

New determinant expressions of multi-indexed orthogonal polynomials in discrete quantum mechanics

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Multi-indexed orthogonal polynomials (the Meixner, little q -Jacobi (Laguerre), $(q-)$ Racah, Wilson, and Askey–Wilson types) satisfying second-order difference equations were constructed in discrete quantum mechanics. They are polynomials in sinusoidal coordinates $\eta(x)$ (x is the coordinate of the quantum system) and are expressed in terms of Casorati determinants whose matrix elements are functions of x at various points. By using shape-invariance properties, we derive various equivalent determinant expressions, especially those whose matrix elements are functions of the same point x . Except for the $(q-)$ Racah case, they can be expressed in terms of η only, without explicit x -dependence.

Subject Index A10, A64

1. Introduction

The exceptional and multi-indexed orthogonal polynomials $\{P_{\mathcal{D},n}(\eta) | n \in \mathbb{Z}_{\geq 0}\}$ (Refs. [1–14]) are a new type of orthogonal polynomials, which form a complete set of orthogonal basis in an appropriate Hilbert space despite missing degrees. Instead of the three-term recurrence relations that characterize ordinary orthogonal polynomials (Refs. [15–17]), they satisfy recurrence relations with more terms (Refs. [18–26]) and the constraints of Bochner’s theorem and its generalizations (Refs. [15–17,27,28]) are avoided. They satisfy second-order differential or difference equations and quantum mechanical formulation has played an important role in constructing these new orthogonal polynomials. The quantum mechanical systems described by classical orthogonal polynomials can be iso-spectrally (or almost iso-spectrally) deformed by applying the multi-step Darboux transformations (Refs. [29–35]) and the main part of the eigenfunctions of the deformed systems are multi-indexed orthogonal polynomials. 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 ℓ is a positive integer. The situation of case (1) is called stable in Ref. [6]. Case (1) is obtained by taking virtual states as the seed solutions of the Darboux transformation (Refs. [8,10,12,14]) and case (2) is obtained by employing eigenstates or pseudo-virtual states (Refs. [36–39]). In the quantum mechanical formulation, multi-indexed orthogonal polynomials appear as polynomials in the sinusoidal coordinate $\eta(x)$ (Refs. [40,41]), $P_{\mathcal{D},n}(\eta(x))$, where x is the coordinate of the quantum system.

The eigenstates of the deformed system are expressed in terms of determinants: Wronskians for ordinary quantum mechanics (in which the Schrödinger equation is a second-order differential

equation) and Casoratians for discrete quantum mechanics (in which the Schrödinger equations are second-order difference equations). In our previous paper Ref. [42], we presented simplified determinant expressions for case (1) multi-indexed Laguerre and Jacobi polynomials in ordinary quantum mechanics. We rewrite the Wronskians by using identities of the original Laguerre and Jacobi polynomials and two simplified expressions A and B are presented. The identities used in case A are essentially forward shift relations. For case B, the Schrödinger equation is used and it is regarded as a combination of the forward and backward shift relations, which are consequences of shape invariance. Thus both expressions A and B are derived by using properties of Wronskians and shape invariance (see Sect. 4 for details). This idea is also applicable to discrete quantum mechanics. In this paper we consider case (1) multi-indexed orthogonal polynomials appearing in discrete quantum mechanics: the Meixner, little q -Laguerre, little q -Jacobi, Racah, q -Racah, Wilson, and Askey–Wilson types. The first five appear in discrete quantum mechanics with real shifts (rdQM) and the last two belong to discrete quantum mechanics with pure imaginary shifts (idQM). We rewrite the Casoratians by using their properties and identities of the original polynomials, which are consequences of shape invariance. Various new determinant expressions of multi-indexed orthogonal polynomials are obtained. Corresponding to cases A and B in Ref. [42], we present two typical expressions explicitly. The matrix elements of the Casoratians are functions of x at various points, $x + j - 1$ for rdQM and $x + i(\frac{n+1}{2} - j)\gamma$ for idQM. In some of the new determinant expressions, the matrix elements are functions of the same point x . Therefore the multi-indexed orthogonal polynomials are expressed in terms of η only, namely, without explicit x -dependence. For the Racah and q -Racah cases, the corresponding matrix elements for multi-indexed polynomials do have explicit x -dependence because of the parameter (λ) dependence of the sinusoidal coordinates $\eta(x; \lambda)$. These new equivalent expressions show explicitly the constituents of the multi-indexed orthogonal polynomials and they help to gain a deeper understanding.

This paper is organized as follows. We derive new equivalent expressions for the multi-indexed Meixner, little q -Laguerre, little q -Jacobi, Racah, and q -Racah polynomials in Sect. 2. Those for the multi-indexed Wilson and Askey–Wilson polynomials are presented in Sect. 3. The discussions in these two sections are parallel. In Sect. 2.1 (Sect. 3.1), discrete quantum mechanics with real (pure imaginary) shifts is recapitulated and the data for the original systems are presented. The virtual state vectors (wave functions) and related functions are introduced in Sect. 2.2 (Sect. 3.2). The original systems have shape invariance, which entails the well-known forward and backward shift relations of the eigenpolynomials P_n . The forward and backward shift relations for virtual state polynomials ξ_v are presented in Sect. 2.3 (Sect. 3.3). In Sect. 2.4 (Sect. 3.4) the definitions of multi-indexed orthogonal polynomials given in Refs. [12,14] (Ref. [10]) are recapitulated. They are expressed in terms of Casoratians. Sections 2.5 and 3.5 are the main contents of this paper. The Casoratians are rewritten by using their properties and the identities stemming from shape invariance, and new determinant expressions of multi-indexed orthogonal polynomials are obtained. We present two typical examples. Section 4 is for a summary and comments.

2. Multi-indexed orthogonal polynomials in rdQM

In this section we derive various equivalent determinant expressions for multi-indexed orthogonal polynomials in the framework of discrete quantum mechanics with real shifts. They are the multi-indexed Meixner, little q -Laguerre, little q -Jacobi, Racah, and q -Racah polynomials.

