi}_{\mathcal{D}}(x + i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\tilde{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \right), \end{aligned} \quad (3.37)$$

and the multi-indexed polynomials  $\check{P}_{\mathcal{D},n}(x)$  are its eigenpolynomials,

$$\tilde{\mathcal{H}}_{\mathcal{D}} \check{P}_{\mathcal{D},n}(x) = \mathcal{E}_n \check{P}_{\mathcal{D},n}(x) \quad (n \in \mathbb{Z}_{\geq 0}). \quad (3.38)$$

### 3.4 Some identities

For the ordered index set  $\mathcal{D} = \{d_1, \dots, d_M\}$ , let us consider the following ordered index sets,

$$\mathcal{D}' = \{d_1, \dots, d_M, d'\}, \quad \mathcal{D}'' = \{d_1, \dots, d_M, d''\}, \quad \mathcal{D}''' = \{d_1, \dots, d_M, d', d''\}, \quad (3.39)$$

where  $d', d'' \notin \mathcal{D}$  and  $d' \neq d''$ . From the properties of the multi-step Darboux transformations given in §3.2, we have the following identities:

$$\phi_{\mathcal{D}''n}(x) = \hat{\mathcal{A}}_{\mathcal{D}''}^{\dagger} \frac{\hat{\mathcal{A}}_{\mathcal{D}'}^{\dagger}}{\mathcal{E}_n - \tilde{\mathcal{E}}_{d'}} \phi_{\mathcal{D}'n}(x), \quad (3.40)$$

$$\phi_{\mathcal{D}'''n}(x) = \hat{\mathcal{A}}_{\mathcal{D}'''} \hat{\mathcal{A}}_{\mathcal{D}'} \phi_{\mathcal{D}n}(x). \quad (3.41)$$

By extracting the polynomial parts from these identities, we obtain the following proposition.

#### Proposition 3.1

(1) When the types of  $d'$  and  $d''$  are the same, (3.40) gives

$$(\mathcal{E}_n - \tilde{\mathcal{E}}_{d'}) \left( \frac{\tilde{\Xi}_{\mathcal{D}'}(x - i\frac{\gamma}{2})}{\tilde{\Xi}_{\mathcal{D}''}(x - i\frac{\gamma}{2})} + \frac{\tilde{\Xi}_{\mathcal{D}'}(x + i\frac{\gamma}{2})}{\tilde{\Xi}_{\mathcal{D}''}(x + i\frac{\gamma}{2})} \right) \check{P}_{\mathcal{D}''n}(x) = (\tilde{\mathcal{H}}_{\mathcal{D}''} + \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) \check{P}_{\mathcal{D}',n}(x). \quad (3.42)$$

(2) When the types of  $d'$  and  $d''$  are different, (3.41) gives

$$\kappa^{2M+\frac{3}{2}}\sqrt{\alpha^I\alpha^{II}}\left(\frac{\check{\Xi}_{\mathcal{D}}(x-i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}'''}(x-i\frac{\gamma}{2})}+\frac{\check{\Xi}_{\mathcal{D}}(x+i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}'''}(x+i\frac{\gamma}{2})}\right)\check{P}_{\mathcal{D}''',n}(x)=(\check{\mathcal{H}}_{\mathcal{D}'''}+\mathcal{E}_n-\check{\mathcal{E}}_{d'}-\check{\mathcal{E}}_{d''})\check{P}_{\mathcal{D},n}(x). \quad (3.43)$$

Since the proof is rather technical, we present it in Appendix A.

**Remark 3.1** The identities (3.42) and (3.43) are invariant under the permutation of  $d_j$ ,  $d'$ ,  $d''$  in  $\mathcal{D}$ ,  $\mathcal{D}'$ ,  $\mathcal{D}''$ ,  $\mathcal{D}'''$ , namely, the order of ordered sets  $\mathcal{D}$ ,  $\mathcal{D}'$ ,  $\mathcal{D}''$  and  $\mathcal{D}'''$  is irrelevant.

**Remark 3.2** For generic values of  $\lambda$ ,  $\check{P}_{\mathcal{D},n}(x)$  and  $\check{\Xi}_{\mathcal{D}}(x \pm i\frac{\gamma}{2})$  do not have a common root.

### 3.5 Discrete orthogonality relations

Let us fix a non-negative integer  $\mathcal{N}$  and set  $\tilde{\mathcal{N}} = \deg P_{\mathcal{D},\mathcal{N}} = \ell_{\mathcal{D}} + \mathcal{N}$ . We denote the zeros of  $P_{\mathcal{D},\mathcal{N}}(\eta)$  as  $\eta_j^{[\mathcal{D},\mathcal{N}]}$  ( $j = 1, 2, \dots, \tilde{\mathcal{N}}$ ), and assume that they are simple. We define  $x_j^{[\mathcal{D},\mathcal{N}]}$  by requiring  $\eta(x_j^{[\mathcal{D},\mathcal{N}]}) = \eta_j^{[\mathcal{D},\mathcal{N}]}$  and  $x_1 \leq \operatorname{Re} x_j^{[\mathcal{D},\mathcal{N}]} \leq x_2$ .

In the following, for simplicity in notation, we write  $\eta_j^{[\mathcal{D},\mathcal{N}]}$  and  $x_j^{[\mathcal{D},\mathcal{N}]}$  as  $\eta_j$  and  $x_j$ , respectively. (Although this notation  $x_j$  conflicts with the end points of the physical range of the coordinate ( $x_1$  and  $x_2$ ), we think this does not cause any confusion.) Then  $\check{P}_{\mathcal{D},\mathcal{N}}(x)$  is expressed as

$$\check{P}_{\mathcal{D},\mathcal{N}}(x) = c_{\mathcal{D},\mathcal{N}}^P \prod_{j=1}^{\tilde{\mathcal{N}}} (\eta(x) - \eta_j). \quad (3.44)$$

#### 3.5.1 polynomials $\mathcal{P}_a$

For the index set  $\mathcal{D}$  (3.25) in the standard order, let us define the index sets  $\mathcal{D}'_{1,jk}$ ,  $\mathcal{D}'_{2,jk}$  and  $\mathcal{D}'_{3,jk}$  as follows [27]:

$$(1) \mathcal{D}'_{1,jk} : E^I \stackrel{\text{def}}{=} \{0, 1, \dots, d_{M_I}^I\} \setminus \mathcal{D}^I, \quad d_j^I \in \mathcal{D}^I, \quad E_j^I \stackrel{\text{def}}{=} \{\epsilon \in E^I \mid \epsilon < d_j^I\}, \quad \epsilon_k^I \in E_j^I, \\ \mathcal{D}_{jk}^{I'} \stackrel{\text{def}}{=} (\mathcal{D}^I \setminus \{d_j^I\}) \cup \{\epsilon_k^I\}, \quad \mathcal{D}'_{1,jk} \stackrel{\text{def}}{=} \mathcal{D}_{jk}^{I'} \cup \mathcal{D}^{II}, \quad (3.45)$$

$$(2) \mathcal{D}'_{2,jk} : E^{II} \stackrel{\text{def}}{=} \{0, 1, \dots, d_{M_{II}}^{II}\} \setminus \mathcal{D}^{II}, \quad d_j^{II} \in \mathcal{D}^{II}, \quad E_j^{II} \stackrel{\text{def}}{=} \{\epsilon \in E^{II} \mid \epsilon < d_j^{II}\}, \quad \epsilon_k^{II} \in E_j^{II}, \\ \mathcal{D}_{jk}^{II'} \stackrel{\text{def}}{=} (\mathcal{D}^{II} \setminus \{d_j^{II}\}) \cup \{\epsilon_k^{II}\}, \quad \mathcal{D}'_{2,jk} \stackrel{\text{def}}{=} \mathcal{D}^I \cup \mathcal{D}_{jk}^{II'}, \quad (3.46)$$

$$(3) \mathcal{D}'_{3,jk} : d_j^I \in \mathcal{D}^I, \quad d_k^{II} \in \mathcal{D}^{II}, \quad \mathcal{D}'_{3,jk} \stackrel{\text{def}}{=} (\mathcal{D}^I \setminus \{d_j^I\}) \cup (\mathcal{D}^{II} \setminus \{d_k^{II}\}). \quad (3.47)$$

As an ordered set, we choose one order of the elements for each  $\mathcal{D}'_{1,jk}$ ,  $\mathcal{D}'_{2,jk}$  and  $\mathcal{D}'_{3,jk}$ , e.g. the standard order. Note that  $|E_j^I| = d_j^I - (j-1)$  and  $|E_j^{II}| = d_j^{II} - (j-1)$ . The numbers of

these sets are

$$\begin{aligned}
\#\{\mathcal{D}'_{1,jk}\} &= \sum_{j=1}^{M_I} (d_j^I - (j-1)) = \sum_{j=1}^{M_I} d_j^I - \frac{1}{2}M_I(M_I-1), \\
\#\{\mathcal{D}'_{2,jk}\} &= \sum_{j=1}^{M_{II}} (d_j^{II} - (j-1)) = \sum_{j=1}^{M_{II}} d_j^{II} - \frac{1}{2}M_{II}(M_{II}-1), \\
\#\{\mathcal{D}'_{3,jk}\} &= M_I M_{II},
\end{aligned} \tag{3.48}$$

and the sum of these numbers is  $\ell_{\mathcal{D}}$  (3.28).

Let us define the polynomials  $\check{\mathcal{P}}_a(x) = \mathcal{P}_a(\eta(x))$  ( $a = 1, \dots, \tilde{\mathcal{N}}$ ) as follows [27]:

$$\begin{aligned}
(0) : \check{\mathcal{P}}_a(x) &= \check{P}_{\mathcal{D},n}(x) \quad (0 \leq n < \mathcal{N}), \\
(1) : \check{\mathcal{P}}_a(x) &= \check{P}_{\mathcal{D}'_{1,jk},\mathcal{N}}(x) \quad (\mathcal{D}'_{1,jk} \text{ in (3.45)}), \\
(2) : \check{\mathcal{P}}_a(x) &= \check{P}_{\mathcal{D}'_{2,jk},\mathcal{N}}(x) \quad (\mathcal{D}'_{2,jk} \text{ in (3.46)}), \\
(3) : \check{\mathcal{P}}_a(x) &= \check{P}_{\mathcal{D}'_{3,jk},\mathcal{N}}(x) \quad (\mathcal{D}'_{3,jk} \text{ in (3.47)}).
\end{aligned} \tag{3.49}$$

The total number of these  $\check{\mathcal{P}}_a(x)$  is actually  $\mathcal{N} + \ell_{\mathcal{D}} = \tilde{\mathcal{N}}$ .

Let us show that the conditions in (2.3) are satisfied. The condition (i) is trivial. The condition (ii) is satisfied, because we have

$$\begin{aligned}
(0) : \deg \mathcal{P}_a &= \ell_{\mathcal{D}} + n, \quad n < \mathcal{N}, \\
(1) : \deg \mathcal{P}_a &= \ell_{\mathcal{D}'_{1,jk}} + \mathcal{N}, \quad \ell_{\mathcal{D}'_{1,jk}} = \ell_{\mathcal{D}} - d_j^I + \epsilon_k^I < \ell_{\mathcal{D}}, \\
(2) : \deg \mathcal{P}_a &= \ell_{\mathcal{D}'_{2,jk}} + \mathcal{N}, \quad \ell_{\mathcal{D}'_{2,jk}} = \ell_{\mathcal{D}} - d_j^{II} + \epsilon_k^{II} < \ell_{\mathcal{D}}, \\
(3) : \deg \mathcal{P}_a &= \ell_{\mathcal{D}'_{3,jk}} + \mathcal{N}, \quad \ell_{\mathcal{D}'_{3,jk}} = \ell_{\mathcal{D}} - d_j^I - d_k^{II} - 1 < \ell_{\mathcal{D}}.
\end{aligned} \tag{3.50}$$

The condition (iii) is satisfied by the following proposition.

**Proposition 3.2** *For  $\check{\mathcal{P}}_a(x)$  (3.49), we have*

$$\tilde{\mathcal{H}}_{\mathcal{D}} \check{\mathcal{P}}_a(x) \big|_{x=x_j} = \mathcal{E}_a^{\mathcal{P}} \mathcal{P}_a(\eta_j), \tag{3.51}$$

where  $\mathcal{E}_a^{\mathcal{P}}$  are given by

$$\begin{aligned}
(0) : \mathcal{E}_a^{\mathcal{P}} &= \mathcal{E}_n, \\
(1) : \mathcal{E}_a^{\mathcal{P}} &= \tilde{\mathcal{E}}_{d_j^I}^I + \tilde{\mathcal{E}}_{\epsilon_k^I}^I - \mathcal{E}_{\mathcal{N}}, \\
(2) : \mathcal{E}_a^{\mathcal{P}} &= \tilde{\mathcal{E}}_{d_j^{II}}^{II} + \tilde{\mathcal{E}}_{\epsilon_k^{II}}^{II} - \mathcal{E}_{\mathcal{N}}, \\
(3) : \mathcal{E}_a^{\mathcal{P}} &= \tilde{\mathcal{E}}_{d_j^I}^I + \tilde{\mathcal{E}}_{d_k^{II}}^{II} - \mathcal{E}_{\mathcal{N}}.
\end{aligned} \tag{3.52}$$

Proof:

(0): Eq. (3.38) gives  $\tilde{\mathcal{H}}_{\mathcal{D}}\check{\mathcal{P}}_a(x) = \mathcal{E}_n\check{\mathcal{P}}_a(x)$ , and (3.51) is obtained by setting  $x = x_j$ .

(1): Eq. (3.42) with the replacement  $(\mathcal{D}', \mathcal{D}'', n, d', d'') \rightarrow (\mathcal{D}'_{1,jk}, \mathcal{D}, \mathcal{N}, \epsilon_k^I, d_j^I)$  gives

$$(\cdots) \times \check{P}_{\mathcal{D},\mathcal{N}}(x) = (\tilde{\mathcal{H}}_{\mathcal{D}} + \mathcal{E}_{\mathcal{N}} - \tilde{\mathcal{E}}_{\epsilon_k^I}^I - \tilde{\mathcal{E}}_{d_j^I}^I)\check{\mathcal{P}}_a(x),$$

and (3.51) is obtained by setting  $x = x_j$ .

(2): Eq. (3.42) with the replacement  $(\mathcal{D}', \mathcal{D}'', n, d', d'') \rightarrow (\mathcal{D}'_{2,jk}, \mathcal{D}, \mathcal{N}, \epsilon_k^{II}, d_j^{II})$  gives

$$(\cdots) \times \check{P}_{\mathcal{D},\mathcal{N}}(x) = (\tilde{\mathcal{H}}_{\mathcal{D}} + \mathcal{E}_{\mathcal{N}} - \tilde{\mathcal{E}}_{\epsilon_k^{II}}^{II} - \tilde{\mathcal{E}}_{d_j^{II}}^{II})\check{\mathcal{P}}_a(x),$$

and (3.51) is obtained by setting  $x = x_j$ .

(3): Eq. (3.43) with the replacement  $(\mathcal{D}, \mathcal{D}''', n, d', d'') \rightarrow (\mathcal{D}'_{3,jk}, \mathcal{D}, \mathcal{N}, d_j^I, d_k^{II})$  gives

$$(\cdots) \times \check{P}_{\mathcal{D},\mathcal{N}}(x) = (\tilde{\mathcal{H}}_{\mathcal{D}} + \mathcal{E}_{\mathcal{N}} - \tilde{\mathcal{E}}_{d_j^I}^I - \tilde{\mathcal{E}}_{d_k^{II}}^{II})\check{\mathcal{P}}_a(x),$$

and (3.51) is obtained by setting  $x = x_j$ . □

By using (3.52) and explicit forms of  $\mathcal{E}_n$  and  $\tilde{\mathcal{E}}_v$ , we can show that the condition (iv) is satisfied for generic values of  $\lambda$ . Thus the polynomials  $\check{\mathcal{P}}_a(x)$  (3.49) (with generic values of  $\lambda$ ) satisfy all the conditions in (2.3).

### 3.5.2 matrices $\tilde{\mathcal{M}}$ and $\mathcal{M}$

Let us show the proposition for  $\tilde{\mathcal{M}}$ .

**Proposition 3.3** *The matrix elements  $\tilde{\mathcal{M}}_{jk}$  (2.8) for  $j \neq k$  are expressed as*

$$\tilde{\mathcal{M}}_{jk} = \frac{1}{(\eta(x_j - i\gamma) - \eta_k)(\eta(x_j + i\gamma) - \eta_k)} \frac{-\tilde{\mathcal{H}}_{\mathcal{D}}(\eta(x)\check{P}_{\mathcal{D},\mathcal{N}}(x))|_{x=x_j}}{P'_{\mathcal{D},\mathcal{N}}(\eta_j)} \quad (j \neq k). \quad (3.53)$$

Proof: The similarity transformed Hamiltonian  $\tilde{\mathcal{H}}_{\mathcal{D}}$  (3.37) has the following form,

$$\tilde{\mathcal{H}}_{\mathcal{D}} = A(x)(e^{\gamma p} - B(x)) + A^*(x)(e^{-\gamma p} - B^*(x)).$$

Recalling (3.44) and evaluating  $\tilde{\mathcal{H}}_{\mathcal{D}}\check{P}_{\mathcal{D},\mathcal{N}}(x) = \mathcal{E}_{\mathcal{N}}\check{P}_{\mathcal{D},\mathcal{N}}(x)$  at  $x = x_j$ , we have

$$A(x_j) \prod_{l=1}^{\tilde{\mathcal{N}}} (\eta(x_j - i\gamma) - \eta_l) + A^*(x_j) \prod_{l=1}^{\tilde{\mathcal{N}}} (\eta(x_j + i\gamma) - \eta_l) = 0. \quad (3.54)$$



For  $j \neq k$ , we have

$$\begin{aligned}
& \widetilde{\mathcal{H}}_{\mathcal{D}} \prod_{\substack{l=1 \\ l \neq k}}^{\widetilde{\mathcal{N}}} (\eta(x) - \eta_l) \Big|_{x=x_j} \\
&= A(x_j) \prod_{\substack{l=1 \\ l \neq k}}^{\widetilde{\mathcal{N}}} (\eta(x_j - i\gamma) - \eta_l) + A^*(x_j) \prod_{\substack{l=1 \\ l \neq k}}^{\widetilde{\mathcal{N}}} (\eta(x_j + i\gamma) - \eta_l) \\
&= \frac{A(x_j) \prod_{l=1}^{\widetilde{\mathcal{N}}} (\eta(x_j - i\gamma) - \eta_l)}{\eta(x_j - i\gamma) - \eta_k} + \frac{A^*(x_j) \prod_{l=1}^{\widetilde{\mathcal{N}}} (\eta(x_j + i\gamma) - \eta_l)}{\eta(x_j + i\gamma) - \eta_k} \\
&\stackrel{(i)}{=} \frac{A(x_j) \prod_{l=1}^{\widetilde{\mathcal{N}}} (\eta(x_j - i\gamma) - \eta_l) \cdot (\eta(x_j + i\gamma) - \eta(x_j - i\gamma))}{(\eta(x_j - i\gamma) - \eta_k)(\eta(x_j + i\gamma) - \eta_k)} \\
&\stackrel{(i)}{=} \frac{-A(x_j)\eta(x_j - i\gamma) \prod_{l=1}^{\widetilde{\mathcal{N}}} (\eta(x_j - i\gamma) - \eta_l) - A^*(x_j)\eta(x_j + i\gamma) \prod_{l=1}^{\widetilde{\mathcal{N}}} (\eta(x_j + i\gamma) - \eta_l)}{(\eta(x_j - i\gamma) - \eta_k)(\eta(x_j + i\gamma) - \eta_k)} \\
&= \frac{-\widetilde{\mathcal{H}}_{\mathcal{D}} \left( \eta(x) \prod_{l=1}^{\widetilde{\mathcal{N}}} (\eta(x) - \eta_l) \right) \Big|_{x=x_j}}{(\eta(x_j - i\gamma) - \eta_k)(\eta(x_j + i\gamma) - \eta_k)},
\end{aligned}$$

where we have used (3.54) in (i). Then the matrix elements  $\widetilde{\mathcal{M}}_{jk}$  (2.8) for  $j \neq k$  become

$$\widetilde{\mathcal{M}}_{jk} = \frac{1}{(\eta(x_j - i\gamma) - \eta_k)(\eta(x_j + i\gamma) - \eta_k)} \frac{-\widetilde{\mathcal{H}}_{\mathcal{D}} \left( \eta(x) \prod_{l=1}^{\widetilde{\mathcal{N}}} (\eta(x) - \eta_l) \right) \Big|_{x=x_j}}{\prod_{\substack{l=1 \\ l \neq j}}^{\widetilde{\mathcal{N}}} (\eta_j - \eta_l)}.$$

By multiply the numerator and denominator of the last factor by  $c_{\mathcal{D}, \mathcal{N}}^P$ , (3.53) is obtained.  $\square$

Let us define  $F_j$  ( $j = 1, \dots, \widetilde{\mathcal{N}}$ ) as

$$F_j \stackrel{\text{def}}{=} -\frac{\widetilde{\mathcal{H}}_{\mathcal{D}}(\eta(x) \check{P}_{\mathcal{D}, \mathcal{N}}(x)) \Big|_{x=x_j}}{P'_{\mathcal{D}, \mathcal{N}}(\eta_j)}. \quad (3.55)$$

Then we have the following proposition.