2.1. Original systems

The Hamiltonian of discrete quantum mechanics with real shifts (rdQM) (Refs. [43,44]) $\mathcal{H} = (\mathcal{H}_{x,y})$ is a tri-diagonal real symmetric (Jacobi) matrix and its rows and columns are indexed by integers x and y , which take values in $\{0, 1, \dots, N\}$ (finite) or $\mathbb{Z}_{\geq 0}$ (semi-infinite),

$$\mathcal{H}_{x,y} \stackrel{\text{def}}{=} -\sqrt{B(x)D(x+1)}\delta_{x+1,y} - \sqrt{B(x-1)D(x)}\delta_{x-1,y} + (B(x) + D(x))\delta_{x,y}, \quad (2.1)$$

where the potential functions $B(x)$ and $D(x)$ are real and positive but vanish at the boundary, $D(0) = 0$ and $B(N) = 0$ for finite cases. This Hamiltonian can be expressed in a factorized form:

$$\mathcal{H} = \mathcal{A}^\dagger \mathcal{A}, \quad \mathcal{A} = (\mathcal{A}_{x,y}), \quad \mathcal{A}^\dagger = ((\mathcal{A}^\dagger)_{x,y}) = (\mathcal{A}_{y,x}), \quad (2.2)$$

$$\begin{aligned} \mathcal{A}_{x,y} &\stackrel{\text{def}}{=} \sqrt{B(x)}\delta_{x,y} - \sqrt{D(x+1)}\delta_{x+1,y}, \\ (\mathcal{A}^\dagger)_{x,y} &= \sqrt{B(x)}\delta_{x,y} - \sqrt{D(x)}\delta_{x-1,y}. \end{aligned} \quad (2.3)$$

For simplicity in notation, we write \mathcal{H} , \mathcal{A} , and \mathcal{A}^\dagger as follows:

$$\begin{aligned} \mathcal{H} &= -\sqrt{B(x)D(x+1)}e^\partial - \sqrt{B(x-1)D(x)}e^{-\partial} + B(x) + D(x) \\ &= -\sqrt{B(x)}e^\partial\sqrt{D(x)} - \sqrt{D(x)}e^{-\partial}\sqrt{B(x)} + B(x) + D(x), \end{aligned} \quad (2.4)$$

$$\mathcal{A} = \sqrt{B(x)} - e^\partial\sqrt{D(x)}, \quad \mathcal{A}^\dagger = \sqrt{B(x)} - \sqrt{D(x)}e^{-\partial}, \quad (2.5)$$

where matrices $e^{\pm\partial}$ are

$$e^{\pm\partial} = ((e^{\pm\partial})_{x,y}), \quad (e^{\pm\partial})_{x,y} \stackrel{\text{def}}{=} \delta_{x\pm 1,y}, \quad (e^\partial)^\dagger = e^{-\partial}, \quad (2.6)$$

and we suppress the unit matrix $\mathbf{1} = (\delta_{x,y})$: $(B(x) + D(x))\mathbf{1}$ in Eq. (2.4), $\sqrt{B(x)}\mathbf{1}$ in Eq. (2.5). (The notation $f(x)Ag(x)$, where $f(x)$ and $g(x)$ are functions of x and A is a matrix $A = (A_{x,y})$, stands for a matrix whose (x, y) -element is $f(x)A_{x,y}g(y)$.) Note that the matrices e^∂ and $e^{-\partial}$ are not inverse to each other: $e^{\pm\partial}e^{\mp\partial} \neq \mathbf{1}$ for finite systems and $e^{-\partial}e^\partial \neq \mathbf{1}$ for semi-infinite systems. The Schrödinger equation is the eigenvalue problem for the hermitian matrix \mathcal{H} ,

$$\mathcal{H}\phi_n(x) = \mathcal{E}_n\phi_n(x) \quad (n = 0, 1, 2, \dots), \quad 0 = \mathcal{E}_0 < \mathcal{E}_1 < \mathcal{E}_2 < \dots \quad (2.7)$$

($n = 0, 1, \dots, N$ for a finite case).

We consider rdQM described by the Meixner (M), little q -Laguerre (lqL), little q -Jacobi (lqJ), Racah (R), and q -Racah (q R) polynomials. The first three are semi-infinite systems and the last two are finite systems. Eigenvectors have the following factorized form:

$$\phi_n(x) = \phi_0(x)\check{P}_n(x), \quad \check{P}_n(x) \stackrel{\text{def}}{=} P_n(\eta(x)). \quad (2.8)$$

Here the ground state eigenvector $\phi_0(x)$, which is characterized by $\mathcal{A}\phi_0(x) = 0$, is chosen as

$$\phi_0(x) = \prod_{y=0}^{x-1} \left(\frac{B(y)}{D(y+1)} \right)^{1/2} > 0. \quad (2.9)$$

We use the convention that $\prod_{k=n}^{n-1} * = 1$, which means the normalization $\phi_0(0) = 1$. The other function $P_n(\eta)$ is a degree- n polynomial in η , and $\eta(x)$ is the sinusoidal coordinate satisfying the boundary condition $\eta(0) = 0$. We adopt the universal normalization condition (Refs. [43,44]) as

$$P_n(0) = 1 \quad (\Leftrightarrow \check{P}_n(0) = 1). \quad (2.10)$$

Various quantities depend on a set of parameters $\lambda = (\lambda_1, \lambda_2, \dots)$ and their dependence is expressed like $\mathcal{H} = \mathcal{H}(\lambda)$, $\mathcal{A} = \mathcal{A}(\lambda)$, $\mathcal{E}_n = \mathcal{E}_n(\lambda)$, $B(x) = B(x; \lambda)$, $\phi_n(x) = \phi_n(x; \lambda)$, $\check{P}_n(x) = \check{P}_n(x; \lambda) = P_n(\eta(x; \lambda); \lambda)$, etc. The parameter q is $0 < q < 1$ and q^λ stands for $q^{(\lambda_1, \lambda_2, \dots)} = (q^{\lambda_1}, q^{\lambda_2}, \dots)$. The symbols $(a)_n$ and $(a; q)_n$ are (q) -shifted factorials (Ref. [45]) and $[x]$ denotes the greatest integer not exceeding x .

The parameters of the systems are

$$M: \lambda = (\beta, c), \quad \delta = (1, 0), \quad \kappa = 1, \quad \beta > 0, \quad 0 < c < 1, \tag{2.11}$$

$$lqL: q^\lambda = a, \quad \delta = 1, \quad \kappa = q^{-1}, \quad 0 < a < q^{-1}, \tag{2.12}$$

$$lqJ: q^\lambda = (a, b), \quad \delta = (1, 1), \quad \kappa = q^{-1}, \quad 0 < a < q^{-1}, \quad b < q^{-1}, \tag{2.13}$$

$$R: \lambda = (a, b, c, d), \quad \delta = (1, 1, 1, 1), \quad \kappa = 1, \tag{2.14}$$

$$qR: q^\lambda = (a, b, c, d), \quad \delta = (1, 1, 1, 1), \quad \kappa = q^{-1}, \tag{2.15}$$

and we adopt the following choice of the parameter ranges for R and qR:

$$R: a = -N, \quad 0 < d < a + b, \quad 0 < c < 1 + d, \tag{2.16}$$

$$qR: a = q^{-N}, \quad 0 < ab < d < 1, \quad qd < c < 1. \tag{2.17}$$

We list the fundamental data (Ref. [43]).

◦ **Meixner:**

We rescale the overall normalization of the Hamiltonian in Ref. [43]: $(\mathcal{H}$ in Ref. [43]) $\times (1 - c) \rightarrow \mathcal{H}$.

$$B(x; \lambda) = c(x + \beta), \quad D(x) = x, \tag{2.18}$$

$$\mathcal{E}_n(\lambda) = (1 - c)n, \quad \eta(x) = x, \quad \varphi(x) = 1, \tag{2.19}$$

$$\check{P}_n(x; \lambda) = {}_2F_1\left(\begin{matrix} -n, -x \\ \beta \end{matrix} \middle| 1 - c^{-1}\right) = M_n(x; \beta, c), \tag{2.20}$$

$$\phi_0(x; \lambda) = \left(\frac{(\beta)_x c^x}{x!}\right)^{1/2}, \tag{2.21}$$

where $M_n(x; \beta, c)$ is the Meixner polynomial (Ref. [45]).

◦ **Little q -Laguerre and little q -Jacobi:**

$$B(x; \lambda) = \begin{cases} aq^{-x} & : lqL, \\ a(q^{-x} - bq) & : lqJ, \end{cases} \quad D(x) = q^{-x} - 1, \tag{2.22}$$

$$\mathcal{E}_n(\lambda) = \begin{cases} q^{-n} - 1 & : lqL, \\ (q^{-n} - 1)(1 - abq^{n+1}) & : lqJ, \end{cases} \quad \eta(x) = 1 - q^x, \quad \varphi(x) = q^x, \tag{2.23}$$

$$\begin{aligned} \check{P}_n(x; \lambda) &= \begin{cases} 2\phi_0\left(\begin{matrix} q^{-n}, q^{-x} \\ - \end{matrix} \middle| q; \frac{q^x}{a}\right) = (a^{-1}q^{-n}; q)_n {}_2\phi_1\left(\begin{matrix} q^{-n}, 0 \\ aq \end{matrix} \middle| q; q^{x+1}\right), \\ 3\phi_1\left(\begin{matrix} q^{-n}, abq^{n+1}, q^{-x} \\ bq \end{matrix} \middle| q; \frac{q^x}{a}\right) = \frac{(a^{-1}q^{-n}; q)_n}{(bq; q)_n} {}_2\phi_1\left(\begin{matrix} q^{-n}, abq^{n+1} \\ aq \end{matrix} \middle| q; q^{x+1}\right), \end{cases} \\ &= \begin{cases} (a^{-1}q^{-n}; q)_n p_n(1 - \eta(x); a|q) & : lqL, \\ (bq; q)_n^{-1} (a^{-1}q^{-n}; q)_n p_n(1 - \eta(x); a, b|q) & : lqJ, \end{cases} \end{aligned} \tag{2.24}$$

$$\phi_0(x; \lambda) = \begin{cases} ((q; q)_x^{-1}(aq)^x)^{1/2} & : lqL, \\ ((bq; q)_x(q; q)_x^{-1}(aq)^x)^{1/2} & : lqJ, \end{cases} \tag{2.25}$$

where $p_n(y; a|q)$ and $p_n(y; a, b|q)$ are the little q -Laguerre and little q -Jacobi polynomials in the conventional definition (Ref. [45]), respectively.

o **Racah and q -Racah:**

$$B(x; \lambda) = \begin{cases} -\frac{(x+a)(x+b)(x+c)(x+d)}{(2x+d)(2x+1+d)} & : R, \\ -\frac{(1-aq^x)(1-bq^x)(1-cq^x)(1-dq^x)}{(1-dq^{2x})(1-dq^{2x+1})} & : qR, \end{cases} \tag{2.26}$$

$$D(x; \lambda) = \begin{cases} -\frac{(x+d-a)(x+d-b)(x+d-c)x}{(2x-1+d)(2x+d)} & : R, \\ -\tilde{d} \frac{(1-a^{-1}dq^x)(1-b^{-1}dq^x)(1-c^{-1}dq^x)(1-q^x)}{(1-dq^{2x-1})(1-dq^{2x})} & : qR, \end{cases} \tag{2.27}$$

$$\mathcal{E}_n(\lambda) = \begin{cases} n(n+\tilde{d}) & : R, \\ (q^{-n}-1)(1-\tilde{d}q^n) & : qR, \end{cases} \quad \eta(x; \lambda) = \begin{cases} x(x+d) & : R, \\ (q^{-x}-1)(1-dq^x) & : qR, \end{cases} \tag{2.28}$$