**Proposition 3.4** *The number  $F_j$  (3.55) is expressed as*

$$F_j = \check{F}(x_j) = F(\eta_j). \quad (3.56)$$

Here  $\check{F}(x)$  is given by

$$\check{F}(x) \stackrel{\text{def}}{=} \frac{-1}{P'_{\mathcal{D},\mathcal{N}}(\eta(x))} \left( \eta(x - i\gamma) V(x; \boldsymbol{\lambda}_{\mathcal{D}}) \frac{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2})} \check{P}_{\mathcal{D},\mathcal{N}}(x - i\gamma) \right. \\ \left. + \eta(x + i\gamma) V^*(x; \boldsymbol{\lambda}_{\mathcal{D}}) \frac{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2})} \check{P}_{\mathcal{D},\mathcal{N}}(x + i\gamma) \right). \quad (3.57)$$

It is a rational function of  $\eta(x)$ , and  $F(\eta)$  is given by  $F(\eta(x)) \stackrel{\text{def}}{=} \check{F}(x)$ .

Proof: By (3.37),  $F_j$  becomes

$$F_j = \frac{-1}{P'_{\mathcal{D},\mathcal{N}}(\eta_j)} \left( V(x_j; \boldsymbol{\lambda}_{\mathcal{D}}) \frac{\check{\Xi}_{\mathcal{D}}(x_j + i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}(x_j - i\frac{\gamma}{2})} \eta(x_j - i\gamma) \check{P}_{\mathcal{D},\mathcal{N}}(x_j - i\gamma) \right. \\ \left. + V^*(x_j; \boldsymbol{\lambda}_{\mathcal{D}}) \frac{\check{\Xi}_{\mathcal{D}}(x_j - i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}(x_j + i\frac{\gamma}{2})} \eta(x_j + i\gamma) \check{P}_{\mathcal{D},\mathcal{N}}(x_j + i\gamma) \right),$$

namely  $F_j = \check{F}(x_j)$ . Let us show that  $\check{F}(x)$  is a rational function of  $\eta(x) = x, x^2$  and  $\cos x$  for cH, W and AW cases, respectively. From (3.57) and explicit form of  $V(x)$ ,  $\check{F}(x)$  is a rational function of  $x$  (cH, W) or  $e^{ix}$  (AW). For cH case, it is trivial that  $\check{F}(x)$  is a rational function of  $x$ . For W and AW cases, the potential function  $V(x)$  satisfies

$$\text{W, AW} : V^*(x) = V(-x). \quad (3.58)$$

By using this and  $\eta(-x) = \eta(x)$ , we obtain  $\check{F}(-x) = \check{F}(x)$ . This means that  $\check{F}(x)$  is a rational function of  $x^2$  (W) or  $e^{ix} + e^{-ix} = 2\cos x$  (AW).  $\square$

**Remark 3.3** By (3.54),  $F_j$  can be written as

$$F_j = \frac{\eta(x_j + i\gamma) - \eta(x_j - i\gamma)}{P'_{\mathcal{D},\mathcal{N}}(\eta_j)} V(x_j; \boldsymbol{\lambda}_{\mathcal{D}}) \frac{\check{\Xi}_{\mathcal{D}}(x_j + i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}(x_j - i\frac{\gamma}{2})} \check{P}_{\mathcal{D},\mathcal{N}}(x_j - i\gamma). \quad (3.59)$$

The sinusoidal coordinates have the following property.

**Lemma 3.1** *The sinusoidal coordinates  $\eta(x) = x, x^2$  and  $\cos x$  satisfy the following identity for any complex numbers  $a, b$  and  $c$ :*

$$(\eta(a - c) - \eta(b))(\eta(a + c) - \eta(b)) = (\eta(b - c) - \eta(a))(\eta(b + c) - \eta(a)). \quad (3.60)$$

Proof: Direct calculation shows this lemma.  $\square$

By the similarity transformation (2.11), we obtain the symmetric matrix  $\mathcal{M}$ .

**Proposition 3.5** *By taking  $g_j = \sqrt{F_j}$  in (2.11), the matrix  $\mathcal{M}$  is symmetric, (2.12).*

Proof: Since the matrix elements  $\widetilde{\mathcal{M}}_{jk}$  ( $j \neq k$ ) are expressed as

$$\widetilde{\mathcal{M}}_{jk} = \frac{F_j}{(\eta(x_j - i\gamma) - \eta_k)(\eta(x_j + i\gamma) - \eta_k)} \quad (j \neq k), \quad (3.61)$$

the matrix elements  $\mathcal{M}_{jk}$  ( $j \neq k$ ) become

$$\mathcal{M}_{jk} = \frac{\sqrt{F_j} \sqrt{F_k}}{(\eta(x_j - i\gamma) - \eta_k)(\eta(x_j + i\gamma) - \eta_k)} \quad (j \neq k). \quad (3.62)$$

By Lemma 3.1,  $\mathcal{M}_{jk}$  are symmetric in  $j$  and  $k$ . □

**Remark 3.4** We have not written down the diagonal elements  $\mathcal{M}_{jj}(= \widetilde{\mathcal{M}}_{jj})$  explicitly, because their concrete forms are not needed to show (2.12). For the sake of completeness, we write down the concrete form of  $\widetilde{\mathcal{M}}_{jj} = \mathcal{M}_{jj}$ ,

$$\begin{aligned} \widetilde{\mathcal{M}}_{jj} = & \frac{F_j}{(\eta(x_j - i\gamma) - \eta_j)(\eta(x_j + i\gamma) - \eta_j)} \\ & - V(x_j; \boldsymbol{\lambda}_{\mathcal{D}}) \frac{\check{\Xi}_{\mathcal{D}}(x_j + i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x_j - i\frac{\gamma}{2}; \boldsymbol{\lambda})} \frac{\check{\Xi}_{\mathcal{D}}(x_j - i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x_j; \boldsymbol{\lambda} + \boldsymbol{\delta})} \\ & - V^*(x_j; \boldsymbol{\lambda}_{\mathcal{D}}) \frac{\check{\Xi}_{\mathcal{D}}(x_j - i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x_j + i\frac{\gamma}{2}; \boldsymbol{\lambda})} \frac{\check{\Xi}_{\mathcal{D}}(x_j + i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x_j; \boldsymbol{\lambda} + \boldsymbol{\delta})}, \end{aligned} \quad (3.63)$$

which is derived from the definition (2.8) by using (3.54), like as (3.53) and (3.57).

### 3.5.3 discrete orthogonality relations

Let us present a main result of this paper.

**Theorem 3.1** *For the case-(1) multi-indexed orthogonal polynomials of  $cH$ ,  $W$  and  $AW$  types  $P_{\mathcal{D},n}(\eta)$ ,  $\mathcal{P}_a(\eta)$  (3.49) and  $F(\eta)$  (3.56), we have the discrete orthogonality relations:*

$$\sum_{j=1}^{\tilde{N}} \frac{1}{F(\eta_j)} \frac{\mathcal{P}_a(\eta_j)}{P'_{\mathcal{D},\mathcal{N}}(\eta_j)} \frac{\mathcal{P}_b(\eta_j)}{P'_{\mathcal{D},\mathcal{N}}(\eta_j)} = k_a^{[\mathcal{D},\mathcal{N}]} \delta_{ab} \quad (a, b = 1, 2, \dots, \tilde{N}), \quad (3.64)$$

where  $k_a^{[\mathcal{D},\mathcal{N}]}$ 's are normalization constants.

Proof: Since the assumptions of Theorem 2.1 are satisfied (for generic values of  $\boldsymbol{\lambda}$ ), Theorem 2.1 gives this theorem. □

**Remark 3.5** In contrast to the weight  $1/c_2(\eta)$  in oQM case, this weight  $1/F(\eta)$  depends on the multi index  $\mathcal{D}$ , see (3.57).

**Remark 3.6** As in Remark 2.1, the weights  $1/F(\eta_j)$  may not be positive and may be complex, and the normalization constants  $k_a^{[\mathcal{D}, \mathcal{N}]}$  may not be positive. As in Remark 2.2, the theorem states nothing about the properties of  $k_a^{[\mathcal{D}, \mathcal{N}]}$ , nor does it state anything for  $\tilde{\mathcal{N}} = 0, 1$  cases.

**Remark 3.7** The property  $P_{\mathcal{D}, \mathcal{N}}^*(\eta) = P_{\mathcal{D}, \mathcal{N}}(\eta)$  (which holds if (3.9)–(3.10) are satisfied) implies

$$\{\eta_1^*, \dots, \eta_{\tilde{\mathcal{N}}}^*\} = \{\eta_1, \dots, \eta_{\tilde{\mathcal{N}}}\} \quad (\text{as a set}). \quad (3.65)$$

Base on this fact, let us define  $\bar{j}$  as  $\eta_{\bar{j}} \stackrel{\text{def}}{=} \eta_j^*$ . If  $\eta_j^* = \eta_j$ , we have  $\bar{j} = j$ . In [27], the vector space  $\tilde{\mathbf{V}} = \{\tilde{v} = (\tilde{v}_j) \in \mathbb{C}^{\tilde{\mathcal{N}}} \mid \tilde{v}_j^* = \tilde{v}_{\bar{j}}\}$  is considered. It is a  $\tilde{\mathcal{N}}$ -dimensional vector space over  $\mathbb{R}$ , and  $(\tilde{v}, \tilde{w}) = \sum_{j=1}^{\tilde{\mathcal{N}}} \tilde{v}_j \tilde{w}_j$  gives an (indefinite) inner product on  $\tilde{\mathbf{V}}$ . By studying  $(\tilde{\mathcal{M}}_{jk}^{\text{HS}})^*$ , it is shown that  $\tilde{\mathbf{V}}$  is invariant under the action of  $\tilde{\mathcal{M}}^{\text{HS}}$  [27]. A similar analysis is possible for our  $\tilde{\mathcal{M}}$ .

**Remark 3.8** The discrete orthogonality relations (3.64) are shown for the multi-indexed orthogonal polynomials  $P_{\mathcal{D}, n}$ . As mentioned in Remark 2.2, the difference equations (3.38) are used in the proof, but the orthogonality relations (3.35) are not explicitly used. In order for  $P_{\mathcal{D}, n}$  to be orthogonal polynomials, the parameters  $\boldsymbol{\lambda}$  are restricted by the conditions such as (3.34). If the parameters  $\boldsymbol{\lambda}$  do not satisfy the conditions, the polynomials  $P_{\mathcal{D}, n}$  are no longer orthogonal polynomials, but may still satisfy the difference equations. Then, the discrete orthogonality relations still hold in that case. Let us discuss this point. For the parameters  $\boldsymbol{\lambda}$  satisfying (3.9)–(3.10), they have 4 real degrees of freedom, and one more degree of freedom  $q$  ( $0 < q < 1$ ) for AW case. Let us consider  $a_1, a_2, a_3, a_4, q \in \mathbb{C}$  ( $a_i$  is  $\lambda_i$  or  $q^{\lambda_i}$ ) without any restriction (except for the condition  $c_{\mathcal{D}}^{\Xi}, c_{\mathcal{D}, \mathcal{N}}^P \neq 0$ ). There are 8 real degrees of freedom for cH and W, and 10 for AW. The definitions of the polynomials  $P_{\mathcal{D}, n}$ , (3.19) of [14] and (3.38) of [9], are meaningful for these complex values of parameters. Note that the property  $P_{\mathcal{D}, n}^* = P_{\mathcal{D}, n}$  is lost and (3.65) does not hold. The difference equations (3.38) hold by replacing  $V^*(x; \boldsymbol{\lambda}_{\mathcal{D}})$  in (3.37) as follows:

$$V^*(x) \rightarrow \begin{cases} (a_3 - ix)(a_4 - ix) & : \text{cH} \\ V(-x) & : \text{W, AW} \end{cases} \quad (3.66)$$

Then Proposition 3.1, the conditions (2.3) for  $\check{\mathcal{P}}_a(x)$  (3.49), Proposition 3.3–3.5 are valid. Thus the discrete orthogonality relations (3.64) hold for any complex values of parameters

(with the condition  $c_{\mathcal{D}}^{\Xi}, c_{\mathcal{D}, \mathcal{N}}^P, F(\eta_j) \neq 0$ ). We can verify this for small  $M, d_j, \mathcal{N}$  and  $n$  by numerical calculation. The normalization constants  $k_a^{[\mathcal{D}, \mathcal{N}]}$  may not be real.

**Remark 3.9** The case-(1) multi-indexed orthogonal polynomials are also constructed for the Meixner-Pollaczek (MP) polynomials [14]. In this case, there is only one type of virtual state. Various formulas are obtained from those of two type case (cH, W, AW) given above, by setting  $M_{\text{II}} = 0$  and neglecting a superscript (or subscript) I. There is no  $D'_{2,jk}$  and  $D'_{3,jk}$ . So, the polynomials  $\check{\mathcal{P}}_a(x)$  (3.49) are only (0) and (1). The condition (iv) in (2.3) may not be satisfied even for generic values of  $\lambda$ . However, the case-(1) multi-indexed MP polynomials  $P_{\mathcal{D}, n}(\eta)$  can be obtained from the case-(1) multi-indexed cH polynomials by taking certain limit of parameters (with appropriate rescalings). By this limit, the discrete orthogonality relations (3.64) for the case-(1) multi-indexed cH polynomials are inherited by the case-(1) multi-indexed MP polynomials. As in Remark 3.8, they hold for any complex values of parameters.

We conjecture the normalization constants  $k_a^{[\mathcal{D}, \mathcal{N}]}$  as follows.

**Conjecture 3.1** *The normalization constants  $k_a^{[\mathcal{D}, \mathcal{N}]}$  are given by*

$$(0) \mathcal{P}_a = P_{\mathcal{D}, n} : k_a^{[\mathcal{D}, \mathcal{N}]} = \frac{h_{\mathcal{D}, n}}{h_{\mathcal{D}, \mathcal{N}}} \times \begin{cases} \frac{1}{2(b_1 + 2\mathcal{N} - 1)} & : \text{cH, W} \\ \frac{q^{\mathcal{N}+1}}{(1 - q^2)(1 - b_4 q^{2\mathcal{N}-1})} & : \text{AW} \end{cases}, \quad (3.67)$$

$$(1) \mathcal{P}_a = P_{\mathcal{D}'_{1,jk}, \mathcal{N}} :$$

$$\begin{aligned} \text{cH} : k_a^{[\mathcal{D}, \mathcal{N}]} &= \frac{h_{\mathcal{D}'_{1,jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{(\epsilon_k^{\text{I}} + 1)_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}}{2} \frac{1}{(a_1 + a_3 - d_j^{\text{I}} - 1, a_2 + a_4 + \epsilon_k^{\text{I}})_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}} \\ &\times \frac{1}{(a_1 - a_2 - d_j^{\text{I}})_{d_j^{\text{I}} - \epsilon_k^{\text{I}}} (a_3 - a_4 - d_j^{\text{I}})_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}} \frac{(b'^{\text{cH}} - d_k^{\text{I}})_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}}{-b'^{\text{cH}} + 1 + 2\epsilon_k^{\text{I}}} \\ &\times \prod_{\substack{i=1 \\ i \neq j}}^{M_{\text{I}}} \frac{d_i^{\text{I}} - \epsilon_k^{\text{I}}}{d_i^{\text{I}} - d_j^{\text{I}}} \frac{-b'^{\text{cH}} + d_i^{\text{I}} + \epsilon_k^{\text{I}} + 1}{-b'^{\text{cH}} + d_i^{\text{I}} + d_j^{\text{I}} + 1} \cdot \prod_{i=1}^{M_{\text{II}}} \frac{d_i^{\text{II}} + \epsilon_k^{\text{I}} + 1}{d_i^{\text{II}} + d_j^{\text{I}} + 1} \frac{b'^{\text{cH}} + d_i^{\text{II}} - \epsilon_k^{\text{I}}}{b'^{\text{cH}} + d_i^{\text{II}} - d_j^{\text{I}}}, \\ \text{W} : k_a^{[\mathcal{D}, \mathcal{N}]} &= \frac{h_{\mathcal{D}'_{1,jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{1}{2(\epsilon_k^{\text{I}} + 1)_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}} \frac{1}{(a_1 + a_2 - d_j^{\text{I}} - 1, a_3 + a_4 + \epsilon_k^{\text{I}})_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}} \\ &\times \prod_{l=1}^2 \prod_{m=3}^4 \frac{1}{(a_l - a_m - d_j^{\text{I}})_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}} \cdot \frac{(b'_1 - d_k^{\text{I}})_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}}{-b'_1 + 1 + 2\epsilon_k^{\text{I}}} \\ &\times \prod_{\substack{i=1 \\ i \neq j}}^{M_{\text{I}}} \frac{d_i^{\text{I}} - \epsilon_k^{\text{I}}}{d_i^{\text{I}} - d_j^{\text{I}}} \frac{-b'_1 + d_i^{\text{I}} + \epsilon_k^{\text{I}} + 1}{-b'_1 + d_i^{\text{I}} + d_j^{\text{I}} + 1} \cdot \prod_{i=1}^{M_{\text{II}}} \frac{d_i^{\text{II}} + \epsilon_k^{\text{I}} + 1}{d_i^{\text{II}} + d_j^{\text{I}} + 1} \frac{b'_1 + d_i^{\text{II}} - \epsilon_k^{\text{I}}}{b'_1 + d_i^{\text{II}} - d_j^{\text{I}}}, \end{aligned} \quad (3.68)$$

$$\begin{aligned}
\text{AW : } k_a^{[\mathcal{D}, \mathcal{N}]} &= \frac{h_{\mathcal{D}'_{1,jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{(a_1 a_2)^{2(d_j^I - \epsilon_k^I) - 1} (a_3 a_4)^{-(d_j^I - \epsilon_k^I)}}{(1 - q^2)(q^{\epsilon_k^I + 1}; q)_{d_j^I - \epsilon_k^I}} \frac{q^{2 - 2d_j^I(d_j^I + 1) + \epsilon_k^I(2\epsilon_k^I + 3)}}{(a_1 a_2 q^{-d_j^I - 1}, a_3 a_4 q^{\epsilon_k^I}; q)_{d_j^I - \epsilon_k^I}} \\
&\times \prod_{l=1}^2 \prod_{m=3}^4 \frac{1}{(a_l a_m^{-1} q^{-d_j^I}; q)_{d_j^I - \epsilon_k^I}} \cdot \frac{(b'_4 q^{-d_k^I}; q)_{d_j^I - \epsilon_k^I}}{1 - b'_4 q^{1 + 2\epsilon_k^I}} \\
&\times \prod_{\substack{i=1 \\ i \neq j}}^{M_I} \frac{1 - q^{d_i^I - \epsilon_k^I}}{1 - q^{d_i^I - d_j^I}} \frac{1 - b'_4 q^{d_i^I + \epsilon_k^I + 1}}{1 - b'_4 q^{d_i^I + d_j^I + 1}} \cdot \prod_{i=1}^{M_{II}} \frac{1 - q^{d_i^{II} + \epsilon_k^I + 1}}{1 - q^{d_i^{II} + d_j^I + 1}} \frac{1 - b'_4 q^{d_i^{II} - \epsilon_k^I}}{1 - b'_4 q^{d_i^{II} - d_j^I}},
\end{aligned}$$

$$(2) \mathcal{P}_a = P_{\mathcal{D}'_{2,jk}, \mathcal{N}} :$$

$$\begin{aligned}
\text{cH : } k_a^{[\mathcal{D}, \mathcal{N}]} &= \frac{h_{\mathcal{D}'_{2,jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{(\epsilon_k^{II} + 1)_{d_j^{II} - \epsilon_k^{II}}}{2} \frac{1}{(a_2 + a_4 - d_j^{II} - 1, a_1 + a_3 + \epsilon_k^{II})_{d_j^{II} - \epsilon_k^{II}}} \\
&\times \frac{1}{(a_2 - a_1 - d_j^{II})_{d_j^{II} - \epsilon_k^{II}} (a_4 - a_3 - d_j^{II})_{d_j^{II} - \epsilon_k^{II}}} \frac{(-b'^{\text{cH}} - d_k^{II})_{d_j^{II} - \epsilon_k^{II}}}{b'^{\text{cH}} + 1 + 2\epsilon_k^{II}} \\
&\times \prod_{\substack{i=1 \\ i \neq j}}^{M_{II}} \frac{d_i^{II} - \epsilon_k^{II}}{d_i^{II} - d_j^{II}} \frac{b'^{\text{cH}} + d_i^{II} + \epsilon_k^{II} + 1}{b'^{\text{cH}} + d_i^{II} + d_j^{II} + 1} \cdot \prod_{i=1}^{M_I} \frac{d_i^I + \epsilon_k^{II} + 1}{d_i^I + d_j^{II} + 1} \frac{-b'^{\text{cH}} + d_i^I - \epsilon_k^{II}}{-b'^{\text{cH}} + d_i^I - d_j^{II}},
\end{aligned}$$