$$\varphi(x; \lambda) = \begin{cases} \frac{2x+d+1}{d+1} & : R, \\ \frac{q^{-x}-dq^{x+1}}{1-dq} & : qR, \end{cases} \quad \tilde{d} \stackrel{\text{def}}{=} \begin{cases} a+b+c-d-1 & : R, \\ abcd^{-1}q^{-1} & : qR, \end{cases} \tag{2.29}$$

$$\check{P}_n(x; \lambda) = P_n(\eta(x; \lambda); \lambda) = \begin{cases} {}_4F_3\left(\begin{matrix} -n, n+\tilde{d}, -x, x+d \\ a, b, c \end{matrix} \middle| 1\right), \\ {}_4\phi_3\left(\begin{matrix} q^{-n}, \tilde{d}q^n, q^{-x}, dq^x \\ a, b, c \end{matrix} \middle| q; q\right), \end{cases} \tag{2.30}$$

$$= \begin{cases} R_n(\eta(x; \lambda); a-1, \tilde{d}-a, c-1, d-c) & : R, \\ R_n(1+d+\eta(x; \lambda); aq^{-1}, \tilde{d}a^{-1}, cq^{-1}, dc^{-1}|q) & : qR, \end{cases}$$

$$\phi_0(x; \lambda) = \begin{cases} \left(\frac{(a, b, c, d)_x}{(d-a+1, d-b+1, d-c+1, 1)_x} \frac{2x+d}{d}\right)^{1/2} & : R, \\ \left(\frac{(a, b, c, d; q)_x}{(a^{-1}dq, b^{-1}dq, c^{-1}dq, q; q)_x} \frac{1-dq^{2x}}{\tilde{d}^x(1-d)}\right)^{1/2} & : qR, \end{cases} \tag{2.31}$$

where $R_n(x(x+\gamma+\delta+1); \alpha, \beta, \gamma, \delta)$ and $R_n(q^{-x}+\gamma\delta q^{x+1}; \alpha, \beta, \gamma, \delta|q)$ are the Racah and q -Racah polynomials (Ref. [45]), respectively. It should be emphasized that for these two polynomials, the sinusoidal coordinates $\eta(x)$ in Eq. (2.28) and the auxiliary function $\varphi(x)$ in Eq. (2.29) depend on the parameters $\eta(x; \lambda)$, $\varphi(x; \lambda)$ as distinct from the other polynomials in this section.

Note that the following relations are valid for all the systems discussed in this section:

$$\varphi(x; \lambda) = \frac{\eta(x+1; \lambda) - \eta(x; \lambda)}{\eta(1; \lambda)}, \tag{2.32}$$

$$\varphi(x; \lambda) = \left(\frac{B(0; \lambda)}{B(x; \lambda)}\right)^{1/2} \frac{\phi_0(x; \lambda + \delta)}{\phi_0(x; \lambda)}, \quad \varphi(x; \lambda) = \left(\frac{B(0; \lambda)}{D(x+1; \lambda)}\right)^{1/2} \frac{\phi_0(x; \lambda + \delta)}{\phi_0(x+1; \lambda)}, \tag{2.33}$$

$$\frac{B(x; \lambda + \delta)}{B(x + 1; \lambda)} = \kappa^{-1} \frac{\varphi(x + 1; \lambda)}{\varphi(x; \lambda)}, \quad \frac{D(x; \lambda + \delta)}{D(x; \lambda)} = \kappa^{-1} \frac{\varphi(x - 1; \lambda)}{\varphi(x; \lambda)}. \tag{2.34}$$

2.2. Virtual states

The virtual state vectors are obtained by using the discrete symmetries of the Hamiltonian (Refs. [12, 14]). We define the twist operation t as

$$t(\lambda) \stackrel{\text{def}}{=} \begin{cases} (\lambda_1, \lambda_2^{-1}) & : M, \\ -\lambda_1 & : lqL, \\ (-\lambda_1, \lambda_2) & : lqJ, \\ (\lambda_4 - \lambda_1 + 1, \lambda_4 - \lambda_2 + 1, \lambda_3, \lambda_4) & : R, qR, \end{cases}$$

namely,
$$\begin{cases} t(\lambda) = (\beta, c^{-1}) & : M, \\ q^{t(\lambda)} = a^{-1} & : lqL, \\ q^{t(\lambda)} = (a^{-1}, b) & : lqJ, \\ t(\lambda) = (d - a + 1, d - b + 1, c, d) & : R, \\ q^{t(\lambda)} = (a^{-1}dq, b^{-1}dq, c, d) & : qR, \end{cases} \tag{2.35}$$

which is an involution $t^2 = \text{id}$ and satisfies

$$t(\lambda) + u\delta = t(\lambda + u\tilde{\delta}) \quad (\forall u \in \mathbb{R}), \quad \tilde{\delta} \stackrel{\text{def}}{=} \begin{cases} (1, 0) & : M, \\ -1 & : lqL, \\ (-1, 1) & : lqJ, \\ (0, 0, 1, 1) & : R, qR. \end{cases} \tag{2.36}$$

Note that this twist operation does not affect $\eta(x; \lambda)$ and $\varphi(x; \lambda)$,

$$\eta(x; t(\lambda)) = \eta(x; \lambda), \quad \varphi(x; t(\lambda)) = \varphi(x; \lambda). \tag{2.37}$$

We define two functions $B'(x; \lambda)$ and $D'(x; \lambda)$:

$$B'(x; \lambda) \stackrel{\text{def}}{=} B(x; t(\lambda)), \quad D'(x; \lambda) \stackrel{\text{def}}{=} D(x; t(\lambda)). \tag{2.38}$$

By using the twist operation, the virtual state vectors $\tilde{\phi}_v(x; \lambda)$ are introduced:

$$\begin{aligned} \tilde{\phi}_v(x; \lambda) &\stackrel{\text{def}}{=} \phi_v(x; t(\lambda)) = \tilde{\phi}_0(x; \lambda) \check{\xi}_v(x; \lambda), & \tilde{\phi}_0(x; \lambda) &\stackrel{\text{def}}{=} \phi_0(x; t(\lambda)), \\ \check{\xi}_v(x; \lambda) &\stackrel{\text{def}}{=} \xi_v(\eta(x; \lambda); \lambda) \stackrel{\text{def}}{=} \check{P}_v(x; t(\lambda)) = P_v(\eta(x; \lambda); t(\lambda)). \end{aligned} \tag{2.39}$$