$$\begin{aligned}
\text{W : } k_a^{[\mathcal{D}, \mathcal{N}]} &= \frac{h_{\mathcal{D}'_{2,jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{1}{2(\epsilon_k^{II} + 1)_{d_j^{II} - \epsilon_k^{II}}} \frac{1}{(a_3 + a_4 - d_j^{II} - 1, a_1 + a_2 + \epsilon_k^{II})_{d_j^{II} - \epsilon_k^{II}}} \\
&\times \prod_{l=3}^4 \prod_{m=1}^2 \frac{1}{(a_l - a_m - d_j^{II})_{d_j^{II} - \epsilon_k^{II}}} \cdot \frac{(-b'_1 - d_k^{II})_{d_j^{II} - \epsilon_k^{II}}}{b'_1 + 1 + 2\epsilon_k^{II}} \\
&\times \prod_{\substack{i=1 \\ i \neq j}}^{M_{II}} \frac{d_i^{II} - \epsilon_k^{II}}{d_i^{II} - d_j^{II}} \frac{b'_1 + d_i^{II} + \epsilon_k^{II} + 1}{b'_1 + d_i^{II} + d_j^{II} + 1} \cdot \prod_{i=1}^{M_I} \frac{d_i^I + \epsilon_k^{II} + 1}{d_i^I + d_j^{II} + 1} \frac{-b'_1 + d_i^I - \epsilon_k^{II}}{-b'_1 + d_i^I - d_j^{II}},
\end{aligned} \tag{3.69}$$

$$\begin{aligned}
\text{AW : } k_a^{[\mathcal{D}, \mathcal{N}]} &= \frac{h_{\mathcal{D}'_{2,jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{(a_3 a_4)^{2(d_j^{II} - \epsilon_k^{II}) - 1} (a_1 a_2)^{-(d_j^{II} - \epsilon_k^{II})}}{(1 - q^2)(q^{\epsilon_k^{II} + 1}; q)_{d_j^{II} - \epsilon_k^{II}}} \frac{q^{2 - 2d_j^{II}(d_j^{II} + 1) + \epsilon_k^{II}(2\epsilon_k^{II} + 3)}}{(a_3 a_4 q^{-d_j^{II} - 1}, a_1 a_2 q^{\epsilon_k^{II}}; q)_{d_j^{II} - \epsilon_k^{II}}} \\
&\times \prod_{l=3}^4 \prod_{m=1}^2 \frac{1}{(a_l a_m^{-1} q^{-d_j^{II}}; q)_{d_j^{II} - \epsilon_k^{II}}} \cdot \frac{(b'_4 q^{-d_k^{II}}; q)_{d_j^{II} - \epsilon_k^{II}}}{1 - b'_4 q^{1 + 2\epsilon_k^{II}}} \\
&\times \prod_{\substack{i=1 \\ i \neq j}}^{M_{II}} \frac{1 - q^{d_i^{II} - \epsilon_k^{II}}}{1 - q^{d_i^{II} - d_j^{II}}} \frac{1 - b'_4 q^{d_i^{II} + \epsilon_k^{II} + 1}}{1 - b'_4 q^{d_i^{II} + d_j^{II} + 1}} \cdot \prod_{i=1}^{M_I} \frac{1 - q^{d_i^I + \epsilon_k^{II} + 1}}{1 - q^{d_i^I + d_j^{II} + 1}} \frac{1 - b'_4 q^{d_i^I - \epsilon_k^{II}}}{1 - b'_4 q^{d_i^I - d_j^{II}}},
\end{aligned}$$

$$(3) \mathcal{P}_a = P_{\mathcal{D}'_{3,jk}, \mathcal{N}} :$$

$$\begin{aligned}
\text{cH : } k_a^{[\mathcal{D}, \mathcal{N}]} &= \frac{h_{\mathcal{D}'_{3,jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{(-1)^{d_j^I + d_k^{II} + 1} d_j^I! d_k^{II}!}{2(d_j^I + d_k^{II} + 1)} \frac{1}{(a_1 + a_3 - d_j^I - 1, a_2 + a_4 - d_k^{II} - 1)_{d_j^I + d_k^{II} + 1}} \\
&\times \frac{(-b'^{\text{cH}} - d_k^{II})_{d_j^I} (b'^{\text{cH}} - d_j^I)_{d_k^{II}}}{(a_1 - a_2 - d_j^I, a_3 - a_4 - d_j^I)_{d_j^I + d_k^{II} + 1}}
\end{aligned}$$

$$\begin{aligned}
& \times \prod_{\substack{i=1 \\ i \neq j}}^{M_I} \frac{1}{(d_i^I - d_j^I)(d_i^I + d_k^{II} + 1)(-b'^{\text{cH}} + d_i^I + d_j^I + 1)(-b'^{\text{cH}} + d_i^I - d_k^{II})} \\
& \times \prod_{\substack{i=1 \\ i \neq k}}^{M_{II}} \frac{1}{(d_i^{II} - d_k^{II})(d_i^{II} + d_j^I + 1)(b'^{\text{cH}} + d_i^{II} + d_k^{II} + 1)(b'^{\text{cH}} + d_i^{II} - d_j^I)}, \\
\text{W : } k_a^{[\mathcal{D}, \mathcal{N}]} &= \frac{h_{\mathcal{D}', \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{(-1)^{d_j^I + d_k^{II} + 1}}{2(d_j^I + d_k^{II} + 1)d_j^I! d_k^{II}!} \frac{1}{(a_1 + a_2 - d_j^I - 1, a_3 + a_4 - d_k^{II} - 1)_{d_j^I + d_k^{II} + 1}} \\
& \times \frac{(-b'_1 - d_k^{II})_{d_j^I} (b'_1 - d_j^I)_{d_k^{II}}}{\prod_{l=1}^2 \prod_{m=3}^4 (a_l - a_m - d_j^I)_{d_j^I + d_k^{II} + 1}} \\
& \times \prod_{\substack{i=1 \\ i \neq j}}^{M_I} \frac{1}{(d_i^I - d_j^I)(d_i^I + d_k^{II} + 1)(-b'_1 + d_i^I + d_j^I + 1)(-b'_1 + d_i^I - d_k^{II})} \\
& \times \prod_{\substack{i=1 \\ i \neq k}}^{M_{II}} \frac{1}{(d_i^{II} - d_k^{II})(d_i^{II} + d_j^I + 1)(b'_1 + d_i^{II} + d_k^{II} + 1)(b'_1 + d_i^{II} - d_j^I)}, \\
\text{AW : } k_a^{[\mathcal{D}, \mathcal{N}]} &= \frac{h_{\mathcal{D}', \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{(-1)^{d_j^I + d_k^{II} + 1} (a_1 a_2)^{3d_j^I + 2} (a_3 a_4)^{d_k^{II} - 2d_j^I}}{(1 - q^2)(1 - q^{d_j^I + d_k^{II} + 1})(q; q)_{d_j^I} (q; q)_{d_k^{II}}} \\
& \times \frac{q^{-\frac{1}{2}(5d_j^{I2} - 2d_j^I d_k^{II} + d_k^{II2} + 3d_j^I - d_k^{II} + 8)}}{(a_1 a_2 q^{-d_j^I - 1}, a_3 a_4 q^{-d_k^{II} - 1}; q)_{d_j^I + d_k^{II} + 1}} \frac{(b'_4{}^{-1} q^{-d_k^{II}}; q)_{d_j^I} (b'_4 q^{-d_j^I}; q)_{d_k^{II}}}{\prod_{l=1}^2 \prod_{m=3}^4 (a_l a_m^{-1} q^{-d_j^I}; q)_{d_j^I + d_k^{II} + 1}} \\
& \times \prod_{\substack{i=1 \\ i \neq j}}^{M_I} \frac{b'_4{}^{-1} q^{2(d_i^I - i - M_{II}) - 1}}{(1 - q^{d_i^I - d_j^I})(1 - q^{d_i^I + d_k^{II} + 1})(1 - b'_4{}^{-1} q^{d_i^I + d_j^I + 1})(1 - b'_4{}^{-1} q^{d_i^I - d_k^{II}})} \\
& \times \prod_{\substack{i=1 \\ i \neq k}}^{M_{II}} \frac{b'_4 q^{2(d_i^{II} - i - M_I) - 1}}{(1 - q^{d_i^{II} - d_k^{II}})(1 - q^{d_i^{II} + d_j^I + 1})(1 - b'_4 q^{d_i^{II} + d_k^{II} + 1})(1 - b'_4 q^{d_i^{II} - d_j^I})},
\end{aligned} \tag{3.70}$$

where  $b_1^{\text{cH}} = a_1 + a_3 - a_2 - a_4$ ,  $b'_1 = a_1 + a_2 - a_3 - a_4$  and  $b'_4 = a_1 a_2 a_3^{-1} a_4^{-1}$ .

By numerical calculation, we can verify this conjecture for small  $M$ ,  $d_j$ ,  $\mathcal{N}$  and  $n$ .

## 4 Krein-Adler Type Multi-Indexed Orthogonal Polynomials

In this section, after recapitulating the Krein-Adler type multi-indexed orthogonal polynomials in idQM, we show their discrete orthogonality relations and conjecture the normalization constants.

In order to distinguish them from the quantities in §3, we add the superscript KA to the quantities in this section, if necessary. The notations  $P_n$  and  $\tilde{\mathcal{H}}$  in §2 correspond to  $P_{\mathcal{D},n}^{\text{KA}}$  and  $\tilde{\mathcal{H}}_{\mathcal{D}}^{\text{KA}}$  in this section, respectively.

## 4.1 Original idQM systems

As the original idQM systems, we consider the systems studied in [15], namely, continuous Hahn (cH) and Meixner-Pollaczek (MP) systems with  $\eta(x) = x$ , Wilson (W) and continuous dual Hahn (cdH) systems with  $\eta(x) = x^2$ , and Askey-Wilson (AW), continuous dual  $q$ -Hahn (cd $q$ H), Al-Salam-Chihara (ASC), continuous big  $q$ -Hermite (cb $q$ H), continuous  $q$ -Hermite (c $q$ H), continuous  $q$ -Jacobi (c $q$ J) and continuous  $q$ -Laguerre (c $q$ L) systems with  $\eta(x) = \cos x$ . For various data of these systems, see [15]. We remark that the potential functions  $V(x)$  satisfy

$$V(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = \kappa^{-1} \frac{\varphi(x - i\gamma)}{\varphi(x)} V(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}), \quad (4.1)$$

which gives the shape invariance of these systems, and

$$V^*(x) = V(-x) \quad \text{for } \eta(x) = x^2, \cos x. \quad (4.2)$$

## 4.2 Darboux transformations

As seed solutions of the Darboux transformations, we take eigenfunctions (3.3),  $\phi_{d_1}(x)$ ,  $\phi_{d_2}(x), \dots, \phi_{d_M}(x)$  ( $d_j$  : mutually distinct). The formulas for the  $M$ -step Darboux transformations are almost the same as in §3. In the  $s$ -step ( $1 \leq s \leq M$ ), we have [17, 9] ( $s = 0$  :  $\mathcal{H} = \hat{\mathcal{A}}_{d_1}^{\text{KA}\dagger} \hat{\mathcal{A}}_{d_1}^{\text{KA}} + \mathcal{E}_{d_1}$ )

$$\mathcal{H}_{d_1 \dots d_s}^{\text{KA}} \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1 \dots d_s}^{\text{KA}} \hat{\mathcal{A}}_{d_1 \dots d_s}^{\text{KA}\dagger} + \mathcal{E}_{d_s} = \hat{\mathcal{A}}_{d_1 \dots d_s d_{s+1}}^{\text{KA}\dagger} \hat{\mathcal{A}}_{d_1 \dots d_s d_{s+1}}^{\text{KA}} + \mathcal{E}_{d_{s+1}}, \quad (4.3)$$

$$\begin{aligned} \hat{\mathcal{A}}_{d_1 \dots d_s}^{\text{KA}} &\stackrel{\text{def}}{=} i \left( e^{\frac{\gamma}{2}p} \sqrt{\hat{V}_{d_1 \dots d_s}^{\text{KA}*}(x)} - e^{-\frac{\gamma}{2}p} \sqrt{\hat{V}_{d_1 \dots d_s}^{\text{KA}}(x)} \right), \\ \hat{\mathcal{A}}_{d_1 \dots d_s}^{\text{KA}\dagger} &\stackrel{\text{def}}{=} -i \left( \sqrt{\hat{V}_{d_1 \dots d_s}^{\text{KA}}(x)} e^{\frac{\gamma}{2}p} - \sqrt{\hat{V}_{d_1 \dots d_s}^{\text{KA}*}(x)} e^{-\frac{\gamma}{2}p} \right), \end{aligned} \quad (4.4)$$

$$\begin{aligned} \hat{V}_{d_1 \dots d_s}^{\text{KA}}(x) &\stackrel{\text{def}}{=} \sqrt{V(x - i\frac{s-1}{2}\gamma) V^*(x - i\frac{s+1}{2}\gamma)} \\ &\quad \times \frac{W_\gamma[\phi_{d_1}, \dots, \phi_{d_{s-1}}](x + i\frac{\gamma}{2})}{W_\gamma[\phi_{d_1}, \dots, \phi_{d_{s-1}}](x - i\frac{\gamma}{2})} \frac{W_\gamma[\phi_{d_1}, \dots, \phi_{d_s}](x - i\gamma)}{W_\gamma[\phi_{d_1}, \dots, \phi_{d_s}](x)}, \end{aligned} \quad (4.5)$$

$$\begin{aligned} \phi_{d_1 \dots d_s n}^{\text{KA}}(x) &\stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1 \dots d_s}^{\text{KA}} \phi_{d_1 \dots d_{s-1} n}^{\text{KA}}(x) = \phi_{d_1 \dots d_s n}^{\text{KA}*}(x) \quad (n \in \mathbb{Z}_{\geq 0} \setminus \{d_1, \dots, d_s\}) \\ &= A(x) W_\gamma[\phi_{d_1}, \dots, \phi_{d_s}, \phi_n](x), \end{aligned} \quad (4.6)$$



$$A(x) = \left( \frac{\sqrt{\prod_{j=0}^{s-1} V(x + i(\frac{s}{2} - j)\gamma) V^*(x - i(\frac{s}{2} - j)\gamma)}}{W_\gamma[\phi_{d_1}, \dots, \phi_{d_s}](x - i\frac{\gamma}{2}) W_\gamma[\phi_{d_1}, \dots, \phi_{d_s}](x + i\frac{\gamma}{2})} \right)^{\frac{1}{2}}, \quad (4.7)$$

$$\mathcal{H}_{d_1 \dots d_s}^{\text{KA}} \phi_{d_1 \dots d_s n}^{\text{KA}}(x) = \mathcal{E}_n \phi_{d_1 \dots d_s n}^{\text{KA}}(x) \quad (n \in \mathbb{Z}_{\geq 0} \setminus \{d_1, \dots, d_s\}), \quad (4.8)$$

$$(\phi_{d_1 \dots d_s n}^{\text{KA}}, \phi_{d_1 \dots d_s m}^{\text{KA}}) = \prod_{j=1}^s (\mathcal{E}_n - \mathcal{E}_{d_j}) \cdot h_n \delta_{nm} \quad (n, m \in \mathbb{Z}_{\geq 0} \setminus \{d_1, \dots, d_s\}). \quad (4.9)$$

The operator  $\hat{\mathcal{A}}_{d_1 \dots d_s}^{\text{KA} \dagger}$  does not have a zero mode, but  $\hat{\mathcal{A}}_{d_1 \dots d_s}^{\text{KA}}$  has a zero mode. Therefore some of the spectrum of the original system are missing in the deformed system. The standard form of  $\mathcal{H}_{d_1 \dots d_s}^{\text{KA}}$  is given by

$$\mathcal{H}_{d_1 \dots d_s}^{\text{KA}} = \mathcal{A}_{d_1 \dots d_s}^{\text{KA} \dagger} \mathcal{A}_{d_1 \dots d_s}^{\text{KA}} + \mathcal{E}_\mu, \quad (4.10)$$

$$\begin{aligned} \mathcal{A}_{d_1 \dots d_s}^{\text{KA}} &\stackrel{\text{def}}{=} i \left( e^{\frac{\gamma}{2}p} \sqrt{V_{d_1 \dots d_s}^{\text{KA}*}(x)} - e^{-\frac{\gamma}{2}p} \sqrt{V_{d_1 \dots d_s}^{\text{KA}}(x)} \right), \\ \mathcal{A}_{d_1 \dots d_s}^{\text{KA} \dagger} &\stackrel{\text{def}}{=} -i \left( \sqrt{V_{d_1 \dots d_s}^{\text{KA}}(x)} e^{\frac{\gamma}{2}p} - \sqrt{V_{d_1 \dots d_s}^{\text{KA}*}(x)} e^{-\frac{\gamma}{2}p} \right), \end{aligned} \quad (4.11)$$

$$\begin{aligned} V_{d_1 \dots d_s}^{\text{KA}}(x) &\stackrel{\text{def}}{=} \sqrt{V(x - i\frac{s}{2}\gamma) V^*(x - i\frac{s+2}{2}\gamma)} \\ &\times \frac{W_\gamma[\phi_{d_1}, \dots, \phi_{d_s}](x + i\frac{\gamma}{2})}{W_\gamma[\phi_{d_1}, \dots, \phi_{d_s}](x - i\frac{\gamma}{2})} \frac{W_\gamma[\phi_{d_1}, \dots, \phi_{d_s}, \phi_\mu](x - i\gamma)}{W_\gamma[\phi_{d_1}, \dots, \phi_{d_s}, \phi_\mu](x)}, \end{aligned} \quad (4.12)$$

where  $\mu$  is

$$\mu \stackrel{\text{def}}{=} \min\{n \mid n \in \mathbb{Z}_{\geq 0} \setminus \{d_1, \dots, d_s\}\}. \quad (4.13)$$

These formulas (4.3)–(4.13) (except for (4.9)) are derived algebraically ((4.9) is derived only formally unless  $\mathcal{H}_{d_1 \dots d_{s'}}^{\text{KA}}$  ( $s' \leq s$ ) are hermite). If the following Krein-Adler condition [24, 25],

$$\prod_{j=1}^s (m - d_j) \geq 0 \quad (\forall m \in \mathbb{Z}_{\geq 0}), \quad (4.14)$$

is satisfied, the deformed Hamiltonian  $\mathcal{H}_{d_1 \dots d_s}$  is hermite [17].

### 4.3 Krein-Adler type multi-indexed orthogonal polynomials

For the index set  $\mathcal{D} = \{d_1, \dots, d_M\}$ , we write  $\mathcal{H}_{d_1 \dots d_M} = \mathcal{H}_{\mathcal{D}}$ ,  $\phi_{d_1 \dots d_M n}(x) = \phi_{\mathcal{D} n}(x)$ , etc. as in § 3. We call an ordered set  $\mathcal{D} = \{d_1, \dots, d_M\}$  with  $0 \leq d_1 < \dots < d_M$  the standard order.

As polynomial parts of the Casoratians  $W_\gamma[\phi_{d_1}, \dots, \phi_{d_M}](x)$  and  $W_\gamma[\phi_{d_1}, \dots, \phi_{d_M}, \phi_n](x)$ , the denominator polynomial  $\Xi_{\mathcal{D}}^{\text{KA}}$  and the multi-indexed polynomials  $P_{\mathcal{D}, n}^{\text{KA}}$  are constructed, respectively. Their definitions are

$$W_\gamma[\check{P}_{d_1}, \dots, \check{P}_{d_M}](x) \stackrel{\text{def}}{=} \varphi_M(x) \check{\Xi}_{\mathcal{D}}^{\text{KA}}(x), \quad \check{\Xi}_{\mathcal{D}}^{\text{KA}}(x) \stackrel{\text{def}}{=} \Xi_{\mathcal{D}}^{\text{KA}}(\eta(x)), \quad (4.15)$$

$$W_\gamma[\check{P}_{d_1}, \dots, \check{P}_{d_M}, \check{P}_n](x) \stackrel{\text{def}}{=} \varphi_{M+1}(x) \check{P}_{\mathcal{D},n}^{\text{KA}}(x), \quad \check{P}_{\mathcal{D},n}^{\text{KA}}(x) \stackrel{\text{def}}{=} P_{\mathcal{D},n}^{\text{KA}}(\eta(x)), \quad (4.16)$$

and

$$W_\gamma[\phi_{d_1}, \dots, \phi_{d_M}](x) = g_{\mathcal{D}}^{\text{KA}}(x) \check{\Xi}_{\mathcal{D}}^{\text{KA}}(x), \quad g_{\mathcal{D}}^{\text{KA}}(x) = \varphi_M(x) \prod_{j=1}^M \phi_0(x_j^{(M)}), \quad (4.17)$$

$$W_\gamma[\phi_{d_1}, \dots, \phi_{d_M}, \phi_n](x) = g_{\mathcal{D}}^{P\text{KA}}(x) \check{P}_{\mathcal{D},n}^{\text{KA}}(x), \quad g_{\mathcal{D}}^{P\text{KA}}(x) = \varphi_{M+1}(x) \prod_{j=1}^{M+1} \phi_0(x_j^{(M+1)}). \quad (4.18)$$

We call  $P_{\mathcal{D},n}^{\text{KA}}$  the Krein-Adler type multi-indexed orthogonal polynomials. Note that, in contrast to §3, there is no essential difference between  $\Xi_{\mathcal{D}}^{\text{KA}}$  and  $P_{\mathcal{D},n}^{\text{KA}}$ . In fact,  $P_{\mathcal{D},n}^{\text{KA}} = \Xi_{d_1 \dots d_M n}^{\text{KA}}$ . The denominator polynomial  $\Xi_{\mathcal{D}}^{\text{KA}}(\eta)$  and the multi-indexed polynomials  $P_{\mathcal{D},n}^{\text{KA}}(\eta)$  are polynomials in  $\eta$  and their degrees are  $\ell_{\mathcal{D}}^{\text{KA}} + M$  and  $\ell_{\mathcal{D}}^{\text{KA}} + n$ , respectively (we assume  $c_{\mathcal{D}}^{\Xi\text{KA}} \neq 0$  and  $c_{\mathcal{D},n}^{P\text{KA}} \neq 0$ ). Here  $\ell_{\mathcal{D}}^{\text{KA}}$  is

$$\ell_{\mathcal{D}}^{\text{KA}} \stackrel{\text{def}}{=} \sum_{j=1}^M d_j - \frac{1}{2}M(M+1), \quad (4.19)$$

and the coefficient of the highest degree term of  $\Xi_{\mathcal{D}}^{\text{KA}}(\eta)$ ,  $c_{\mathcal{D}}^{\Xi\text{KA}}$ , is

$$c_{\mathcal{D}}^{\Xi\text{KA}} = \prod_{j=1}^M c_{d_j} \times \begin{cases} \prod_{1 \leq j < k \leq M} (d_k - d_j) & : \eta(x) = x, x^2 \\ \prod_{1 \leq j < k \leq M} q^{\frac{1}{2}(d_j - d_k)} (1 - q^{d_k - d_j}) \cdot 2^{-\sum_{j=1}^M d_j} & : \eta(x) = \cos x \end{cases}, \quad (4.20)$$

( $c_n$  is that of  $P_n(\eta)$ ) and that of  $P_{\mathcal{D},n}^{\text{KA}}(\eta)$  is  $c_{\mathcal{D},n}^{P\text{KA}} = c_{d_1 \dots d_M n}^{\Xi\text{KA}}$ .