The virtual state polynomials $\xi_v(\eta; \lambda)$ are polynomials of degree v in η . The virtual state vectors satisfy the Schrödinger equation $\mathcal{H}(\lambda)\tilde{\phi}_v(x; \lambda) = \tilde{\mathcal{E}}_v(\lambda)\tilde{\phi}_v(x; \lambda)$ (except for the upper boundary $x = N$ for finite cases) with virtual energies $\tilde{\mathcal{E}}_v(\lambda)$,

$$\tilde{\mathcal{E}}_v(\lambda) = \begin{cases} -(1 - c)(v + \beta) & : M, \\ -(1 - aq^{-v}) & : lqL, \\ -(1 - aq^{-v})(1 - bq^{v+1}) & : lqJ, \\ -(c + v)(a + b - d - v - 1) & : R, \\ -(1 - cq^v)(1 - abd^{-1}q^{-v-1}) & : qR. \end{cases} \tag{2.40}$$

The other data $\alpha(\lambda)$ and $\alpha'(\lambda)$ (see Refs. [12,14] for details) are

$$\alpha(\lambda) = \begin{cases} c & : M, \\ a & : lqL, lqJ, \\ 1 & : R, \\ abd^{-1}q^{-1} & : qR, \end{cases} \quad \alpha'(\lambda) = \begin{cases} -(1-c)\beta & : M, \\ -(1-a) & : lqL, \\ -(1-a)(1-bq) & : lqJ, \\ -c(a+b-d-1) & : R, \\ -(1-c)(1-abd^{-1}q^{-1}) & : qR. \end{cases} \quad (2.41)$$

In order to obtain well-defined quantum systems, we have to restrict the degree v and parameters λ so that the conditions $\tilde{\mathcal{E}}_v(\lambda) < 0$, $\alpha(\lambda) > 0$, $\alpha'(\lambda) < 0$, no zeros of $\xi_v(\eta; \lambda)$ in the domain, etc. are satisfied; see Refs. [12,14]. In this paper, however, we consider algebraic properties only and we do not bother about the ranges of v and λ .

The function $v(x; \lambda)$ is defined as the ratio of ϕ_0 and $\tilde{\phi}_0$:

$$v(x; \lambda) \stackrel{\text{def}}{=} \frac{\phi_0(x; \lambda)}{\tilde{\phi}_0(x; \lambda)}. \quad (2.42)$$

Since the potential functions $B(x; \lambda)$ and $D(x; \lambda)$ are rational functions of x or q^x , this function $v(x; \lambda)$ can be analytically continued into a meromorphic function of x or q^x through the functional relations

$$v(x+1; \lambda) = \frac{B(x; \lambda)}{\alpha(\lambda)B'(x; \lambda)}v(x; \lambda), \quad v(x-1; \lambda) = \frac{D(x; \lambda)}{\alpha(\lambda)D'(x; \lambda)}v(x; \lambda). \quad (2.43)$$

Explicitly it is

$$v(x; \lambda) = \begin{cases} c^x & : M, \\ a^x & : lqL, lqJ, \\ \frac{\Gamma(1-a)\Gamma(x+b)\Gamma(d-a+1)\Gamma(b-d-x)}{\Gamma(1-a-x)\Gamma(b)\Gamma(x+d-a+1)\Gamma(b-d)} & : R, \\ \frac{(a^{-1}q^{1-x}, b, a^{-1}dq^{x+1}, bd^{-1}; q)_\infty}{(a^{-1}q, bq^x, a^{-1}dq, bd^{-1}q^{-x}; q)_\infty} & : qR. \end{cases} \quad (2.44)$$

For a non-negative integer x , it reduces to

$$v(x; \lambda) = \frac{(1-a-x, b)_x}{(d-a+1, b-d-x)_x} : R, \quad v(x; \lambda) = \frac{(a^{-1}q^{1-x}, b; q)_x}{(a^{-1}dq, bd^{-1}q^{-x}; q)_x} : qR. \quad (2.45)$$

The functions $r_j(x; \lambda, M)$ are defined as the ratio of v 's:

$$r_j(x+j-1; \lambda, M) \stackrel{\text{def}}{=} \frac{v(x+j-1; \lambda)}{v(x; \lambda + M\tilde{\delta})} \quad (1 \leq j \leq M+1), \quad (2.46)$$

whose explicit forms are

$$r_j(x+j-1; \lambda, M) = \begin{cases} c^{j-1} & : M, \\ a^{j-1}q^{Mx} & : lqL, lqJ, \\ \frac{(x+a, x+b)_{j-1}(x+d-a+j, x+d-b+j)_{M+1-j}}{(d-a+1, d-b+1)_M} & : R, \\ \frac{(aq^x, bq^x; q)_{j-1}(a^{-1}dq^{x+j}, b^{-1}dq^{x+j}; q)_{M+1-j}}{(abd^{-1}q^{-1})^{j-1}q^{Mx}(a^{-1}dq, b^{-1}dq; q)_M} & : qR. \end{cases} \quad (2.47)$$

The auxiliary function $\varphi_M(x)$ (Ref. [35]) is defined by

$$\begin{aligned} \varphi_M(x; \lambda) &\stackrel{\text{def}}{=} \prod_{1 \leq j < k \leq M} \frac{\eta(x+k-1; \lambda) - \eta(x+j-1; \lambda)}{\eta(k-j; \lambda)} \\ &= \prod_{1 \leq j < k \leq M} \varphi(x+j-1; \lambda + (k-j-1)\delta), \end{aligned} \tag{2.48}$$

and $\varphi_0(x) = \varphi_1(x) = 1$. For M , lqL , and lqJ , its explicit form is

$$\varphi_M(x) = \kappa^{-\frac{1}{2}M(M-1)x - \frac{1}{6}M(M-1)(M-2)}.$$

In the following we adopt the convention

$$\check{P}_n(x; \lambda) \stackrel{\text{def}}{=} 0 \quad (n \in \mathbb{Z}_{<0}), \quad \check{\xi}_v(x; \lambda) \stackrel{\text{def}}{=} 0 \quad (v \in \mathbb{Z}_{<0}). \tag{2.49}$$

2.3. Shape invariance

The original systems in Sect. 2.1 are shape invariant (Ref. [43]) and they satisfy the relation

$$\mathcal{A}(\lambda)\mathcal{A}(\lambda)^\dagger = \kappa\mathcal{A}(\lambda + \delta)^\dagger\mathcal{A}(\lambda + \delta) + \mathcal{E}_1(\lambda), \tag{2.50}$$

which is a sufficient condition for exact solvability. As a consequence of the shape invariance, the action of the operators $\mathcal{A}(\lambda)$ and $\mathcal{A}(\lambda)^\dagger$ on the eigenvectors is

$$\mathcal{A}(\lambda)\phi_n(x; \lambda) = \frac{\mathcal{E}_n(\lambda)}{\sqrt{B(0; \lambda)}} \phi_{n-1}(x; \lambda + \delta), \quad \mathcal{A}(\lambda)^\dagger\phi_{n-1}(x; \lambda + \delta) = \sqrt{B(0; \lambda)} \phi_n(x; \lambda). \tag{2.51}$$

The relations in Eq. (2.51) are equivalent to the forward and backward shift relations of the orthogonal polynomials P_n (Ref. [45]),

$$\mathcal{F}(\lambda)\check{P}_n(x; \lambda) = \mathcal{E}_n(\lambda)\check{P}_{n-1}(x; \lambda + \delta), \quad \mathcal{B}(\lambda)\check{P}_{n-1}(x; \lambda + \delta) = \check{P}_n(x; \lambda), \tag{2.52}$$

where the forward and backward shift operators $\mathcal{F}(\lambda)$ and $\mathcal{B}(\lambda)$ are defined by

$$\mathcal{F}(\lambda) \stackrel{\text{def}}{=} \sqrt{B(0; \lambda)} \phi_0(x; \lambda + \delta)^{-1} \circ \mathcal{A}(\lambda) \circ \phi_0(x; \lambda) = B(0; \lambda) \varphi(x; \lambda)^{-1} (1 - e^\delta), \tag{2.53}$$

$$\begin{aligned} \mathcal{B}(\lambda) &\stackrel{\text{def}}{=} \frac{1}{\sqrt{B(0; \lambda)}} \phi_0(x; \lambda)^{-1} \circ \mathcal{A}(\lambda)^\dagger \circ \phi_0(x; \lambda + \delta) \\ &= B(0; \lambda)^{-1} (B(x; \lambda) - D(x; \lambda)e^{-\delta}) \varphi(x; \lambda). \end{aligned} \tag{2.54}$$

(For a finite system, the first equation in Eq. (2.52) holds for $x \leq N - 1$ as a matrix and vector equation.) The similarity transformed Hamiltonian $\tilde{\mathcal{H}}(\lambda)$ acting on the polynomial eigenvectors is square-root-free. It is defined by

$$\begin{aligned} \tilde{\mathcal{H}}(\lambda) &\stackrel{\text{def}}{=} \phi_0(x; \lambda)^{-1} \circ \mathcal{H}(\lambda) \circ \phi_0(x; \lambda) = \mathcal{B}(\lambda)\mathcal{F}(\lambda) \\ &= B(x; \lambda)(1 - e^\delta) + D(x; \lambda)(1 - e^{-\delta}), \end{aligned} \tag{2.55}$$

$$\tilde{\mathcal{H}}(\lambda)\check{P}_n(x; \lambda) = \mathcal{E}_n(\lambda)\check{P}_n(x; \lambda). \tag{2.56}$$

Note that the relations (2.52) and (2.56) (after writing down in components) are valid for any $x \in \mathbb{R}$, because they are ‘‘polynomial’’ equations.

The actions of $\mathcal{F}(\lambda)$ and $\mathcal{B}(\lambda)$ on $(v^{-1}\check{\xi}_v)(x; \lambda) \stackrel{\text{def}}{=} v(x; \lambda)^{-1}\check{\xi}_v(x; \lambda)$ are

$$\begin{aligned} \mathcal{F}(\lambda)(v^{-1}\check{\xi}_v)(x; \lambda) &= \tilde{\mathcal{E}}_v(\lambda)(v^{-1}\check{\xi}_v)(x; \lambda + \delta), \\ \mathcal{B}(\lambda)(v^{-1}\check{\xi}_v)(x; \lambda + \delta) &= (v^{-1}\check{\xi}_v)(x; \lambda). \end{aligned} \tag{2.57}$$

(For a finite system, the first equation holds for $x \leq N - 1$ as a matrix and vector equation.) Explicitly they are equivalent to the following forward and backward shift relations of the virtual state polynomial $\check{\xi}_v$:

$$A\check{\xi}_v(x; \lambda) - B\check{\xi}_v(x + 1; \lambda) = C\check{\xi}_v(x; \lambda + \delta), \tag{2.58}$$

$$\begin{aligned} A &= \begin{cases} 1 & : \text{M, } lqL, lqJ, \\ (x + a)(x + b) & : \text{R,} \\ (1 - aq^x)(1 - bq^x) & : qR, \end{cases} \\ B &= \begin{cases} c^{-1} & : \text{M,} \\ a^{-1} & : lqL, lqJ, \\ (x + d - a + 1)(x + d - b + 1) & : \text{R,} \\ \frac{ab}{dq}(1 - a^{-1}dq^{x+1})(1 - b^{-1}dq^{x+1}) & : qR, \end{cases} \\ C &= \begin{cases} -(c\beta)^{-1}(1 - c)(v + \beta) & : \text{M,} \\ -a^{-1}(1 - aq^{-v}) & : lqL, \\ -a^{-1}(1 - bq)^{-1}(1 - aq^{-v})(1 - bq^{v+1}) & : lqJ, \\ c^{-1}(c + v)(a + b - d - 1 - v)(2x + d + 1) & : \text{R,} \\ (1 - c)^{-1}(1 - cq^v)(1 - abd^{-1}q^{-v-1})(1 - dq^{2x+1}) & : qR, \end{cases} \end{aligned}$$