The eigenfunctions of the deformed system (4.6) are expressed as

$$\phi_{\mathcal{D},n}^{\text{KA}}(x) = \kappa^{\frac{1}{4}M(M-1)} \psi_{\mathcal{D}}^{\text{KA}}(x) \check{P}_{\mathcal{D},n}^{\text{KA}}(x) \quad (n \in \mathbb{Z}_{\geq 0} \setminus \mathcal{D}), \quad (4.21)$$

$$\psi_{\mathcal{D}}^{\text{KA}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{\phi_0(x; \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}})}{\sqrt{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}}^{\text{KA}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}}, \quad (4.22)$$

where  $\boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}}$  is

$$\boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}} \stackrel{\text{def}}{=} \boldsymbol{\lambda} + M\boldsymbol{\delta}. \quad (4.23)$$

The potential function  $V_{\mathcal{D}}^{\text{KA}}$  (4.12) of the deformed Hamiltonian  $\mathcal{H}_{\mathcal{D}}^{\text{KA}}$  in the standard form (4.10) is expressed as

$$V_{\mathcal{D}}^{\text{KA}}(x; \boldsymbol{\lambda}) = V(x; \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}}) \frac{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{P}_{\mathcal{D},\mu}^{\text{KA}}(x - i\gamma; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{P}_{\mathcal{D},\mu}(x; \boldsymbol{\lambda})}. \quad (4.24)$$

If the Krein-Adler condition (4.14) (with the replacement  $s \rightarrow M$ ) is satisfied, the deformed Hamiltonian  $\mathcal{H}_{\mathcal{D}}^{\text{KA}}$  is hermite. The orthogonality of the eigenfunctions (4.9), namely, those of the multi-indexed polynomials  $\check{P}_{\mathcal{D},n}^{\text{KA}}(x)$  are

$$\int_{x_1}^{x_2} dx \psi_{\mathcal{D}}^{\text{KA}}(x)^2 \check{P}_{\mathcal{D},n}^{\text{KA}}(x) \check{P}_{\mathcal{D},m}^{\text{KA}}(x) = h_{\mathcal{D},n}^{\text{KA}} \delta_{nm} \quad (n, m \in \mathbb{Z}_{\geq 0} \setminus \mathcal{D}), \quad (4.25)$$

$$h_{\mathcal{D},n}^{\text{KA}} = \kappa^{-\frac{1}{2}M(M-1)} h_n \prod_{j=1}^M (\mathcal{E}_n - \mathcal{E}_{d_j}). \quad (4.26)$$

Let us write  $\mathbb{Z}_{\geq 0} \setminus \mathcal{D} = \{n_0, n_1, \dots\}$  ( $n_0 < n_1 < \dots$ ). Then, for  $n = n_k$ , the multi-indexed orthogonal polynomial  $P_{\mathcal{D},n}^{\text{KA}}(\eta)$  has  $k$  zeros in the physical region  $\eta_{\min} < \eta < \eta_{\max}$  ( $\eta_{\min} \stackrel{\text{def}}{=} \min(\eta(x_1), \eta(x_2))$ ,  $\eta_{\max} \stackrel{\text{def}}{=} \max(\eta(x_1), \eta(x_2))$ ), which interlace the  $k+1$  zeros of  $P_{\mathcal{D},n_{k+1}}(\eta)$  in the physical region, and  $\ell_{\mathcal{D}}^{\text{KA}} + n_k - k$  zeros in the unphysical region  $\eta \in \mathbb{C} \setminus (\eta_{\min}, \eta_{\max})$ .

The similarity transformed Hamiltonian in terms of  $\psi_{\mathcal{D}}^{\text{KA}}(x)$  is square root free,

$$\begin{aligned} \tilde{\mathcal{H}}_{\mathcal{D}}^{\text{KA}} &\stackrel{\text{def}}{=} \psi_{\mathcal{D}}^{\text{KA}}(x)^{-1} \circ \mathcal{H}_{\mathcal{D}}^{\text{KA}} \circ \psi_{\mathcal{D}}^{\text{KA}}(x) \\ &= V(x; \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}}) \frac{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x + i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x - i\frac{\gamma}{2})} \left( e^{\gamma p} - \frac{\check{P}_{\mathcal{D},\mu}(x - i\gamma)}{\check{P}_{\mathcal{D},\mu}(x)} \right) \\ &\quad + V^*(x; \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}}) \frac{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x - i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x + i\frac{\gamma}{2})} \left( e^{-\gamma p} - \frac{\check{P}_{\mathcal{D},\mu}(x + i\gamma)}{\check{P}_{\mathcal{D},\mu}(x)} \right) + \mathcal{E}_{\mu}, \end{aligned} \quad (4.27)$$

and the multi-indexed polynomials  $\check{P}_{\mathcal{D},n}^{\text{KA}}(x)$  are its eigenpolynomials,

$$\tilde{\mathcal{H}}_{\mathcal{D}}^{\text{KA}} \check{P}_{\mathcal{D},n}^{\text{KA}}(x) = \mathcal{E}_n \check{P}_{\mathcal{D},n}^{\text{KA}}(x) \quad (n \in \mathbb{Z}_{\geq 0} \setminus \mathcal{D}). \quad (4.28)$$

## 4.4 Some identities

For the ordered index set  $\mathcal{D} = \{d_1, \dots, d_M\}$ , let us consider the following ordered index sets,

$$\mathcal{D}' = \{d_1, \dots, d_M, d'\}, \quad \mathcal{D}'' = \{d_1, \dots, d_M, d''\}, \quad (4.29)$$

where  $d', d'' \notin \mathcal{D}$  and  $d' \neq d''$ . From the properties of the multi-step Darboux transformation given in §4.2, we have the following identity:

$$\phi_{\mathcal{D}''}^{\text{KA}}(x) = \hat{\mathcal{A}}_{\mathcal{D}''}^{\text{KA}} \frac{\hat{\mathcal{A}}_{\mathcal{D}'}^{\text{KA}\dagger}}{\mathcal{E}_n - \mathcal{E}_{d'}} \phi_{\mathcal{D}'}^{\text{KA}}(x). \quad (4.30)$$

By extracting the polynomial parts from this identity, we obtain the following proposition.

### Proposition 4.1

$$(\mathcal{E}_n - \mathcal{E}_{d'}) \left( \frac{\check{\Xi}_{\mathcal{D}'}^{\text{KA}}(x - i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}''}^{\text{KA}}(x - i\frac{\gamma}{2})} + \frac{\check{\Xi}_{\mathcal{D}'}^{\text{KA}}(x + i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}''}^{\text{KA}}(x + i\frac{\gamma}{2})} \right) \check{P}_{\mathcal{D}'',n}^{\text{KA}}(x) = (\widetilde{\mathcal{H}}_{\mathcal{D}''}^{\text{KA}} + \mathcal{E}_n - \mathcal{E}_{d'} - \mathcal{E}_{d''}) \check{P}_{\mathcal{D}',n}^{\text{KA}}(x). \quad (4.31)$$

Since this proposition can be proved in the same way as Proposition 3.1 (1), we omit the proof.

**Remark 4.1** The identity (4.31) is invariant under the permutation of  $d_j$ ,  $d'$ ,  $d''$  in  $\mathcal{D}$ ,  $\mathcal{D}'$ ,  $\mathcal{D}''$ , namely, the order of ordered sets  $\mathcal{D}$ ,  $\mathcal{D}'$  and  $\mathcal{D}''$  are irrelevant.

**Remark 4.2** For generic values of  $\lambda$ ,  $\check{P}_{\mathcal{D},n}^{\text{KA}}(x)$  and  $\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x \pm i\frac{\gamma}{2})$  do not have a common root.

## 4.5 Discrete orthogonality relations

Let us fix an index set  $\mathcal{D} = \{d_1, \dots, d_M\}$  and a non-negative integer  $\mathcal{N} \notin \mathcal{D}$ , and set  $\tilde{\mathcal{N}} = \deg P_{\mathcal{D},\mathcal{N}}^{\text{KA}} = \ell_{\mathcal{D}}^{\text{KA}} + \mathcal{N}$ . We denote the zeros of  $P_{\mathcal{D},\mathcal{N}}^{\text{KA}}(\eta)$  as  $\eta_j^{[\mathcal{D},\mathcal{N}] \text{KA}}$  ( $j = 1, 2, \dots, \tilde{\mathcal{N}}$ ), and assume that they are simple. We define  $x_j^{[\mathcal{D},\mathcal{N}] \text{KA}}$  by requiring  $\eta(x_j^{[\mathcal{D},\mathcal{N}] \text{KA}}) = \eta_j^{[\mathcal{D},\mathcal{N}] \text{KA}}$  and  $x_1 \leq \text{Re } x_j^{[\mathcal{D},\mathcal{N}] \text{KA}} \leq x_2$ .

In the following, for simplicity in notation, we write  $\eta_j^{[\mathcal{D},\mathcal{N}] \text{KA}}$  and  $x_j^{[\mathcal{D},\mathcal{N}] \text{KA}}$  as  $\eta_j$  and  $x_j$ , respectively. Then  $\check{P}_{\mathcal{D},\mathcal{N}}^{\text{KA}}(x)$  is expressed as

$$\check{P}_{\mathcal{D},\mathcal{N}}^{\text{KA}}(x) = c_{\mathcal{D},\mathcal{N}}^{\text{KA}} \prod_{j=1}^{\tilde{\mathcal{N}}} (\eta(x) - \eta_j). \quad (4.32)$$

### 4.5.1 polynomials $\mathcal{P}_a$

For the index set  $\mathcal{D} = \{d_1, \dots, d_M\}$  in the standard order, let us define the index set  $\mathcal{D}'_{jk}$  as follows [27]:

$$\begin{aligned} \mathcal{D}'_{jk} : E &\stackrel{\text{def}}{=} \{0, 1, \dots, d_M\} \setminus (\mathcal{D} \cup \{\mathcal{N}\}), \quad d_j \in \mathcal{D}, \quad E_j \stackrel{\text{def}}{=} \{\epsilon \in E \mid \epsilon < d_j\}, \quad \epsilon_k \in E_j, \\ \mathcal{D}'_{jk} &\stackrel{\text{def}}{=} (\mathcal{D} \setminus \{d_j\}) \cup \{\epsilon_k\}. \end{aligned} \quad (4.33)$$

As an ordered set, we choose one order of the elements for  $\mathcal{D}'_{jk}$ , e.g. the standard order. Let us define  $\tilde{M} \stackrel{\text{def}}{=} \max\{j \mid d_j < \mathcal{N}\}$  for  $d_1 < \mathcal{N}$  and  $\tilde{M} \stackrel{\text{def}}{=} 0$  for  $d_1 > \mathcal{N}$ . Then we have  $\mathcal{D} \cap \{0, 1, \dots, \mathcal{N} - 1\} = \{d_1, \dots, d_{\tilde{M}}\}$ , and  $|E_j| = d_j - (j - 1)$  for  $1 \leq j \leq \tilde{M}$  and  $|E_j| = d_j - (j - 1) - 1$  for  $\tilde{M} + 1 \leq j \leq M$ . The number of this set  $\mathcal{D}'_{jk}$  is

$$\#\{\mathcal{D}'_{jk}\} = \sum_{j=1}^{\tilde{M}} (d_j - (j - 1)) + \sum_{j=\tilde{M}+1}^M (d_j - (j - 1) - 1) = \ell_{\mathcal{D}}^{\text{KA}} + \tilde{M}. \quad (4.34)$$

Let us define the polynomials  $\check{\mathcal{P}}_a^{\text{KA}}(x) = \mathcal{P}_a^{\text{KA}}(\eta(x))$  ( $a = 1, \dots, \tilde{\mathcal{N}}$ ) as follows [27]:

$$\begin{aligned} (0) : \check{\mathcal{P}}_a^{\text{KA}}(x) &= \check{P}_{\mathcal{D},n}^{\text{KA}}(x) \quad (n \in \{0, 1, \dots, \mathcal{N} - 1\} \setminus \{d_1, \dots, d_{\tilde{M}}\}), \\ (1) : \check{\mathcal{P}}_a^{\text{KA}}(x) &= \check{P}_{\mathcal{D}'_{jk}, \mathcal{N}}^{\text{KA}}(x) \quad (\mathcal{D}'_{jk} \text{ in (4.33)}). \end{aligned} \quad (4.35)$$

The total number of these  $\check{\mathcal{P}}_a^{\text{KA}}(x)$  is actually  $(\mathcal{N} - \tilde{M}) + (\ell_{\mathcal{D}}^{\text{KA}} + \tilde{M}) = \mathcal{N} + \ell_{\mathcal{D}}^{\text{KA}} = \tilde{\mathcal{N}}$ .

Let us show that the conditions in (2.3) are satisfied. The condition (i) is trivial. The condition (ii) is satisfied, because we have

$$\begin{aligned} (0) : \deg \mathcal{P}_a^{\text{KA}} &= \ell_{\mathcal{D}}^{\text{KA}} + n, \quad n < \mathcal{N}, \\ (1) : \deg \mathcal{P}_a^{\text{KA}} &= \ell_{\mathcal{D}'_{jk}}^{\text{KA}} + \mathcal{N}, \quad \ell_{\mathcal{D}'_{jk}}^{\text{KA}} = \ell_{\mathcal{D}}^{\text{KA}} - d_j + \epsilon_k < \ell_{\mathcal{D}}^{\text{KA}}. \end{aligned} \quad (4.36)$$

The condition (iii) is satisfied by the following proposition.

**Proposition 4.2** *For  $\check{\mathcal{P}}_a^{\text{KA}}(x)$  (4.35), we have*

$$\tilde{\mathcal{H}}_{\mathcal{D}}^{\text{KA}} \check{\mathcal{P}}_a^{\text{KA}}(x) \big|_{x=x_j} = \mathcal{E}_a^{\mathcal{P}\text{KA}} \mathcal{P}_a^{\text{KA}}(\eta_j), \quad (4.37)$$

where  $\mathcal{E}_a^{\mathcal{P}\text{KA}}$  are given by

$$\begin{aligned} (0) : \mathcal{E}_a^{\mathcal{P}\text{KA}} &= \mathcal{E}_n, \\ (1) : \mathcal{E}_a^{\mathcal{P}\text{KA}} &= \mathcal{E}_{d_j} + \mathcal{E}_{\epsilon_k} - \mathcal{E}_{\mathcal{N}}. \end{aligned} \quad (4.38)$$

Proof:

(0): Eq. (4.28) gives  $\tilde{\mathcal{H}}_{\mathcal{D}}^{\text{KA}} \check{\mathcal{P}}_a^{\text{KA}}(x) = \mathcal{E}_n \check{\mathcal{P}}_a^{\text{KA}}(x)$ , and (4.37) is obtained by setting  $x = x_j$ .

(1): Eq. (4.31) with the replacement  $(\mathcal{D}', \mathcal{D}'', n, d', d'') \rightarrow (\mathcal{D}'_{jk}, \mathcal{D}, \mathcal{N}, \epsilon_k, d_j)$  gives

$$(\dots) \times \check{P}_{\mathcal{D}, \mathcal{N}}^{\text{KA}}(x) = (\tilde{\mathcal{H}}_{\mathcal{D}}^{\text{KA}} + \mathcal{E}_{\mathcal{N}} - \mathcal{E}_{\epsilon_k} - \mathcal{E}_{d_j}) \check{\mathcal{P}}_a^{\text{KA}}(x),$$

and (4.37) is obtained by setting  $x = x_j$ . □

By using (4.38) and explicit forms of  $\mathcal{E}_n$  [15], we can show that the condition (iv) is satisfied for generic values of  $\boldsymbol{\lambda}$  for cH, W, AW and cqJ cases. For other cases, there may be a degeneracy in  $\mathcal{E}_a^{\mathcal{P}\text{KA}}$  even for generic values of  $\boldsymbol{\lambda}$ . Thus, for cH, W, AW and cqJ cases, the polynomials  $\check{\mathcal{P}}_a^{\text{KA}}(x)$  (4.35) (with generic values of  $\boldsymbol{\lambda}$ ) satisfy all the conditions in (2.3). For other cases, the polynomials  $\check{\mathcal{P}}_a^{\text{KA}}(x)$  satisfy the conditions (i)–(iii) in (2.3) but not (iv). However, we remark that the multi-indexed polynomials  $P_{\mathcal{D},n}^{\text{KA}}(\eta)$  for other cases can be obtained from those for cH, W, AW and cqJ cases by taking certain limits of parameters (with appropriate rescalings).

### 4.5.2 matrices $\widetilde{\mathcal{M}}$ and $\mathcal{M}$

Let us show the proposition for  $\widetilde{\mathcal{M}}$ .

**Proposition 4.3** *The matrix elements  $\widetilde{\mathcal{M}}_{jk}$  (2.8) for  $j \neq k$  are expressed as*

$$\widetilde{\mathcal{M}}_{jk} = \frac{1}{(\eta(x_j - i\gamma) - \eta_k)(\eta(x_j + i\gamma) - \eta_k)} \frac{-\widetilde{\mathcal{H}}_{\mathcal{D}}^{\text{KA}}(\eta(x)\check{P}_{\mathcal{D},\mathcal{N}}^{\text{KA}}(x))|_{x=x_j}}{P_{\mathcal{D},\mathcal{N}}^{\text{KA}'}(\eta_j)} \quad (j \neq k). \quad (4.39)$$

The proof is the same as in Proposition 3.3, so we omit it.

Let us define  $F_j^{\text{KA}}$  ( $j = 1, \dots, \widetilde{\mathcal{N}}$ ) as

$$F_j^{\text{KA}} \stackrel{\text{def}}{=} -\frac{\widetilde{\mathcal{H}}_{\mathcal{D}}^{\text{KA}}(\eta(x)\check{P}_{\mathcal{D},\mathcal{N}}^{\text{KA}}(x))|_{x=x_j}}{P_{\mathcal{D},\mathcal{N}}^{\text{KA}'}(\eta_j)}. \quad (4.40)$$

Then we have the following proposition.

**Proposition 4.4** *The number  $F_j^{\text{KA}}$  (4.40) is expressed as*

$$F_j^{\text{KA}} = \check{F}^{\text{KA}}(x_j) = F^{\text{KA}}(\eta_j). \quad (4.41)$$

Here  $\check{F}^{\text{KA}}(x)$  is given by

$$\begin{aligned} \check{F}^{\text{KA}}(x) \stackrel{\text{def}}{=} \frac{-1}{P_{\mathcal{D},\mathcal{N}}^{\text{KA}'}(\eta(x))} & \left( \eta(x - i\gamma)V(x; \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}}) \frac{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x + i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x - i\frac{\gamma}{2})} \check{P}_{\mathcal{D},\mathcal{N}}^{\text{KA}}(x - i\gamma) \right. \\ & \left. + \eta(x + i\gamma)V^*(x; \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}}) \frac{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x - i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x + i\frac{\gamma}{2})} \check{P}_{\mathcal{D},\mathcal{N}}^{\text{KA}}(x + i\gamma) \right). \end{aligned} \quad (4.42)$$

It is a rational function of  $\eta(x)$ , and  $F^{\text{KA}}(\eta)$  is given by  $F^{\text{KA}}(\eta(x)) \stackrel{\text{def}}{=} \check{F}^{\text{KA}}(x)$ .

The proof is the same as in Proposition 3.3 (recall (4.2)), so we omit it.

**Remark 4.3** As in Remark 3.3,  $F_j^{\text{KA}}$  can be written as

$$F_j^{\text{KA}} = \frac{\eta(x_j + i\gamma) - \eta(x_j - i\gamma)}{P_{\mathcal{D},\mathcal{N}}^{\text{KA}'}(\eta_j)} V(x_j; \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}}) \frac{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x_j + i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x_j - i\frac{\gamma}{2})} \check{P}_{\mathcal{D},\mathcal{N}}^{\text{KA}}(x_j - i\gamma). \quad (4.43)$$

By the similarity transformation (2.11), we obtain the symmetric matrix  $\mathcal{M}$ .