and

$$A\check{\xi}_v(x; \lambda + \delta) - B\check{\xi}_v(x - 1; \lambda + \delta) = C\check{\xi}_v(x; \lambda), \tag{2.59}$$

$$\begin{aligned} A &= \begin{cases} x + \beta & : \text{M,} \\ 1 & : lqL, \\ 1 - bq^{x+1} & : lqJ, \\ (x + c)(x + d) & : \text{R,} \\ (1 - cq^x)(1 - dq^x) & : qR, \end{cases} & B &= \begin{cases} x & : \text{M,} \\ 1 - q^x & : lqL, lqJ, \\ (x + d - c)x & : \text{R,} \\ c(1 - c^{-1}dq^x)(1 - q^x) & : qR, \end{cases} \\ C &= \begin{cases} \beta & : \text{M,} \\ q^x & : lqL, \\ (1 - bq)q^x & : lqJ, \\ c(2x + d) & : \text{R,} \\ (1 - c)(1 - dq^{2x}) & : qR. \end{cases} \end{aligned}$$

Note that the relations (2.57) (after writing down in components) and (2.58)–(2.59) are valid for any $x \in \mathbb{R}$ because $\check{\xi}_v(x)$ is a “polynomial” and $v(x)$ is a meromorphic function.

2.4. Multi-indexed orthogonal polynomials

The original systems in Sect. 2.1 are iso-spectrally deformed by applying multiple Darboux transformations with virtual state vectors $\{\tilde{\phi}_v(x)\}$ as seed solutions. The virtual state vectors are labeled by the degree v of the polynomial part ξ_v . We take M virtual state vectors specified by the multi-index set $\mathcal{D} = \{d_1, \dots, d_M\}$ (ordered set). The deformed Hamiltonian is denoted $\mathcal{H}_{\mathcal{D}}(\lambda)$. The general formula for the eigenfunctions $\{\phi_{\mathcal{D}n}^{\text{gen}}(x; \lambda)\}$ of the deformed system $\mathcal{H}_{\mathcal{D}}(\lambda)\phi_{\mathcal{D}n}^{\text{gen}}(x; \lambda) = \mathcal{E}_n(\lambda)\phi_{\mathcal{D}n}^{\text{gen}}(x; \lambda)$ is (Refs. [12,14])

$$\phi_{\mathcal{D}n}^{\text{gen}}(x; \lambda) = \frac{\mathcal{S}_{\mathcal{D}}(\lambda) \left(\prod_{j=1}^M \alpha(\lambda) B'(x+j-1; \lambda) \right)^{1/2} \tilde{\phi}_0(x; \lambda) \text{W}_C[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}, \nu \check{P}_n](x; \lambda)}{\left(\text{W}_C[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}](x; \lambda) \text{W}_C[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}](x+1; \lambda) \right)^{1/2}},$$

$$\mathcal{S}_{\mathcal{D}}(\lambda) \stackrel{\text{def}}{=} (-1)^M \prod_{1 \leq i < j \leq M} \text{sgn}(\tilde{\mathcal{E}}_{d_i}(\lambda) - \tilde{\mathcal{E}}_{d_j}(\lambda)), \tag{2.60}$$

where $\text{W}_C[f_1, \dots, f_n](x)$ is the Casoratian (2.69).

The multi-indexed orthogonal polynomials $\{\check{P}_{\mathcal{D},n}(x; \lambda)\}$ are the main parts of the eigenfunctions $\{\phi_{\mathcal{D}n}(x; \lambda)\}$ of the deformed system $\mathcal{H}_{\mathcal{D}}(\lambda)\phi_{\mathcal{D}n}(x; \lambda) = \mathcal{E}_n(\lambda)\phi_{\mathcal{D}n}(x; \lambda)$ (Refs. [12,14]):

$$\phi_{\mathcal{D}n}(x; \lambda) \stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x; \lambda) \check{P}_{\mathcal{D},n}(x; \lambda) \propto \phi_{\mathcal{D}n}^{\text{gen}}(x; \lambda), \quad \phi_{\mathcal{D}n}(0; \lambda) = 1, \tag{2.61}$$

$$\psi_{\mathcal{D}}(x; \lambda) \stackrel{\text{def}}{=} \left(\check{\Xi}_{\mathcal{D}}(1; \lambda) \right)^{1/2} \frac{\phi_0(x; \lambda + M\tilde{\delta})}{\left(\check{\Xi}_{\mathcal{D}}(x; \lambda) \check{\Xi}_{\mathcal{D}}(x+1; \lambda) \right)^{1/2}}, \quad \psi_{\mathcal{D}}(0; \lambda) = 1, \tag{2.62}$$

$$\check{\Xi}_{\mathcal{D}}(x; \lambda) \stackrel{\text{def}}{=} \text{W}_C[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}](x; \lambda) \times \mathcal{C}_{\mathcal{D}}(\lambda)^{-1} \varphi_M(x; \lambda)^{-1}, \tag{2.63}$$

$$\check{P}_{\mathcal{D},n}(x; \lambda) \stackrel{\text{def}}{=} \text{W}[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}, \nu \check{P}_n](x; \lambda) \times \mathcal{C}_{\mathcal{D},n}(\lambda)^{-1} \varphi_{M+1}(x; \lambda)^{-1} \nu(x; \lambda + M\tilde{\delta})^{-1}, \tag{2.64}$$

$$\check{P}_{\mathcal{D},n}(x; \lambda) \stackrel{\text{def}}{=} P_{\mathcal{D},n}(\eta(x; \lambda + M\delta); \lambda), \quad \check{\Xi}_{\mathcal{D}}(x; \lambda) \stackrel{\text{def}}{=} \Xi_{\mathcal{D}}(\eta(x; \lambda + (M-1)\delta); \lambda). \tag{2.65}$$