**Proposition 4.5** *By taking  $g_j = \sqrt{F_j^{\text{KA}}}$  in (2.11), the matrix  $\mathcal{M}$  is symmetric, (2.12).*

The proof is the same as in Proposition 3.5, so we omit it.

**Remark 4.4** The matrix elements  $\widetilde{\mathcal{M}}_{jk}$  and  $\mathcal{M}_{jk}$  ( $j \neq k$ ) are given by (3.61) and (3.62) with the replacement  $F_j \rightarrow F_j^{\text{KA}}$ , respectively. The diagonal elements  $\widetilde{\mathcal{M}}_{jj} = \mathcal{M}_{jj}$  are given by

$$\begin{aligned} \widetilde{\mathcal{M}}_{jj} = & \frac{F_j^{\text{KA}}}{(\eta(x_j - i\gamma) - \eta_j)(\eta(x_j + i\gamma) - \eta_j)} \\ & - V(x_j; \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}}) \frac{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x_j + i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x_j - i\frac{\gamma}{2})} \frac{\check{P}_{\mathcal{D},\mu}^{\text{KA}}(x_j - i\gamma)}{\check{P}_{\mathcal{D},\mu}^{\text{KA}}(x_j)} \\ & - V^*(x_j; \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}}) \frac{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x_j - i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x_j + i\frac{\gamma}{2})} \frac{\check{P}_{\mathcal{D},\mu}^{\text{KA}}(x_j + i\gamma)}{\check{P}_{\mathcal{D},\mu}^{\text{KA}}(x_j)} + \mathcal{E}_{\mu}. \end{aligned} \quad (4.44)$$

### 4.5.3 discrete orthogonality relations

The discrete orthogonality relations are as follows.

**Theorem 4.1** *For the Krein-Adler type multi-indexed orthogonal polynomials studied in this section  $\check{P}_{\mathcal{D},n}^{\text{KA}}(x)$ ,  $\mathcal{P}_a^{\text{KA}}(\eta)$  (4.35) and  $F^{\text{KA}}(\eta)$  (4.41), we have the discrete orthogonality relations:*

$$\sum_{j=1}^{\tilde{\mathcal{N}}} \frac{1}{F^{\text{KA}}(\eta_j)} \frac{\mathcal{P}_a^{\text{KA}}(\eta_j)}{P_{\tilde{\mathcal{N}}}^{\text{KA}'}(\eta_j)} \frac{\mathcal{P}_b^{\text{KA}}(\eta_j)}{P_{\tilde{\mathcal{N}}}^{\text{KA}'}(\eta_j)} = k_a^{[\mathcal{D}, \tilde{\mathcal{N}}]^{\text{KA}}} \delta_{ab} \quad (a, b = 1, 2, \dots, \tilde{\mathcal{N}}), \quad (4.45)$$

where  $k_a^{[\mathcal{D}, \tilde{\mathcal{N}}]^{\text{KA}}}$ 's are normalization constants.

Proof: For cH, W, AW and cqJ cases, since the assumptions of Theorem 2.1 are satisfied (for generic values of  $\boldsymbol{\lambda}$ ), Theorem 2.1 gives this theorem. For other cases, the condition (iv) in (2.3) may not be satisfied. For such  $\mathcal{P}_a^{\text{KA}}$  and  $\mathcal{P}_b^{\text{KA}}$  with  $\mathcal{E}_a^{\mathcal{P}^{\text{KA}}} = \mathcal{E}_b^{\mathcal{P}^{\text{KA}}}$ , Theorem 2.1 do not state the discrete orthogonality relations. However, the multi-indexed polynomials  $P_{\mathcal{D},n}^{\text{KA}}(\eta)$  for other cases can be obtained from those for cH, W, AW and cqJ cases by taking certain limits of parameters (with appropriate rescalings). By these limits, the discrete orthogonality relations (4.45) for other cases are obtained from those for cH, W, AW and cqJ cases.  $\square$

**Remark 4.5** We have similar remarks as in Remark 3.6, 3.7 and 3.8 (see (4.2)). Moreover the discrete orthogonality relations (4.45) hold for the index set  $\mathcal{D}$  without the Krein-Adler condition (4.14).

We conjecture the normalization constants  $k_a^{[\mathcal{D}, \tilde{\mathcal{N}}]^{\text{KA}}}$  for cH, W, AW and cqJ cases as follows.

**Conjecture 4.1** *The normalization constants  $k_a^{[\mathcal{D}, \mathcal{N}] \text{KA}}$  are given by*

$$(0) \mathcal{P}_a^{\text{KA}} = P_{\mathcal{D}, n}^{\text{KA}} : k_a^{[\mathcal{D}, \mathcal{N}] \text{KA}} = \frac{h_{\mathcal{D}, n}}{h_{\mathcal{D}, \mathcal{N}}} \times \begin{cases} \frac{1}{2(b_1 + 2\mathcal{N} - 1)} & : \text{cH, W} \\ \frac{q^{\mathcal{N}+1-M}}{(1-q^2)(1-b_4q^{2\mathcal{N}-1})} & : \text{AW} \\ \frac{q^{\mathcal{N}+1-M}}{(1-q^2)(1-q^{\alpha+\beta+1+2\mathcal{N}})} & : \text{cqJ} \end{cases}, \quad (4.46)$$

$$(1) \mathcal{P}_a^{\text{KA}} = P_{\mathcal{D}'_{jk}, \mathcal{N}}^{\text{KA}} :$$

$$\begin{aligned} \text{cH} : k_a^{[\mathcal{D}, \mathcal{N}] \text{KA}} &= \frac{h_{\mathcal{D}'_{jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{(\epsilon_k + 1)_{d_j - \epsilon_k}}{2} \prod_{l=1,3} \prod_{m=2,4} \frac{1}{(a_l + a_m + \epsilon_k)_{d_j - \epsilon_k}} \cdot \frac{(b_1 + \epsilon_k - 1)_{d_j - \epsilon_k}}{b_1 + 2\epsilon_k - 1} \\ &\quad \times \prod_{\substack{i=1 \\ i \neq j}}^M \frac{d_i - \epsilon_k}{d_i - d_j} \frac{b_1 + d_i + \epsilon_k - 1}{b_1 + d_i + d_j - 1}, \\ \text{W} : k_a^{[\mathcal{D}, \mathcal{N}] \text{KA}} &= \frac{h_{\mathcal{D}'_{jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{1}{2(\epsilon_k + 1)_{d_j - \epsilon_k}} \prod_{1 \leq l < m \leq 4} \frac{1}{(a_l + a_m + \epsilon_k)_{d_j - \epsilon_k}} \cdot \frac{(b_1 + \epsilon_k - 1)_{d_j - \epsilon_k}}{b_1 + 2\epsilon_k - 1} \\ &\quad \times \prod_{\substack{i=1 \\ i \neq j}}^M \frac{d_i - \epsilon_k}{d_i - d_j} \frac{b_1 + d_i + \epsilon_k - 1}{b_1 + d_i + d_j - 1}, \\ \text{AW} : k_a^{[\mathcal{D}, \mathcal{N}] \text{KA}} &= \frac{h_{\mathcal{D}'_{jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{q^{d_j}}{(1-q^2)(q^{\epsilon_k+1}; q)_{d_j - \epsilon_k}} \prod_{1 \leq l < m \leq 4} \frac{1}{(a_l a_m q^{\epsilon_k}; q)_{d_j - \epsilon_k}} \cdot \frac{(b_4 q^{\epsilon_k-1}; q)_{d_j - \epsilon_k}}{1 - b_4 q^{2\epsilon_k-1}} \\ &\quad \times \prod_{\substack{i=1 \\ i \neq j}}^M q^{-1} \frac{1 - q^{d_i - \epsilon_k}}{1 - q^{d_i - d_j}} \frac{1 - b_4 q^{d_i + \epsilon_k - 1}}{1 - b_4 q^{d_i + d_j - 1}}, \\ \text{cqJ} : k_a^{[\mathcal{D}, \mathcal{N}] \text{KA}} &= \frac{h_{\mathcal{D}'_{jk}, \mathcal{N}}}{h_{\mathcal{D}, \mathcal{N}}} \frac{q^{(\alpha+\frac{1}{2})(\epsilon_k - d_j) + d_j} (q^{\epsilon_k+1}; q)_{d_j - \epsilon_k}}{1 - q^2} \\ &\quad \times \frac{(q^{\alpha+\beta+\epsilon_k+1}; q)_{d_j - \epsilon_k}}{(1 - q^{\frac{1}{2}(\alpha+\beta+1)+\epsilon_k})(1 + q^{\frac{1}{2}(\alpha+\beta+1)+d_j})(q^{\alpha+\epsilon_k+1}, q^{\beta+\epsilon_k+1}; q)_{d_j - \epsilon_k}} \\ &\quad \times \prod_{\substack{i=1 \\ i \neq j}}^M q^{-1} \frac{1 - q^{d_i - \epsilon_k}}{1 - q^{d_i - d_j}} \frac{1 - q^{\alpha+\beta+d_i+\epsilon_k+1}}{1 - q^{\alpha+\beta+d_i+d_j+1}}. \end{aligned} \quad (4.47)$$

By numerical calculation, we can verify this conjecture for small  $M$ ,  $d_j$ ,  $\mathcal{N}$  and  $n$ . We do not write down the normalization constants for other cases (MP, cdH, cdqH, ASC, cbqH, cqH, cqL), but they can be obtained from the above results.



## 5 Summary and Comments

Ordinary orthogonal polynomials satisfy the discrete orthogonal relations (1.2). For the multi-indexed orthogonal polynomials in oQM, which satisfy the second order differential equations, the discrete orthogonal relations also hold [27]. We have generalized this result to the multi-indexed orthogonal polynomials in idQM, which satisfy the second order difference equations. The discrete orthogonal relations hold for the case-(1) multi-indexed orthogonal polynomials of continuous Hahn, Wilson and Askey-Wilson types, Theorem 3.1, and for the Krein-Adler type multi-indexed orthogonal polynomials, Theorem 4.1. Their normalization constants are conjectured, Conjecture 3.1 and 4.1. The discrete orthogonal relations for the multi-indexed orthogonal polynomials in oQM are revisited in Appendix B, and the normalization constants are conjectured, Conjecture B.1 and B.2. We hope that these conjectures will be proved.

In addition to oQM and idQM, we have another quantum mechanical system, rdQM. Orthogonal polynomials appearing in rdQM are the  $q$ -Racah polynomial, its various limits, and their multi-indexed versions. The discrete orthogonal relations are expected to hold for the multi-indexed orthogonal polynomials in rdQM as well. It is an interesting problem to study these discrete orthogonal relations concretely.

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## A Proof of Proposition 3.1

In this appendix we prove Proposition 3.1. We use the following abbreviated notations:

$$\begin{aligned}
w(x) &= W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}](x), & u(x) &= W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \phi_n](x), \\
w_1(x) &= W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \tilde{\phi}_{d'}](x), & u_1(x) &= W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \tilde{\phi}_{d'}, \phi_n](x), \\
w_2(x) &= W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \tilde{\phi}_{d''}](x), & u_2(x) &= W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \tilde{\phi}_{d''}, \phi_n](x), \\
w_3(x) &= W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \tilde{\phi}_{d'}, \tilde{\phi}_{d''}](x), & u_3(x) &= W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \tilde{\phi}_{d'}, \tilde{\phi}_{d''}, \phi_n](x).
\end{aligned} \tag{A.1}$$

For example, we have

$$\begin{aligned}\hat{V}_{\mathcal{D}''}(x) &= \sqrt{V(x - i\frac{M}{2}\gamma)V^*(x - i\frac{M+2}{2}\gamma)} \frac{w(x + i\frac{\gamma}{2})}{w(x - i\frac{\gamma}{2})} \frac{w_2(x - i\gamma)}{w_2(x)}, \\ \phi_{\mathcal{D}''n}(x) &= \left( \prod_{j=0}^M V(x + i(\frac{M+1}{2} - j)\gamma) V^*(x - i(\frac{M+1}{2} - j)\gamma) \right)^{\frac{1}{4}} \frac{u_2(x)}{\sqrt{w_2(x - i\frac{\gamma}{2})w_2(x + i\frac{\gamma}{2})}} \\ &= c_{\mathcal{D}''}^\phi \psi_{\mathcal{D}''}(x) \check{P}_{\mathcal{D}''n}(x) = c_{\mathcal{D}''}^\phi \psi_{\mathcal{D}''}(x) g_{\mathcal{D}''}^P(x)^{-1} u_2(x).\end{aligned}$$

## A.1 Proof of Proposition 3.1 (1)

From  $\mathcal{H}_{\mathcal{D}''} = \hat{\mathcal{A}}_{\mathcal{D}''} \hat{\mathcal{A}}_{\mathcal{D}''}^\dagger + \tilde{\mathcal{E}}_{d''}$  and

$$\begin{aligned}\tilde{\mathcal{H}}'_{\mathcal{D}''} &\stackrel{\text{def}}{=} g_{\mathcal{D}''}^P(x) \circ \tilde{\mathcal{H}}_{\mathcal{D}''} \circ g_{\mathcal{D}''}^P(x)^{-1} = g_{\mathcal{D}''}^P(x) \psi_{\mathcal{D}''}(x)^{-1} \circ \mathcal{H}_{\mathcal{D}''} \circ \psi_{\mathcal{D}''}(x) g_{\mathcal{D}''}^P(x)^{-1} \\ &= \left( \prod_{j=0}^M V(x + i(\frac{M+1}{2} - j)\gamma) V^*(x - i(\frac{M+1}{2} - j)\gamma) \right)^{-\frac{1}{4}} \sqrt{w_2(x - i\frac{\gamma}{2})w_2(x + i\frac{\gamma}{2})} \\ &\quad \circ \mathcal{H}_{\mathcal{D}''} \circ \left( \prod_{j=0}^M V(x + i(\frac{M+1}{2} - j)\gamma) V^*(x - i(\frac{M+1}{2} - j)\gamma) \right)^{\frac{1}{4}} \frac{1}{\sqrt{w_2(x - i\frac{\gamma}{2})w_2(x + i\frac{\gamma}{2})}} \\ &= \sqrt{V(x - i\frac{M+1}{2}\gamma)V^*(x - i\frac{M+3}{2}\gamma)} \frac{w_2(x + i\frac{\gamma}{2})}{w_2(x - i\frac{\gamma}{2})} e^{\gamma p} \\ &\quad + \sqrt{V(x + i\frac{M+3}{2}\gamma)V^*(x + i\frac{M+1}{2}\gamma)} \frac{w_2(x - i\frac{\gamma}{2})}{w_2(x + i\frac{\gamma}{2})} e^{-\gamma p} \\ &\quad - \sqrt{V(x - i\frac{M-1}{2}\gamma)V^*(x - i\frac{M+1}{2}\gamma)} \frac{w(x + i\gamma)}{w(x)} \frac{w_2(x - i\frac{\gamma}{2})}{w_2(x + i\frac{\gamma}{2})} \\ &\quad - \sqrt{V(x + i\frac{M+1}{2}\gamma)V^*(x + i\frac{M-1}{2}\gamma)} \frac{w(x - i\gamma)}{w(x)} \frac{w_2(x + i\frac{\gamma}{2})}{w_2(x - i\frac{\gamma}{2})} + \tilde{\mathcal{E}}_{d''},\end{aligned}\tag{A.2}$$

we have

$$\begin{aligned}\tilde{\mathcal{H}}'_{\mathcal{D}''} u_1(x) &= \sqrt{V(x - i\frac{M+1}{2}\gamma)V^*(x - i\frac{M+3}{2}\gamma)} \frac{w_2(x + i\frac{\gamma}{2})}{w_2(x - i\frac{\gamma}{2})} u_1(x - i\gamma) \\ &\quad + \sqrt{V(x + i\frac{M+3}{2}\gamma)V^*(x + i\frac{M+1}{2}\gamma)} \frac{w_2(x - i\frac{\gamma}{2})}{w_2(x + i\frac{\gamma}{2})} u_1(x + i\gamma) \\ &\quad - \sqrt{V(x - i\frac{M-1}{2}\gamma)V^*(x - i\frac{M+1}{2}\gamma)} \frac{w(x + i\gamma)}{w(x)} \frac{w_2(x - i\frac{\gamma}{2})}{w_2(x + i\frac{\gamma}{2})} u_1(x) \\ &\quad - \sqrt{V(x + i\frac{M+1}{2}\gamma)V^*(x + i\frac{M-1}{2}\gamma)} \frac{w(x - i\gamma)}{w(x)} \frac{w_2(x + i\frac{\gamma}{2})}{w_2(x - i\frac{\gamma}{2})} u_1(x) + \tilde{\mathcal{E}}_{d''} u_1(x).\end{aligned}\tag{A.3}$$

From  $\mathcal{H}_{\mathcal{D}'} = \hat{\mathcal{A}}_{\mathcal{D}'} \hat{\mathcal{A}}_{\mathcal{D}'}^\dagger + \tilde{\mathcal{E}}_{d'}$  and  $\mathcal{H}_{\mathcal{D}'} \phi_{\mathcal{D}'n}(x) = \mathcal{E}_n \phi_{\mathcal{D}'n}(x)$ , we have

$$\mathcal{E}_n u_1(x) = \sqrt{V(x - i\frac{M+1}{2}\gamma)V^*(x - i\frac{M+3}{2}\gamma)} \frac{w_1(x + i\frac{\gamma}{2})}{w_1(x - i\frac{\gamma}{2})} u_1(x - i\gamma)$$

$$\begin{aligned}
& + \sqrt{V(x + i\frac{M+3}{2}\gamma)V^*(x + i\frac{M+1}{2}\gamma)} \frac{w_1(x - i\frac{\gamma}{2})}{w_1(x + i\frac{\gamma}{2})} u_1(x + i\gamma) \\
& - \sqrt{V(x - i\frac{M-1}{2}\gamma)V^*(x - i\frac{M+1}{2}\gamma)} \frac{w(x + i\gamma)}{w(x)} \frac{w_1(x - i\frac{\gamma}{2})}{w_1(x + i\frac{\gamma}{2})} u_1(x) \\
& - \sqrt{V(x + i\frac{M+1}{2}\gamma)V^*(x + i\frac{M-1}{2}\gamma)} \frac{w(x - i\gamma)}{w(x)} \frac{w_1(x + i\frac{\gamma}{2})}{w_1(x - i\frac{\gamma}{2})} u_1(x) + \tilde{\mathcal{E}}_{d'} u_1(x). \quad (\text{A.4})
\end{aligned}$$

By rewriting these (A.4) and (A.3) as

$$\begin{pmatrix} \alpha_1 a_1 & \alpha_1^* a_1^* \\ \alpha_1 a_2 & \alpha_1^* a_2^* \end{pmatrix} \begin{pmatrix} u_1(x - i\gamma) \\ u_1(x + i\gamma) \end{pmatrix} = \begin{pmatrix} b_1 u_1(x) \\ b_2 u_1(x) \end{pmatrix}, \quad (\text{A.5})$$

where

$$\begin{aligned}
\alpha_1 &= \sqrt{V(x - i\frac{M+1}{2}\gamma)V^*(x - i\frac{M+3}{2}\gamma)}, \quad \alpha_2 = \sqrt{V(x - i\frac{M-1}{2}\gamma)V^*(x - i\frac{M+1}{2}\gamma)}, \\
a_1 &= \frac{w_1(x + i\frac{\gamma}{2})}{w_1(x - i\frac{\gamma}{2})} = \frac{1}{a_1^*}, \quad a_2 = \frac{w_2(x + i\frac{\gamma}{2})}{w_2(x - i\frac{\gamma}{2})} = \frac{1}{a_2^*}, \quad c = \frac{w(x + i\gamma)}{w(x)}, \\
b_1 &= \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} + \alpha_2 c a_1^* + \alpha_2^* c^* a_1, \quad b_2 = \tilde{\mathcal{H}}'_{\mathcal{D}''} - \tilde{\mathcal{E}}_{d''} + \alpha_2 c a_2^* + \alpha_2^* c^* a_2,
\end{aligned}$$

we obtain

$$\begin{pmatrix} \alpha_1 u_1(x - i\gamma) \\ \alpha_1^* u_1(x + i\gamma) \end{pmatrix} = \frac{1}{a_1 a_2^* - a_1^* a_2} \begin{pmatrix} a_2^* & -a_1^* \\ -a_2 & a_1 \end{pmatrix} \begin{pmatrix} b_1 u_1(x) \\ b_2 u_1(x) \end{pmatrix}. \quad (\text{A.6})$$

By writing down the identity (3.40) and multiplying by

$$(\mathcal{E}_n - \tilde{\mathcal{E}}_{d'}) \left( \prod_{j=0}^M V(x + i(\frac{M+1}{2} - j)\gamma) V^*(x - i(\frac{M+1}{2} - j)\gamma) \right)^{-\frac{1}{4}} \sqrt{w_2(x - i\frac{\gamma}{2}) w_2(x + i\frac{\gamma}{2})},$$

we obtain

$$\begin{aligned}
(\mathcal{E}_n - \tilde{\mathcal{E}}_{d'}) u_2(x) &= \alpha_1 \frac{w_2(x + i\frac{\gamma}{2})}{w_1(x - i\frac{\gamma}{2})} u_1(x - i\gamma) + \alpha_1^* \frac{w_2(x - i\frac{\gamma}{2})}{w_1(x + i\frac{\gamma}{2})} u_1(x + i\gamma) \\
&\quad - \alpha_2 \frac{w_2(x - i\frac{\gamma}{2})}{w_1(x + i\frac{\gamma}{2})} c u_1(x) - \alpha_2^* \frac{w_2(x + i\frac{\gamma}{2})}{w_1(x - i\frac{\gamma}{2})} c^* u_1(x). \quad (\text{A.7})
\end{aligned}$$

By substituting  $u_1(x \mp i\gamma)$  in (A.6) into (A.7), we obtain

$$(a_1 a_2^* - a_1^* a_2) (\mathcal{E}_n - \tilde{\mathcal{E}}_{d'}) u_2(x) = \left( \frac{w_2(x - i\frac{\gamma}{2})}{w_1(x - i\frac{\gamma}{2})} - \frac{w_2(x + i\frac{\gamma}{2})}{w_1(x + i\frac{\gamma}{2})} \right) (\tilde{\mathcal{H}}'_{\mathcal{D}''} u_1(x) + (\mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) u_1(x)). \quad (\text{A.8})$$

Since  $u_1(x) = g_{\mathcal{D}'}^P(x) \check{P}_{\mathcal{D}',n}(x)$ , we have

$$\tilde{\mathcal{H}}'_{\mathcal{D}''} u_1(x) + (\mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) u_1(x)$$

$$\begin{aligned}
&= g_{\mathcal{D}''}^P(x) (g_{\mathcal{D}''}^P(x)^{-1} \circ \tilde{\mathcal{H}}'_{\mathcal{D}''} \circ g_{\mathcal{D}''}^P(x) + \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) \frac{g_{\mathcal{D}'}^P(x)}{g_{\mathcal{D}''}^P(x)} \check{P}_{\mathcal{D}',n}(x) \\
&= g_{\mathcal{D}''}^P(x) (\tilde{\mathcal{H}}_{\mathcal{D}''} + \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) \frac{g_{\mathcal{D}'}^P(x)}{g_{\mathcal{D}''}^P(x)} \check{P}_{\mathcal{D}',n}(x).
\end{aligned}$$

Therefore (A.8) gives

$$\left( \frac{w_1(x - i\frac{\gamma}{2})}{w_2(x - i\frac{\gamma}{2})} + \frac{w_1(x + i\frac{\gamma}{2})}{w_2(x + i\frac{\gamma}{2})} \right) (\mathcal{E}_n - \tilde{\mathcal{E}}_{d'}) \check{P}_{\mathcal{D}',n}(x) = (\tilde{\mathcal{H}}_{\mathcal{D}''} + \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) \frac{g_{\mathcal{D}'}^P(x)}{g_{\mathcal{D}''}^P(x)} \check{P}_{\mathcal{D}',n}(x),$$

namely,

$$\begin{aligned}
&(\mathcal{E}_n - \tilde{\mathcal{E}}_{d'}) \left( \frac{g_{\mathcal{D}'}(x - i\frac{\gamma}{2})}{g_{\mathcal{D}''}(x - i\frac{\gamma}{2})} \frac{\check{\Xi}_{\mathcal{D}'}(x - i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}''}(x - i\frac{\gamma}{2})} + \frac{g_{\mathcal{D}'}(x + i\frac{\gamma}{2})}{g_{\mathcal{D}''}(x + i\frac{\gamma}{2})} \frac{\check{\Xi}_{\mathcal{D}'}(x + i\frac{\gamma}{2})}{\check{\Xi}_{\mathcal{D}''}(x + i\frac{\gamma}{2})} \right) \check{P}_{\mathcal{D}',n}(x) \\
&= (\tilde{\mathcal{H}}_{\mathcal{D}''} + \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) \frac{g_{\mathcal{D}'}^P(x)}{g_{\mathcal{D}''}^P(x)} \check{P}_{\mathcal{D}',n}(x). \tag{A.9}
\end{aligned}$$

When the types of  $d'$  and  $d''$  are the same, we have  $g_{\mathcal{D}'}(x) = g_{\mathcal{D}''}(x)$  and  $g_{\mathcal{D}'}^P(x) = g_{\mathcal{D}''}^P(x)$ .

Thus (A.9) gives (3.42).  $\square$

## A.2 Proof of Proposition 3.1 (2)

Like as (A.2),  $\tilde{\mathcal{H}}'_{\mathcal{D}'''} \stackrel{\text{def}}{=} g_{\mathcal{D}'''}^P(x) \circ \tilde{\mathcal{H}}_{\mathcal{D}'''} \circ g_{\mathcal{D}'''}^P(x)^{-1}$  is expressed as

$$\begin{aligned}
\tilde{\mathcal{H}}'_{\mathcal{D}'''} &= \sqrt{V(x - i\frac{M+2}{2}\gamma)V^*(x - i\frac{M+4}{2}\gamma)} \frac{w_3(x + i\frac{\gamma}{2})}{w_3(x - i\frac{\gamma}{2})} e^{\gamma p} \\
&\quad + \sqrt{V(x + i\frac{M+4}{2}\gamma)V^*(x + i\frac{M+2}{2}\gamma)} \frac{w_3(x - i\frac{\gamma}{2})}{w_3(x + i\frac{\gamma}{2})} e^{-\gamma p} \\
&\quad - \sqrt{V(x - i\frac{M}{2}\gamma)V^*(x - i\frac{M+2}{2}\gamma)} \frac{w_1(x + i\gamma)}{w_1(x)} \frac{w_3(x - i\frac{\gamma}{2})}{w_3(x + i\frac{\gamma}{2})} \\
&\quad - \sqrt{V(x + i\frac{M+2}{2}\gamma)V^*(x + i\frac{M}{2}\gamma)} \frac{w_1(x - i\gamma)}{w_1(x)} \frac{w_3(x + i\frac{\gamma}{2})}{w_3(x - i\frac{\gamma}{2})} + \tilde{\mathcal{E}}_{d''}.
\end{aligned}$$

Then we have

$$\begin{aligned}
g_{\mathcal{D}}^P(x) \circ \tilde{\mathcal{H}}_{\mathcal{D}'''} \circ g_{\mathcal{D}}^P(x)^{-1} &= \frac{g_{\mathcal{D}}^P(x)}{g_{\mathcal{D}'''}^P(x)} \circ \tilde{\mathcal{H}}'_{\mathcal{D}'''} \circ \frac{g_{\mathcal{D}'''}^P(x)}{g_{\mathcal{D}}^P(x)} \\
&= \sqrt{V(x - i\frac{M+2}{2}\gamma)V^*(x - i\frac{M+4}{2}\gamma)} \frac{w_3(x + i\frac{\gamma}{2})}{w_3(x - i\frac{\gamma}{2})} \frac{g_{\mathcal{D}}^P(x)}{g_{\mathcal{D}}^P(x - i\gamma)} \frac{g_{\mathcal{D}'''}^P(x - i\gamma)}{g_{\mathcal{D}'''}^P(x)} e^{\gamma p} \\
&\quad + \sqrt{V(x + i\frac{M+4}{2}\gamma)V^*(x + i\frac{M+2}{2}\gamma)} \frac{w_3(x - i\frac{\gamma}{2})}{w_3(x + i\frac{\gamma}{2})} \frac{g_{\mathcal{D}}^P(x)}{g_{\mathcal{D}}^P(x + i\gamma)} \frac{g_{\mathcal{D}'''}^P(x + i\gamma)}{g_{\mathcal{D}'''}^P(x)} e^{-\gamma p} \\
&\quad - \sqrt{V(x - i\frac{M}{2}\gamma)V^*(x - i\frac{M+2}{2}\gamma)} \frac{w_1(x + i\gamma)}{w_1(x)} \frac{w_3(x - i\frac{\gamma}{2})}{w_3(x + i\frac{\gamma}{2})} \\
&\quad - \sqrt{V(x + i\frac{M+2}{2}\gamma)V^*(x + i\frac{M}{2}\gamma)} \frac{w_1(x - i\gamma)}{w_1(x)} \frac{w_3(x + i\frac{\gamma}{2})}{w_3(x - i\frac{\gamma}{2})}
\end{aligned}$$

$$- \sqrt{V(x + i\frac{M+2}{2}\gamma)V^*(x + i\frac{M}{2}\gamma)} \frac{w_1(x - i\gamma)}{w_1(x)} \frac{w_3(x + i\frac{\gamma}{2})}{w_3(x - i\frac{\gamma}{2})} + \tilde{\mathcal{E}}_{d''},$$

and obtain

$$\begin{aligned} & (g_{\mathcal{D}}^P(x) \circ \tilde{\mathcal{H}}_{\mathcal{D}'''} \circ g_{\mathcal{D}}^P(x)^{-1})u(x) \\ &= \sqrt{V(x - i\frac{M+2}{2}\gamma)V^*(x - i\frac{M+4}{2}\gamma)} \frac{w_3(x + i\frac{\gamma}{2})}{w_3(x - i\frac{\gamma}{2})} \frac{g_{\mathcal{D}}^P(x)}{g_{\mathcal{D}}^P(x - i\gamma)} \frac{g_{\mathcal{D}'''}^P(x - i\gamma)}{g_{\mathcal{D}'''}^P(x)} u(x - i\gamma) \\ &+ \sqrt{V(x + i\frac{M+4}{2}\gamma)V^*(x + i\frac{M+2}{2}\gamma)} \frac{w_3(x - i\frac{\gamma}{2})}{w_3(x + i\frac{\gamma}{2})} \frac{g_{\mathcal{D}}^P(x)}{g_{\mathcal{D}}^P(x + i\gamma)} \frac{g_{\mathcal{D}'''}^P(x + i\gamma)}{g_{\mathcal{D}'''}^P(x)} u(x + i\gamma) \\ &- \sqrt{V(x - i\frac{M}{2}\gamma)V^*(x - i\frac{M+2}{2}\gamma)} \frac{w_1(x + i\gamma)}{w_1(x)} \frac{w_3(x - i\frac{\gamma}{2})}{w_3(x + i\frac{\gamma}{2})} u(x) \\ &- \sqrt{V(x + i\frac{M+2}{2}\gamma)V^*(x + i\frac{M}{2}\gamma)} \frac{w_1(x - i\gamma)}{w_1(x)} \frac{w_3(x + i\frac{\gamma}{2})}{w_3(x - i\frac{\gamma}{2})} u(x) + \tilde{\mathcal{E}}_{d''} u(x). \end{aligned} \quad (\text{A.10})$$

From  $\mathcal{H}_{\mathcal{D}} = \hat{\mathcal{A}}_{\mathcal{D}}^\dagger \hat{\mathcal{A}}_{\mathcal{D}'} + \tilde{\mathcal{E}}_{d'}$  and  $\mathcal{H}_{\mathcal{D}} \phi_{\mathcal{D}n}(x) = \mathcal{E}_n \phi_{\mathcal{D}n}(x)$ , we have

$$\begin{aligned} \mathcal{E}_n u(x) &= \sqrt{V(x - i\frac{M}{2}\gamma)V^*(x - i\frac{M+2}{2}\gamma)} \frac{w(x + i\frac{\gamma}{2})}{w(x - i\frac{\gamma}{2})} u(x - i\gamma) \\ &+ \sqrt{V(x + i\frac{M+2}{2}\gamma)V^*(x + i\frac{M}{2}\gamma)} \frac{w(x - i\frac{\gamma}{2})}{w(x + i\frac{\gamma}{2})} u(x + i\gamma) \\ &- \sqrt{V(x - i\frac{M}{2}\gamma)V^*(x - i\frac{M+2}{2}\gamma)} \frac{w(x + i\frac{\gamma}{2})}{w(x - i\frac{\gamma}{2})} \frac{w_1(x - i\gamma)}{w_1(x)} u(x) \\ &- \sqrt{V(x + i\frac{M+2}{2}\gamma)V^*(x + i\frac{M}{2}\gamma)} \frac{w(x - i\frac{\gamma}{2})}{w(x + i\frac{\gamma}{2})} \frac{w_1(x + i\gamma)}{w_1(x)} u(x) + \tilde{\mathcal{E}}_{d'} u(x). \end{aligned} \quad (\text{A.11})$$

By rewriting these (A.11) and (A.10) as

$$\begin{pmatrix} \alpha_1 a_1 & \alpha_1^* a_1^* \\ \alpha_2 a_2 \beta^* & \alpha_2^* a_2^* \beta \end{pmatrix} \begin{pmatrix} u(x - i\gamma) \\ u(x + i\gamma) \end{pmatrix} = \begin{pmatrix} b_1 u(x) \\ b_2 u(x) \end{pmatrix}, \quad (\text{A.12})$$

where

$$\begin{aligned} \alpha_1 &= \sqrt{V(x - i\frac{M}{2}\gamma)V^*(x - i\frac{M+2}{2}\gamma)}, \quad \alpha_2 = \sqrt{V(x - i\frac{M+2}{2}\gamma)V^*(x - i\frac{M+4}{2}\gamma)}, \\ a_1 &= \frac{w(x + i\frac{\gamma}{2})}{w(x - i\frac{\gamma}{2})} = \frac{1}{a_1^*}, \quad a_2 = \frac{w_3(x + i\frac{\gamma}{2})}{w_3(x - i\frac{\gamma}{2})} = \frac{1}{a_2^*}, \quad c = \frac{w_1(x + i\gamma)}{w_1(x)}, \\ \beta_1 &= \frac{g_{\mathcal{D}}^P(x + i\gamma)}{g_{\mathcal{D}}^P(x)}, \quad \beta_2 = \frac{g_{\mathcal{D}'''}^P(x + i\gamma)}{g_{\mathcal{D}'''}^P(x)}, \quad \beta = \frac{\beta_2}{\beta_1}, \\ b_1 &= \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} + \alpha_1 a_1 c^* + \alpha_1^* a_1^* c, \quad b_2 = g_{\mathcal{D}}^P(x) \circ \tilde{\mathcal{H}}_{\mathcal{D}'''} \circ g_{\mathcal{D}}^P(x)^{-1} - \tilde{\mathcal{E}}_{d''} + \alpha_1 a_2^* c + \alpha_1^* a_2 c^*, \end{aligned}$$

we obtain

$$\begin{pmatrix} u(x - i\gamma) \\ u(x + i\gamma) \end{pmatrix} = \frac{1}{\alpha_1 \alpha_2^* a_1 a_2^* \beta - \alpha_1^* \alpha_2 a_1^* a_2 \beta^*} \begin{pmatrix} \alpha_2^* a_2^* \beta & -\alpha_1^* a_1^* \\ -\alpha_2 a_2 \beta^* & \alpha_1 a_1 \end{pmatrix} \begin{pmatrix} b_1 u(x) \\ b_2 u(x) \end{pmatrix}. \quad (\text{A.13})$$

By using the explicit forms of  $g_{\mathcal{D}}^P(x)$  and  $g_{\mathcal{D}'''}^P(x)$  ( $d', d''$  : different types), a lengthy but straightforward calculation shows the following:

$$\alpha_1 - \alpha_2^* \beta = 0. \quad (\text{A.14})$$

By writing down the identity (3.41) and multiplying by

$$\left( \prod_{j=0}^{M+1} V\left(x + i\left(\frac{M+2}{2} - j\right)\gamma\right) V^*\left(x - i\left(\frac{M+2}{2} - j\right)\gamma\right) \right)^{-\frac{1}{4}} \sqrt{w_3(x - i\frac{\gamma}{2}) w_3(x + i\frac{\gamma}{2})},$$

we obtain

$$\begin{aligned} u_3(x) = & -\frac{w_3(x + i\frac{\gamma}{2})}{w(x - i\frac{\gamma}{2})} u(x - i\gamma) - \frac{w_3(x - i\frac{\gamma}{2})}{w(x + i\frac{\gamma}{2})} u(x + i\gamma) \\ & + \frac{w_3(x - i\frac{\gamma}{2})}{w(x + i\frac{\gamma}{2})} c u(x) + \frac{w_3(x + i\frac{\gamma}{2})}{w(x - i\frac{\gamma}{2})} c^* u(x). \end{aligned} \quad (\text{A.15})$$

By substituting  $u(x \mp i\gamma)$  in (A.13) into (A.15) and using  $u(x) = g_{\mathcal{D}}^P(x) \check{P}_{\mathcal{D},n}(x)$ , a short calculation gives

$$\begin{aligned} & (\alpha_1 \alpha_2^* a_1 a_2^* \beta - \alpha_1^* \alpha_2 a_1^* a_2 \beta^*) u_3(x) \\ & = g_{\mathcal{D}}^P(x) \left( \alpha_1^* \frac{w_3(x + i\frac{\gamma}{2})}{w(x + i\frac{\gamma}{2})} - \alpha_1 \frac{w_3(x - i\frac{\gamma}{2})}{w(x - i\frac{\gamma}{2})} \right) (\tilde{\mathcal{H}}_{\mathcal{D}'''} + \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) \check{P}_{\mathcal{D},n}(x), \end{aligned}$$

where (A.14) is used. Dividing this equation by  $\alpha_1 \alpha_1^*$  and using (A.14) and  $u_3(x) = g_{\mathcal{D}'''}^P(x) \check{P}_{\mathcal{D}''',n}(x)$ , we obtain

$$\begin{aligned} & \left( \frac{\alpha_1}{\alpha_1^*} a_1 a_2^* - \frac{\alpha_1^*}{\alpha_1} a_1^* a_2 \right) \check{P}_{\mathcal{D}''',n}(x) \\ & = \frac{g_{\mathcal{D}}^P(x)}{g_{\mathcal{D}'''}^P(x)} \left( \frac{1}{\alpha_1} \frac{w_3(x + i\frac{\gamma}{2})}{w(x + i\frac{\gamma}{2})} - \frac{1}{\alpha_1^*} \frac{w_3(x - i\frac{\gamma}{2})}{w(x - i\frac{\gamma}{2})} \right) (\tilde{\mathcal{H}}_{\mathcal{D}'''} + \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) \check{P}_{\mathcal{D},n}(x). \end{aligned} \quad (\text{A.16})$$

By using the explicit forms of  $g_{\mathcal{D}}^P(x)$ ,  $g_{\mathcal{D}'''}^P(x)$ ,  $g_{\mathcal{D}}(x)$  and  $g_{\mathcal{D}'''}(x)$ , a lengthy but straightforward calculation shows that (A.16) is expressed as (3.43).  $\square$

## B Discrete Orthogonality Relations in oQM

In this appendix, we revisit the discrete orthogonality relations for the multi-indexed orthogonal polynomials in ordinary quantum mechanics studied in [27].

For the multi-step Darboux transformations of oQM, see Appendix A in [31].

## B.1 Multi-indexed orthogonal polynomials

We consider the discrete orthogonality relations for the case-(1) multi-indexed Laguerre and Jacobi orthogonal polynomials. The outline is the same as in § 3, and the results are described briefly.

By the  $M$ -step Darboux transformations, the deformed Hamiltonian  $\mathcal{H}_{\mathcal{D}}$  and its eigenfunctions  $\phi_{\mathcal{D}n}(x)$  are expressed as

$$\mathcal{H}_{\mathcal{D}} = -\frac{d^2}{dx^2} + U(x) - 2\partial_x^2 \log |W[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}](x)|, \quad U(x) = \frac{\phi_0''(x)}{\phi_0(x)}, \quad (\text{B.1})$$

$$\begin{aligned} \phi_{\mathcal{D}n}(x) &= \frac{W[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \phi_n](x)}{W[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}](x)} \quad (n \in \mathbb{Z}_{\geq 0}), \\ &= c_{\mathcal{F}}^M \psi_{\mathcal{D}}(x) \check{P}_{\mathcal{D},n}(x), \quad \psi_{\mathcal{D}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{\phi_0(x; \boldsymbol{\lambda}_{\mathcal{D}})}{\Xi_{\mathcal{D}}(x; \boldsymbol{\lambda})}, \end{aligned} \quad (\text{B.2})$$

where  $\boldsymbol{\lambda}_{\mathcal{D}}$  is given by (3.32),  $c_{\mathcal{F}}$  is given by (2.132) in [18],  $\tilde{\phi}_v(x)$  is given by (B.3)–(B.6) in [31],  $\Xi_{\mathcal{D}}(x)$  and  $\check{P}_{\mathcal{D},n}(x)$  are given by (B.9)–(B.10) in [31]. The functions  $g_{\mathcal{D}}(x)$  and  $g_{\mathcal{D}}^P(x)$  are defined by (3.26)–(3.27) with the replacement  $W_{\gamma} \rightarrow W$ , and their explicit forms are given in (B.7)–(B.8) in [31]. We remark that  $g_{\mathcal{D}}(x)$  and  $g_{\mathcal{D}}^P(x)$  depend on  $M_{\text{I}}$  and  $M_{\text{II}}$ , but not on the specific values of  $d_j$  and  $n$ . The degrees of  $\Xi_{\mathcal{D}}(\eta)$  and  $P_{\mathcal{D},n}(\eta)$  are same as § 3. The orthogonality of the multi-indexed polynomials are (3.35)–(3.36) with the replacement  $c_{\mathcal{D}}^{\phi} \rightarrow c_{\mathcal{F}}^M$ . A direct calculation shows

$$U(x) - U(x; \boldsymbol{\lambda}_{\mathcal{D}}) - 2\partial_x^2 \log \left| \frac{W[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}](x)}{\Xi_{\mathcal{D}}(x)} \right| = 0. \quad (\text{B.3})$$

The similarity transformed deformed Hamiltonian  $\tilde{\mathcal{H}}_{\mathcal{D}} = \psi_{\mathcal{D}}(x)^{-1} \circ \mathcal{H}_{\mathcal{D}} \circ \psi_{\mathcal{D}}(x)$  is expressed as

$$\begin{aligned} \tilde{\mathcal{H}}_{\mathcal{D}} &= -\frac{d^2}{dx^2} - 2\frac{\psi'_{\mathcal{D}}(x)}{\psi_{\mathcal{D}}(x)} \frac{d}{dx} + 2\frac{\phi_0'(x; \boldsymbol{\lambda}_{\mathcal{D}})}{\phi_0(x; \boldsymbol{\lambda}_{\mathcal{D}})} \frac{\Xi'_{\mathcal{D}}(x)}{\Xi_{\mathcal{D}}(x)} - \frac{\Xi''_{\mathcal{D}}(x)}{\Xi_{\mathcal{D}}(x)} \\ &= -4 \left( c_2(\eta) \frac{d^2}{d\eta^2} + \left( c_1(\eta, \boldsymbol{\lambda}_{\mathcal{D}}) - 2c_2(\eta) \frac{\Xi'_{\mathcal{D}}(\eta)}{\Xi_{\mathcal{D}}(\eta)} \right) \frac{d}{d\eta} \right. \\ &\quad \left. + c_2(\eta) \frac{\Xi''_{\mathcal{D}}(\eta)}{\Xi_{\mathcal{D}}(\eta)} - c_1(\eta, \boldsymbol{\lambda}_{\mathcal{D}} - \boldsymbol{\delta}) \frac{\Xi'_{\mathcal{D}}(\eta)}{\Xi_{\mathcal{D}}(\eta)} \right), \end{aligned} \quad (\text{B.4})$$

where  $c_1(\eta, \boldsymbol{\lambda})$  is given by (2.132) in [18].

From the identities (3.40)–(3.41) with  $\hat{\mathcal{A}}_{d_1 \dots d_s} = \frac{d}{dx} - \partial_x \log |\tilde{\phi}_{d_1 \dots d_s}(x)|$  and  $\hat{\mathcal{A}}_{d_1 \dots d_s}^{\dagger} = -\frac{d}{dx} - \partial_x \log |\tilde{\phi}_{d_1 \dots d_s}(x)|$ , we obtain Proposition 3.1 with the following replacements,

$$(3.42) \rightarrow 2(\mathcal{E}_n - \tilde{\mathcal{E}}_{d'}) \frac{\Xi_{\mathcal{D}'}(\eta)}{\Xi_{\mathcal{D}'}(\eta)} P_{\mathcal{D}'',n}(\eta) = (\tilde{\mathcal{H}}_{\mathcal{D}''} + \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) P_{\mathcal{D}'',n}(\eta), \quad (\text{B.5})$$

$$(3.43) \rightarrow -2c_{\mathcal{F}}^2 \frac{\Xi_{\mathcal{D}}(\eta)}{\Xi_{\mathcal{D}'''}(\eta)} P_{\mathcal{D}''',n}(\eta) = (\tilde{\mathcal{H}}_{\mathcal{D}'''} + \mathcal{E}_n - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) P_{\mathcal{D},n}(\eta). \quad (\text{B.6})$$

These properties (B.5)–(B.6) with  $n = \mathcal{N}$  are given as Theorem 4.3, 4.5 and 4.6 in [27], but their reader-friendly concrete proofs are not presented. So we present them in § B.3, in which explicit expressions of  $\Xi_{\mathcal{D}}$  and  $P_{\mathcal{D},n}$  ((B.9)–(B.10) in [31]) are not used. We have Proposition 3.2.

Since  $\tilde{\mathcal{H}}_{\mathcal{D}}$  has the form  $\tilde{\mathcal{H}}_{\mathcal{D}} = -\frac{d^2}{dx^2} + A(x)\frac{d}{dx} + B(x)$ , we obtain Proposition 3.3 with the replacement,

$$(3.53) \rightarrow \tilde{\mathcal{M}}_{jk} = \frac{1}{(\eta_j - \eta_k)^2} \frac{-\tilde{\mathcal{H}}_{\mathcal{D}}(\eta(x)\check{P}_{\mathcal{D},\mathcal{N}}(x))|_{x=x_j}}{P'_{\mathcal{D},\mathcal{N}}(\eta_j)} \quad (j \neq k). \quad (\text{B.7})$$

By using the explicit form of  $\tilde{\mathcal{H}}_{\mathcal{D}}$  (B.4), we obtain Proposition 3.4 with the replacement

$$(3.57) \rightarrow \check{F}(x) = 2\eta'(x)^2, \quad F(\eta) = 8c_2(\eta). \quad (\text{B.8})$$

Then we have Proposition 3.5, and (3.61)–(3.62) become

$$\tilde{\mathcal{M}}_{jk} = \frac{F_j}{(\eta_j - \eta_k)^2}, \quad \mathcal{M}_{jk} = \frac{\sqrt{F_j}\sqrt{F_k}}{(\eta_j - \eta_k)^2} \quad (j \neq k). \quad (\text{B.9})$$

We have Remark 3.4 with the replacement,

$$(3.63) \rightarrow \tilde{\mathcal{M}}_{jj} = 4c_2(\eta_j) \left( \sum_{\substack{m=1 \\ m \neq j}}^{\tilde{\mathcal{N}}} \frac{1}{(\eta_j - \eta_m)^2} + \left( \sum_{\substack{m=1 \\ m \neq j}}^{\tilde{\mathcal{N}}} \frac{1}{\eta_j - \eta_m} \right)^2 - \frac{\Xi''_{\mathcal{D}}(\eta_j)}{\Xi_{\mathcal{D}}(\eta_j)} \right) \\ + 4c_1(\eta_j, \boldsymbol{\lambda}_{\mathcal{D}} - \boldsymbol{\delta}) \frac{\Xi'_{\mathcal{D}}(\eta_j)}{\Xi_{\mathcal{D}}(\eta_j)}, \quad (\text{B.10})$$

which agrees to  $\tilde{\mathcal{M}}_{jj}^{\text{HS}} + \mathcal{E}_{\mathcal{N}}$  in [27].

For the case-(1) multi-indexed Jacobi polynomials, the assumptions of Theorem 2.1 are satisfied (for generic values of  $\boldsymbol{\lambda}$ ). Therefore Theorem 2.1 gives the following.

**Theorem B.1** *For the case-(1) multi-indexed orthogonal polynomials of  $L$  and  $J$  types  $P_{\mathcal{D},n}(\eta)$ ,  $\mathcal{P}_a(\eta)$  (3.49) and  $F(\eta)$  (B.8), we have the discrete orthogonality relations:*

$$\sum_{j=1}^{\tilde{\mathcal{N}}} \frac{1}{F(\eta_j)} \frac{\mathcal{P}_a(\eta_j)}{P'_{\mathcal{D},\mathcal{N}}(\eta_j)} \frac{\mathcal{P}_b(\eta_j)}{P'_{\mathcal{D},\mathcal{N}}(\eta_j)} = k_a^{[\mathcal{D},\mathcal{N}]} \delta_{ab} \quad (a, b = 1, 2, \dots, \tilde{\mathcal{N}}), \quad (\text{B.11})$$

where  $k_a^{[\mathcal{D},\mathcal{N}]}$ 's are normalization constants.



**Remark B.1** For L case, there may be a degeneracy in  $\mathcal{E}_a^{\mathcal{P}}$  even for generic values of  $\lambda$ , namely, the condition (iv) in (2.3) may not be satisfied. Theorem 2.1 can not be applied to such cases. However, the case-(1) multi-indexed L polynomials  $P_{\mathcal{D},n}(\eta)$  can be obtained from those of J by taking certain limit of parameters (with appropriate rescalings). So, the discrete orthogonality relations (B.11) for J are inherited by L. This point is not mentioned in [27].

**Remark B.2** Like as Remark 3.8, the discrete orthogonality relations (B.11) hold for any complex values of parameters  $\lambda$  (with the condition  $c_{\mathcal{D}}^{\bar{\mathcal{P}}}, c_{\mathcal{D},\mathcal{N}}^{\mathcal{P}} \neq 0$ ).

We conjecture the normalization constants  $k_a^{[\mathcal{D},\mathcal{N}]}$  as follows.

**Conjecture B.1** The normalization constants  $k_a^{[\mathcal{D},\mathcal{N}]}$  are given by

$$(0) \mathcal{P}_a = P_{\mathcal{D},n} : k_a^{[\mathcal{D},\mathcal{N}]} = \frac{1}{8} \frac{h_{\mathcal{D},n}}{h_{\mathcal{D},\mathcal{N}}} \times \begin{cases} 1 & : \text{L} \\ \frac{1}{2\mathcal{N}+g+h} & : \text{J} \end{cases}, \quad (\text{B.12})$$

$$(1) \mathcal{P}_a = P_{\mathcal{D}'_{1,jk},\mathcal{N}} :$$

$$k_a^{[\mathcal{D},\mathcal{N}]} = \frac{1}{8} \frac{h_{\mathcal{D}'_{1,jk},\mathcal{N}}}{h_{\mathcal{D},\mathcal{N}}} \frac{(\epsilon_k^{\text{I}} + 1)_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}}{(\epsilon_k^{\text{I}} + g + \frac{1}{2})_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}} \prod_{\substack{i=1 \\ i \neq j}}^{M_{\text{I}}} \frac{d_i^{\text{I}} - \epsilon_k^{\text{I}}}{d_i^{\text{I}} - d_j^{\text{I}}} \cdot \prod_{i=1}^{M_{\text{II}}} \frac{d_i^{\text{II}} + \epsilon_k^{\text{I}} + 1}{d_i^{\text{II}} + d_j^{\text{I}} + 1} \\ \times \begin{cases} (-1) & : \text{L} \\ \frac{(\epsilon_k^{\text{I}} + g - h + 1)_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}}{(2\epsilon_k^{\text{I}} + g - h + 1)(\epsilon_k^{\text{I}} - h + \frac{3}{2})_{d_j^{\text{I}} - \epsilon_k^{\text{I}}}} & \\ \times \prod_{\substack{i=1 \\ i \neq j}}^{M_{\text{I}}} \frac{d_i^{\text{I}} + \epsilon_k^{\text{I}} + g - h + 1}{d_i^{\text{I}} + d_j^{\text{I}} + g - h + 1} \cdot \prod_{i=1}^{M_{\text{II}}} \frac{d_i^{\text{II}} - \epsilon_k^{\text{I}} - g + h}{d_i^{\text{II}} - d_j^{\text{I}} - g + h} & : \text{J} \end{cases}, \quad (\text{B.13})$$

$$(2) \mathcal{P}_a = P_{\mathcal{D}'_{2,jk},\mathcal{N}} :$$

$$k_a^{[\mathcal{D},\mathcal{N}]} = \frac{1}{8} \frac{h_{\mathcal{D}'_{2,jk},\mathcal{N}}}{h_{\mathcal{D},\mathcal{N}}} \frac{(\epsilon_k^{\text{II}} + 1)_{d_j^{\text{II}} - \epsilon_k^{\text{II}}}}{(\epsilon_k^{\text{II}} - g + \frac{3}{2})_{d_j^{\text{II}} - \epsilon_k^{\text{II}}}} \prod_{\substack{i=1 \\ i \neq j}}^{M_{\text{II}}} \frac{d_i^{\text{II}} - \epsilon_k^{\text{II}}}{d_i^{\text{II}} - d_j^{\text{II}}} \cdot \prod_{i=1}^{M_{\text{I}}} \frac{d_i^{\text{I}} + \epsilon_k^{\text{II}} + 1}{d_i^{\text{I}} + d_j^{\text{II}} + 1} \\ \times \begin{cases} 1 & : \text{L} \\ \frac{(\epsilon_k^{\text{II}} + h - g + 1)_{d_j^{\text{II}} - \epsilon_k^{\text{II}}}}{(2\epsilon_k^{\text{II}} + h - g + 1)(\epsilon_k^{\text{II}} + h + \frac{1}{2})_{d_j^{\text{II}} - \epsilon_k^{\text{II}}}} & \\ \times \prod_{\substack{i=1 \\ i \neq k}}^{M_{\text{II}}} \frac{d_i^{\text{II}} + \epsilon_k^{\text{II}} + h - g + 1}{d_i^{\text{II}} + d_j^{\text{II}} + h - g + 1} \cdot \prod_{i=1}^{M_{\text{I}}} \frac{d_i^{\text{I}} - \epsilon_k^{\text{II}} - h + g}{d_i^{\text{I}} - d_j^{\text{II}} - h + g} & : \text{J} \end{cases}, \quad (\text{B.14})$$

$$(3) \mathcal{P}_a = P_{\mathcal{D}'_{3,jk},\mathcal{N}} :$$

$$k_a^{[\mathcal{D},\mathcal{N}]} = \frac{1}{8} \frac{h_{\mathcal{D}'_{3,jk},\mathcal{N}}}{h_{\mathcal{D},\mathcal{N}}} \frac{-16d_j^{\text{I}}! d_k^{\text{II}}!}{(d_j^{\text{I}} + d_k^{\text{II}} + 1)(g - \frac{1}{2})(g + \frac{1}{2})_{d_j^{\text{I}}}(\frac{3}{2} - g)_{d_k^{\text{II}}}}$$

$$\begin{aligned}
& \times \prod_{\substack{i=1 \\ i \neq j}}^{M_I} \frac{1}{(d_i^I - d_j^I)(d_i^I + d_k^I + 1)} \cdot \prod_{\substack{i=1 \\ i \neq k}}^{M_{II}} \frac{1}{(d_i^{II} - d_k^{II})(d_i^{II} + d_j^I + 1)} \\
& \times \left\{ \begin{array}{l} 1 \\ \frac{4^{2M-1}(g-h)(g-h+1)_{d_j^I} (h-g+1)_{d_k^{II}}}{(h-\frac{1}{2})(g-h+d_j^I-d_k^{II})(\frac{3}{2}-h)_{d_j^I} (h+\frac{1}{2})_{d_k^{II}}} \\ \times \prod_{\substack{i=1 \\ i \neq j}}^{M_I} \frac{1}{(d_i^I - d_k^{II} + g - h)(d_i^I + d_j^I + g - h + 1)} \\ \times \prod_{\substack{i=1 \\ i \neq k}}^{M_{II}} \frac{1}{(d_i^{II} - d_j^I + h - g)(d_i^{II} + d_k^{II} + h - g + 1)} \end{array} \right. : \text{L} \\
& \quad \quad \quad : \text{J}
\end{aligned} \quad . \quad (\text{B.15})$$

By numerical calculation, we can verify this conjecture for small  $M$ ,  $d_j$ ,  $\mathcal{N}$  and  $n$ .

## B.2 Krein-Adler type multi-indexed orthogonal polynomials

We consider the discrete orthogonality relations for the Krein-Adler type multi-indexed orthogonal polynomials of Hermite, Laguerre and Jacobi types. The outline is the same as in § 4, and the results are described briefly.

By the  $M$ -step Darboux transformations, the deformed Hamiltonian  $\mathcal{H}_{\mathcal{D}}$ , which is hermite for (4.14) with  $s \rightarrow M$ , and its eigenfunctions  $\phi_{\mathcal{D}n}(x)$  are expressed as

$$\mathcal{H}_{\mathcal{D}} = -\frac{d^2}{dx^2} + U(x) - 2\partial_x^2 \log |W[\phi_{d_1}, \dots, \phi_{d_M}](x)|, \quad (\text{B.16})$$

$$\begin{aligned}
\phi_{\mathcal{D}n}^{\text{KA}}(x) &= \frac{W[\phi_{d_1}, \dots, \phi_{d_M}, \phi_n](x)}{W[\phi_{d_1}, \dots, \phi_{d_M}](x)} \quad (n \in \mathbb{Z}_{\geq 0} \setminus \mathcal{D}), \\
&= c_{\mathcal{F}}^M \psi_{\mathcal{D}}^{\text{KA}}(x) \check{P}_{\mathcal{D},n}^{\text{KA}}(x), \quad \psi_{\mathcal{D}}^{\text{KA}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{\phi_0(x; \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}})}{\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x; \boldsymbol{\lambda})},
\end{aligned} \quad (\text{B.17})$$

where  $\boldsymbol{\lambda}_{\mathcal{D}}$  is given by (4.23), and  $\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x)$  and  $\check{P}_{\mathcal{D},n}^{\text{KA}}(x)$  are given by

$$\check{\Xi}_{\mathcal{D}}^{\text{KA}}(x) \stackrel{\text{def}}{=} \Xi_{\mathcal{D}}^{\text{KA}}(\eta(x)), \quad \Xi_{\mathcal{D}}^{\text{KA}}(\eta) \stackrel{\text{def}}{=} W[P_{d_1}, \dots, P_{d_M}](\eta), \quad (\text{B.18})$$

$$\check{P}_{\mathcal{D},n}^{\text{KA}}(x) \stackrel{\text{def}}{=} P_{\mathcal{D},n}^{\text{KA}}(\eta(x)), \quad P_{\mathcal{D},n}^{\text{KA}}(\eta) \stackrel{\text{def}}{=} W[P_{d_1}, \dots, P_{d_M}, P_n](\eta). \quad (\text{B.19})$$

Note that  $P_{\mathcal{D},n}^{\text{KA}}(\eta) = \Xi_{d_1, \dots, d_M n}^{\text{KA}}(\eta)$ . By the property of the Wronskian, we have

$$W[\phi_{d_1}, \dots, \phi_{d_M}](x) = g_{\mathcal{D}}^{\text{KA}}(x) \check{\Xi}_{\mathcal{D}}^{\text{KA}}(x), \quad g_{\mathcal{D}}^{\text{KA}}(x) = (\eta'(x))^{\frac{1}{2}M(M-1)} \phi_0(x)^M, \quad (\text{B.20})$$

$$W[\phi_{d_1}, \dots, \phi_{d_M}, \phi_n](x) = g_{\mathcal{D}}^{P\text{KA}}(x) \check{P}_{\mathcal{D},n}^{\text{KA}}(x), \quad g_{\mathcal{D}}^{P\text{KA}}(x) = (\eta'(x))^{\frac{1}{2}M(M+1)} \phi_0(x)^{M+1}. \quad (\text{B.21})$$

The degrees of  $\Xi_D^{\text{KA}}(\eta)$  and  $P_{\mathcal{D},n}^{\text{KA}}(\eta)$  are same as §4. The coefficient of the highest degree term of  $\Xi_D^{\text{KA}}(\eta)$ ,  $c_D^{\Xi \text{KA}}$ , is

$$c_D^{\Xi \text{KA}} = \prod_{j=1}^M c_{d_j} \cdot \prod_{1 \leq j < k \leq M} (d_k - d_j), \quad (\text{B.22})$$

and that of  $P_{\mathcal{D},n}^{\text{KA}}(\eta)$  is  $c_{\mathcal{D},n}^{P \text{KA}} = c_{d_1 \dots d_M n}^{\Xi \text{KA}}$ . The orthogonality of the multi-indexed polynomials are (4.25)–(4.26) with the replacement  $\kappa^{-\frac{1}{2}M(M-1)} \rightarrow c_{\mathcal{F}}^{-2M}$ . A direct calculation shows

$$U(x) - U(x; \boldsymbol{\lambda}_D^{\text{KA}}) - 2\partial_x^2 \log \left| \frac{W[\phi_{d_1}, \dots, \phi_{d_M}](x)}{\Xi_D^{\text{KA}}(x)} \right| = \mathcal{E}_M. \quad (\text{B.23})$$

The similarity transformed deformed Hamiltonian  $\tilde{\mathcal{H}}_D^{\text{KA}} = \psi_D^{\text{KA}}(x)^{-1} \circ \mathcal{H}_D^{\text{KA}} \circ \psi_D^{\text{KA}}(x)$  is expressed as

$$\begin{aligned} \tilde{\mathcal{H}}_D^{\text{KA}} &= -\frac{d^2}{dx^2} - 2\frac{\psi_D^{\text{KA}'}(x)}{\psi_D^{\text{KA}}(x)} \frac{d}{dx} + 2\frac{\phi_0'(x; \boldsymbol{\lambda}_D^{\text{KA}})}{\phi_0(x; \boldsymbol{\lambda}_D^{\text{KA}})} \frac{\check{\Xi}_D^{\text{KA}'}(x)}{\check{\Xi}_D^{\text{KA}}(x)} - \frac{\check{\Xi}_D^{\text{KA}''}(x)}{\check{\Xi}_D^{\text{KA}}(x)} + \mathcal{E}_M \\ &= -4 \left( c_2(\eta) \frac{d^2}{d\eta^2} + \left( c_1(\eta, \boldsymbol{\lambda}_D^{\text{KA}}) - 2c_2(\eta) \frac{\Xi_D^{\text{KA}'}(\eta)}{\Xi_D^{\text{KA}}(\eta)} \right) \frac{d}{d\eta} \right. \\ &\quad \left. + c_2(\eta) \frac{\Xi_D^{\text{KA}''}(\eta)}{\Xi_D^{\text{KA}}(\eta)} - c_1(\eta, \boldsymbol{\lambda}_D^{\text{KA}} - \boldsymbol{\delta}) \frac{\Xi_D^{\text{KA}'}(\eta)}{\Xi_D^{\text{KA}}(\eta)} \right) + \mathcal{E}_M. \end{aligned} \quad (\text{B.24})$$

From the identity (4.30) with  $\hat{\mathcal{A}}_{d_1 \dots d_s} = \frac{d}{dx} - \partial_x \log |\phi_{d_1 \dots d_s}(x)|$  and  $\hat{\mathcal{A}}_{d_1 \dots d_s}^\dagger = -\frac{d}{dx} - \partial_x \log |\phi_{d_1 \dots d_s}(x)|$ , we obtain Proposition 4.1 with the following replacements,

$$(4.31) \rightarrow 2(\mathcal{E}_n - \mathcal{E}_{d'}) \frac{\Xi_{\mathcal{D}'}^{\text{KA}}(\eta)}{\Xi_{\mathcal{D}''}^{\text{KA}}(\eta)} P_{\mathcal{D}'',n}^{\text{KA}}(\eta) = (\tilde{\mathcal{H}}_{\mathcal{D}''}^{\text{KA}} + \mathcal{E}_n - \mathcal{E}_{d'} - \mathcal{E}_{d''}) P_{\mathcal{D}'',n}^{\text{KA}}(\eta), \quad (\text{B.25})$$

which can be shown in a similar way to (B.5). We have Proposition 4.2.

Like as §B.1, we obtain Proposition 4.3 with the replacement,

$$(4.39) \rightarrow \widetilde{\mathcal{M}}_{jk} = \frac{1}{(\eta_j - \eta_k)^2} \frac{-\tilde{\mathcal{H}}_D^{\text{KA}}(\eta(x) \check{P}_{\mathcal{D},\mathcal{N}}^{\text{KA}}(x))|_{x=x_j}}{P_{\mathcal{D},\mathcal{N}}^{\text{KA}'}(\eta_j)} \quad (j \neq k), \quad (\text{B.26})$$

and Proposition 4.4 with the replacement

$$(4.42) \rightarrow \check{F}^{\text{KA}}(x) = 2\eta'(x)^2, \quad F^{\text{KA}}(\eta) = 8c_2(\eta). \quad (\text{B.27})$$

Then we have Proposition 4.5, and the matrix elements  $\widetilde{\mathcal{M}}_{jk}$  and  $\mathcal{M}_{jk}$  ( $j \neq k$ ) are given by (B.9) with the replacement  $F_j \rightarrow F_j^{\text{KA}}$ . The diagonal elements  $\widetilde{\mathcal{M}}_{jj} = \mathcal{M}_{jj}$  are given by

$$\widetilde{\mathcal{M}}_{jj} = 4c_2(\eta_j) \left( \sum_{\substack{m=1 \\ m \neq j}}^{\tilde{N}} \frac{1}{(\eta_j - \eta_m)^2} + \left( \sum_{\substack{m=1 \\ m \neq j}}^{\tilde{N}} \frac{1}{\eta_j - \eta_m} \right)^2 - \frac{\Xi_D^{\text{KA}''}(\eta_j)}{\Xi_D^{\text{KA}}(\eta_j)} \right)$$

$$+ 4c_1(\eta_j, \boldsymbol{\lambda}_{\mathcal{D}}^{\text{KA}} - \boldsymbol{\delta}) \frac{\Xi_{\mathcal{D}}^{\text{KA}'}(\eta_j)}{\Xi_{\mathcal{D}}^{\text{KA}}(\eta_j)} + \mathcal{E}_M. \quad (\text{B.28})$$

For the Krein-Adler type multi-indexed Jacobi polynomials, the assumptions of Theorem 2.1 are satisfied (for generic values of  $\boldsymbol{\lambda}$ ). Therefore Theorem 2.1 gives the following.

**Theorem B.2** *For the Krein-Adler type multi-indexed orthogonal polynomials of H, L and J types  $P_{\mathcal{D},n}^{\text{KA}}(\eta)$ ,  $\mathcal{P}_a^{\text{KA}}(\eta)$  (4.35) and  $F^{\text{KA}}(\eta)$  (B.27), we have the discrete orthogonality relations:*

$$\sum_{j=1}^{\tilde{\mathcal{N}}} \frac{1}{F^{\text{KA}}(\eta_j)} \frac{\mathcal{P}_a^{\text{KA}}(\eta_j)}{P_{\mathcal{N}}^{\text{KA}'}(\eta_j)} \frac{\mathcal{P}_b^{\text{KA}}(\eta_j)}{P_{\mathcal{N}}^{\text{KA}'}(\eta_j)} = k_a^{[\mathcal{D},\mathcal{N}] \text{KA}} \delta_{ab} \quad (a, b = 1, 2, \dots, \tilde{\mathcal{N}}), \quad (\text{B.29})$$

where  $k_a^{[\mathcal{D},\mathcal{N}]}$ 's are normalization constants.

**Remark B.3** We have the same remark as Remark B.1. For L and H cases, there may be a degeneracy in  $\mathcal{E}_a^{\mathcal{P} \text{KA}}$  even for generic values of  $\boldsymbol{\lambda}$ . Since the Krein-Adler type multi-indexed L and H polynomials  $P_{\mathcal{D},n}^{\text{KA}}(\eta)$  can be obtained from those of J by taking certain limit of parameters (with appropriate rescalings), the discrete orthogonality relations (B.29) for J are inherited by L and H. This point is not mentioned in [27].

**Remark B.4** Like as Remark 4.5, the discrete orthogonality relations (B.29) hold for any complex values of parameters  $\boldsymbol{\lambda}$  (with the condition  $c_{\mathcal{D}}^{\Xi \text{KA}}, c_{\mathcal{D},\mathcal{N}}^{\mathcal{P} \text{KA}} \neq 0$ ), and for the index set  $\mathcal{D}$  without the Krein-Adler condition (4.14). For H case without (4.14), however,  $P_{\mathcal{N}}(\eta)$  may have zero  $\eta = 0$  with multiplicity. For such case,  $P_{\mathcal{N}}^{\text{KA}'}(0)$  vanishes and (B.29) does not hold.

We conjecture the normalization constants  $k_a^{[\mathcal{D},\mathcal{N}] \text{KA}}$  as follows.

**Conjecture B.2** *The normalization constants  $k_a^{[\mathcal{D},\mathcal{N}] \text{KA}}$  are given by*

$$(0) \quad \mathcal{P}_a^{\text{KA}} = P_{\mathcal{D},n}^{\text{KA}} : k_a^{[\mathcal{D},\mathcal{N}] \text{KA}} = \frac{1}{8} \frac{h_{\mathcal{D},n}}{h_{\mathcal{D},\mathcal{N}}} \times \begin{cases} 2 & : \text{H} \\ 1 & : \text{L} \\ \frac{1}{2\mathcal{N}+g+h} & : \text{J} \end{cases}, \quad (\text{B.30})$$

$$(1) \quad \mathcal{P}_a^{\text{KA}} = P_{\mathcal{D}'_{jk},\mathcal{N}}^{\text{KA}} :$$

$$k_a^{[\mathcal{D},\mathcal{N}] \text{KA}} = \frac{1}{8} \frac{h_{\mathcal{D}'_{jk},\mathcal{N}}}{h_{\mathcal{D},\mathcal{N}}} \prod_{\substack{i=1 \\ i \neq j}}^M \frac{d_i - \epsilon_k}{d_i - d_j}$$

$$\times \left\{ \begin{array}{ll} \frac{2^{\epsilon_k - d_j + 1}}{(\epsilon_k + 1)_{d_j - \epsilon_k}} & : \text{H} \\ \frac{(\epsilon_k + 1)_{d_j - \epsilon_k}}{(\epsilon_k + g + \frac{1}{2})_{d_j - \epsilon_k}} & : \text{L} \\ \frac{(\epsilon_k + 1)_{d_j - \epsilon_k}}{(\epsilon_k + g + \frac{1}{2})_{d_j - \epsilon_k}} \frac{(\epsilon_k + g + h)_{d_j - \epsilon_k}}{(2\epsilon_k + g + h)(\epsilon_k + h + \frac{1}{2})_{d_j - \epsilon_k}} & \\ \times \prod_{\substack{i=1 \\ i \neq j}}^M \frac{d_i + \epsilon_k + g + h}{d_i + d_j + g + h} & : \text{J} \end{array} \right. . \quad (\text{B.31})$$

By numerical calculation, we can verify this conjecture for small  $M$ ,  $d_j$ ,  $\mathcal{N}$  and  $n$ .

### B.3 Proofs of (B.5) and (B.6)

In this subsection we prove (B.5) and (B.6). We use the abbreviated notations (A.1). For example, we have

$$\mathcal{H}_{\mathcal{D}''} = -\frac{d^2}{dx^2} + U(x) - 2\partial_x^2 \log |w_2(x)|, \quad \phi_{\mathcal{D}''n}(x) = \frac{u_2(x)}{w_2(x)} = c_{\mathcal{F}}^{M+1} \psi_{\mathcal{D}''}(x) \check{P}_{\mathcal{D}''n}(x).$$

For simplicity in notation, we omit the argument “(x)” and write  $\partial_x^2 \log |w_2(x)|$  as  $\partial_x^2 \log w_2$ .

From  $\mathcal{H}_{\mathcal{D}} \tilde{\phi}_{\mathcal{D}d'} = \tilde{\mathcal{E}}_{d'} \tilde{\phi}_{\mathcal{D}d'}$  and  $\tilde{\phi}_{\mathcal{D}d'} = w_1/w$  (see Appendix A in [31]), we obtain

$$-\frac{w_1''}{w_1} + 2\frac{w'}{w} \frac{w_1'}{w_1} + U - \frac{w''}{w} = \tilde{\mathcal{E}}_{d'}. \quad (\text{B.32})$$

Similarly we have

$$-\frac{w_2''}{w_2} + 2\frac{w'}{w} \frac{w_2'}{w_2} + U - \frac{w''}{w} = \tilde{\mathcal{E}}_{d''}, \quad (\text{B.33})$$

and  $\mathcal{H}_{\mathcal{D}'} \tilde{\phi}_{\mathcal{D}'d''} = \tilde{\mathcal{E}}_{d''} \tilde{\phi}_{\mathcal{D}'d''}$  with  $\tilde{\phi}_{\mathcal{D}'d''} = w_3/w_1$  gives

$$-\frac{w_3''}{w_3} + 2\frac{w_1'}{w_1} \frac{w_3'}{w_3} + U - \frac{w_1''}{w_1} = \tilde{\mathcal{E}}_{d''}. \quad (\text{B.34})$$

From the form of  $\mathcal{H}_{\mathcal{D}}$ , we have

$$-2\frac{d^2}{dx^2} = \mathcal{H}_{\mathcal{D}'} + \mathcal{H}_{\mathcal{D}''} - 2U + 2\partial_x^2 \log w_1 w_2 = \mathcal{H}_{\mathcal{D}} + \mathcal{H}_{\mathcal{D}'''} - 2U + 2\partial_x^2 \log w w_3. \quad (\text{B.35})$$

#### B.3.1 proof of (B.5)

Since  $d'$  and  $d''$  are the same type, we have  $\lambda_{\mathcal{D}'} = \lambda_{\mathcal{D}''}$  and  $g_{\mathcal{D}'} = g_{\mathcal{D}''}$ , namely

$$\frac{\psi_{\mathcal{D}'}}{\psi_{\mathcal{D}''}} = \frac{\check{\Xi}_{\mathcal{D}''}}{\check{\Xi}_{\mathcal{D}'}} = \frac{w_2}{w_1}. \quad (\text{B.36})$$

Then we have

$$\begin{aligned} \frac{\psi_{\mathcal{D}''}}{\psi_{\mathcal{D}'}} \circ \tilde{\mathcal{H}}_{\mathcal{D}''} \circ \frac{\psi_{\mathcal{D}'}}{\psi_{\mathcal{D}''}} &= \frac{w_1}{w_2} \circ \tilde{\mathcal{H}}_{\mathcal{D}''} \circ \frac{w_2}{w_1} \\ &= \tilde{\mathcal{H}}_{\mathcal{D}''} - 2\partial_x \log \frac{w_2}{w_1} \cdot \frac{d}{dx} - \frac{w_1}{w_2} \left( \frac{w_2}{w_1} \right)'' - 2\partial_x \log \psi_{\mathcal{D}''} \cdot \partial_x \log \frac{w_2}{w_1}. \end{aligned} \quad (\text{B.37})$$

By writing down the identity (3.40) and multiplying by  $2(\mathcal{E}_n - \tilde{\mathcal{E}}_{d'})$ , we have

$$\begin{aligned} &2(\mathcal{E}_n - \tilde{\mathcal{E}}_{d'})\phi_{\mathcal{D}''n} \\ &= \left( -2\frac{d^2}{dx^2} + 2\partial_x \log \frac{w_2}{w_1} \cdot \frac{d}{dx} + 2\partial_x \log \frac{w_2}{w_1} \cdot \partial_x \log \frac{w_1}{w} - 2\partial_x^2 \log \frac{w_1}{w} \right) \phi_{\mathcal{D}'n} \\ &\stackrel{(i)}{=} \left( \mathcal{H}_{\mathcal{D}'} + \mathcal{H}_{\mathcal{D}''} + 2\partial_x \log \frac{w_2}{w_1} \cdot \frac{d}{dx} - 2U + 2\partial_x^2 \log ww_2 + 2\partial_x \log \frac{w_2}{w_1} \cdot \partial_x \log \frac{w_1}{w} \right) \phi_{\mathcal{D}'n} \\ &\stackrel{(ii)}{=} c_{\mathcal{F}}^{M+1} \psi_{\mathcal{D}'} \left( \mathcal{E}_n + \frac{\psi_{\mathcal{D}''}}{\psi_{\mathcal{D}'}} \circ \tilde{\mathcal{H}}_{\mathcal{D}''} \circ \frac{\psi_{\mathcal{D}'}}{\psi_{\mathcal{D}''}} + 2\partial_x \log \frac{w_2}{w_1} \cdot \frac{1}{\psi_{\mathcal{D}'}} \circ \frac{d}{dx} \circ \psi_{\mathcal{D}'} \right. \\ &\quad \left. - 2U + 2\partial_x^2 \log ww_2 + 2\partial_x \log \frac{w_2}{w_1} \cdot \partial_x \log \frac{w_1}{w} \right) \check{P}_{\mathcal{D}',n} \\ &\stackrel{(iii)}{=} c_{\mathcal{F}}^{M+1} \psi_{\mathcal{D}'} \left( \mathcal{E}_n + \tilde{\mathcal{H}}_{\mathcal{D}''} - \frac{w_1}{w_2} \left( \frac{w_2}{w_1} \right)'' + 2\partial_x \log \frac{\psi_{\mathcal{D}'}}{\psi_{\mathcal{D}''}} \cdot \partial_x \log \frac{w_2}{w_1} \right. \\ &\quad \left. - 2U + 2\partial_x^2 \log ww_2 + 2\partial_x \log \frac{w_2}{w_1} \cdot \partial_x \log \frac{w_1}{w} \right) \check{P}_{\mathcal{D}',n} \\ &\stackrel{(iv)}{=} c_{\mathcal{F}}^{M+1} \psi_{\mathcal{D}'} \left( \mathcal{E}_n + \tilde{\mathcal{H}}_{\mathcal{D}''} + \frac{w_1''}{w_1} - 2\frac{w'}{w} \frac{w_1'}{w_1} - U + \frac{w''}{w} + \frac{w_2''}{w_2} - 2\frac{w'}{w} \frac{w_2'}{w_2} - U + \frac{w''}{w} \right) \check{P}_{\mathcal{D}',n} \\ &\stackrel{(v)}{=} c_{\mathcal{F}}^{M+1} \psi_{\mathcal{D}'} (\mathcal{E}_n + \tilde{\mathcal{H}}_{\mathcal{D}''} - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) \check{P}_{\mathcal{D}',n}, \end{aligned} \quad (\text{B.38})$$

where we have used (i): (B.35), (ii):  $\mathcal{H}_{\mathcal{D}'}\phi_{\mathcal{D}'n} = \mathcal{E}_n\phi_{\mathcal{D}'n}$  and (B.2), (iii): (B.37), (iv): (B.36), (v): (B.32) and (B.33). By dividing (B.38) by  $c_{\mathcal{F}}^{M+1}\psi_{\mathcal{D}'}$  and using (B.2) and (B.36), we obtain (B.5).  $\square$

### B.3.2 proof of (B.6)

Since  $d'$  and  $d''$  are different types, we have  $\boldsymbol{\lambda}_{\mathcal{D}} = \boldsymbol{\lambda}_{\mathcal{D}'''}$  and  $c_{\mathcal{F}}^{2M+1}g_{\mathcal{D}} = g_{\mathcal{D}'''}$ , namely

$$\frac{\psi_{\mathcal{D}}}{\psi_{\mathcal{D}'''}} = \frac{\check{\Xi}_{\mathcal{D}'''}}{\check{\Xi}_{\mathcal{D}}} = c_{\mathcal{F}}^{-2M-1} \frac{w_3}{w}. \quad (\text{B.39})$$

Then we have

$$\begin{aligned} \frac{\psi_{\mathcal{D}'''}}{\psi_{\mathcal{D}}} \circ \tilde{\mathcal{H}}_{\mathcal{D}'''} \circ \frac{\psi_{\mathcal{D}}}{\psi_{\mathcal{D}'''}} &= \frac{w}{w_3} \circ \tilde{\mathcal{H}}_{\mathcal{D}'''} \circ \frac{w_3}{w} \\ &= \tilde{\mathcal{H}}_{\mathcal{D}'''} - 2\partial_x \log \frac{w_3}{w} \cdot \frac{d}{dx} - \frac{w}{w_3} \left( \frac{w_3}{w} \right)'' - 2\partial_x \log \psi_{\mathcal{D}'''} \cdot \partial_x \log \frac{w_3}{w}. \end{aligned} \quad (\text{B.40})$$

By writing down the identity (3.41) and multiplying by  $-2$ , we have

$$\begin{aligned}
& -2\phi_{\mathcal{D}'''}_n \\
&= \left( -2\frac{d^2}{dx^2} + 2\partial_x \log \frac{w_3}{w} \cdot \frac{d}{dx} - 2\partial_x \log \frac{w_3}{w_1} \cdot \partial_x \log \frac{w_1}{w} + 2\partial_x^2 \log \frac{w_1}{w} \right) \phi_{\mathcal{D}n} \\
&\stackrel{(i)}{=} \left( \mathcal{H}_{\mathcal{D}} + \mathcal{H}_{\mathcal{D}'''} + 2\partial_x \log \frac{w_3}{w} \cdot \frac{d}{dx} - 2U + 2\partial_x^2 \log w_1 w_3 - 2\partial_x \log \frac{w_3}{w_1} \cdot \partial_x \log \frac{w_1}{w} \right) \phi_{\mathcal{D}n} \\
&\stackrel{(ii)}{=} c_{\mathcal{F}}^M \psi_{\mathcal{D}} \left( \mathcal{E}_n + \frac{\psi_{\mathcal{D}'''}}{\psi_{\mathcal{D}}} \circ \tilde{\mathcal{H}}_{\mathcal{D}'''} \circ \frac{\psi_{\mathcal{D}}}{\psi_{\mathcal{D}'''}} + 2\partial_x \log \frac{w_3}{w} \cdot \frac{1}{\psi_{\mathcal{D}}} \circ \frac{d}{dx} \circ \psi_{\mathcal{D}} \right. \\
&\quad \left. - 2U + 2\partial_x^2 \log w_1 w_3 - 2\partial_x \log \frac{w_3}{w_1} \cdot \partial_x \log \frac{w_1}{w} \right) \check{P}_{\mathcal{D},n} \\
&\stackrel{(iii)}{=} c_{\mathcal{F}}^M \psi_{\mathcal{D}} \left( \mathcal{E}_n + \tilde{\mathcal{H}}_{\mathcal{D}'''} - \frac{w}{w_3} \left( \frac{w_3}{w} \right)'' + 2\partial_x \log \frac{\psi_{\mathcal{D}}}{\psi_{\mathcal{D}'''}} \cdot \partial_x \log \frac{w_3}{w} \right. \\
&\quad \left. - 2U + 2\partial_x^2 \log w_1 w_3 + 2\partial_x \log \frac{w_3}{w_1} \cdot \partial_x \log \frac{w}{w_1} \right) \check{P}_{\mathcal{D},n} \\
&\stackrel{(iv)}{=} c_{\mathcal{F}}^M \psi_{\mathcal{D}} \left( \mathcal{E}_n + \tilde{\mathcal{H}}_{\mathcal{D}'''} + \frac{w_1''}{w_1} - 2\frac{w'}{w} \frac{w_1'}{w_1} - U + \frac{w''}{w} + \frac{w_3''}{w_3} - 2\frac{w_1'}{w_1} \frac{w_3'}{w_3} - U + \frac{w_1''}{w_1} \right) \check{P}_{\mathcal{D},n} \\
&\stackrel{(v)}{=} c_{\mathcal{F}}^M \psi_{\mathcal{D}} (\mathcal{E}_n + \tilde{\mathcal{H}}_{\mathcal{D}'''} - \tilde{\mathcal{E}}_{d'} - \tilde{\mathcal{E}}_{d''}) \check{P}_{\mathcal{D},n}, \tag{B.41}
\end{aligned}$$

where we have used (i): (B.35), (ii):  $\mathcal{H}_{\mathcal{D}}\phi_{\mathcal{D}n} = \mathcal{E}_n\phi_{\mathcal{D}n}$  and (B.2), (iii): (B.40), (iv): (B.39), (v): (B.32) and (B.34). By dividing (B.41) by  $c_{\mathcal{F}}^M \psi_{\mathcal{D}}$  and using (B.2) and (B.39), we obtain (B.6).  $\square$

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