Here the universal normalizations $\check{\Xi}_{\mathcal{D}}(0; \lambda) = 1$ and $\check{P}_{\mathcal{D},n}(0; \lambda) = 1$ are adopted, which determines the constants $\mathcal{C}_{\mathcal{D}}(\lambda)$ and $\mathcal{C}_{\mathcal{D},n}(\lambda)$ (convention: $\prod_{1 \leq j < k \leq M} * = 1$ for $M = 1$),

$$\mathcal{C}_{\mathcal{D}}(\lambda) \stackrel{\text{def}}{=} \frac{1}{\varphi_M(0; \lambda)} \prod_{1 \leq j < k \leq M} \frac{\tilde{\mathcal{E}}_{d_j}(\lambda) - \tilde{\mathcal{E}}_{d_k}(\lambda)}{\alpha(\lambda) B'(j-1; \lambda)}, \tag{2.66}$$

$$\mathcal{C}_{\mathcal{D},n}(\lambda) \stackrel{\text{def}}{=} (-1)^M \mathcal{C}_{\mathcal{D}}(\lambda) \tilde{d}_{\mathcal{D},n}(\lambda)^2, \quad \tilde{d}_{\mathcal{D},n}(\lambda)^2 \stackrel{\text{def}}{=} \frac{\varphi_M(0; \lambda)}{\varphi_{M+1}(0; \lambda)} \prod_{j=1}^M \frac{\mathcal{E}_n(\lambda) - \tilde{\mathcal{E}}_{d_j}(\lambda)}{\alpha(\lambda) B'(j-1; \lambda)}. \tag{2.67}$$

The denominator polynomial $\Xi_{\mathcal{D}}(\eta; \lambda)$ and the multi-indexed orthogonal polynomial $P_{\mathcal{D},n}(\eta; \lambda)$ in Eq. (2.65) are polynomials in η and their degrees are generically $\ell_{\mathcal{D}}$ and $\ell_{\mathcal{D}} + n$, respectively. Here $\ell_{\mathcal{D}}$ is $\ell_{\mathcal{D}} \stackrel{\text{def}}{=} \sum_{j=1}^M d_j - \frac{1}{2}M(M-1)$. Note that $\check{P}_{\mathcal{D},0}(x; \lambda) = \check{\Xi}_{\mathcal{D}}(x; \lambda + \delta)$.

In Ref. [12], the multi-indexed orthogonal polynomials $\check{P}_{\mathcal{D},n}(x; \lambda)$ in Eq. (2.64) for R and qR are expressed as

$$\check{P}_{\mathcal{D},n}(x; \lambda) = C_{\mathcal{D},n}(\lambda)^{-1} \varphi_{M+1}(x; \lambda)^{-1} \times \begin{vmatrix} \check{\xi}_{d_1}(x_1) & \cdots & \check{\xi}_{d_M}(x_1) & r_1(x_1)\check{P}_n(x_1) \\ \check{\xi}_{d_1}(x_2) & \cdots & \check{\xi}_{d_M}(x_2) & r_2(x_2)\check{P}_n(x_2) \\ \vdots & \cdots & \vdots & \vdots \\ \check{\xi}_{d_1}(x_{M+1}) & \cdots & \check{\xi}_{d_M}(x_{M+1}) & r_{M+1}(x_{M+1})\check{P}_n(x_{M+1}) \end{vmatrix}, \tag{2.68}$$

where $x_j \stackrel{\text{def}}{=} x + j - 1$ and $r_j(x) = r_j(x; \lambda, M)$ ($1 \leq j \leq M + 1$) are given by Eq. (2.46). This expression is also valid for M, lqL , and lqJ .

In the next subsection we will rewrite Eqs. (2.63)–(2.64) using the identities implied by the shape invariance and the properties of the Casoratians.

2.5. New determinant expressions

2.5.1. Casoratian

The Casorati determinant of a set of n functions $\{f_j(x)\}$ is defined by

$$W_C[f_1, f_2, \dots, f_n](x) \stackrel{\text{def}}{=} \det\left(f_k(x + j - 1)\right)_{1 \leq j, k \leq n} \tag{2.69}$$

(for $n = 0$, we set $W_C[\cdot](x) = 1$), which satisfies

$$W_C[gf_1, gf_2, \dots, gf_n](x) = \prod_{k=0}^{n-1} g(x + k) \cdot W_C[f_1, f_2, \dots, f_n](x). \tag{2.70}$$

In the rest of this section we consider the Casoratians for $\check{P}_n(x)$, $\check{\xi}_v(x)$, and $v(x)$. Since they are polynomials or meromorphic functions, we can realize the shift operator as an exponential of the differential operator, $\exp\left(a \frac{d}{dx}\right)f(x) = f(x + a)$ ($a \in \mathbb{R}$). In contrast to the matrices e^∂ and $e^{-\partial}$, the operators $\exp\left(\frac{d}{dx}\right)$ and $\exp\left(-\frac{d}{dx}\right)$ are inverse to each other.

The following determinant formula holds for any smooth functions $q_j(x)$ and $r_j(x)$ ($j = 1, 2, \dots$):

$$\det\left(\prod_{l=1}^{\overleftarrow{j-1}} \hat{D}_l \cdot f_k(x)\right)_{1 \leq j, k \leq n} = \prod_{l=1}^n \prod_{m=1}^{n-l} r_m(x + l - 1) \cdot W_C[f_1, \dots, f_n](x), \tag{2.71}$$

where the operators \hat{D}_j ($j = 1, 2, \dots$) are

$$\hat{D}_j = q_j(x) + r_j(x) \exp\left(\frac{d}{dx}\right), \tag{2.72}$$

and the ordered product is

$$\prod_{j=1}^{\overleftarrow{n}} a_j \stackrel{\text{def}}{=} a_n \cdots a_2 a_1. \tag{2.73}$$

This formula is shown by using the properties of the determinants (row properties) and induction on n .

We define the operators $\hat{\mathcal{F}}'(\lambda)$ and $\hat{\mathcal{B}}'(\lambda)$ as $\mathcal{F}(t(\lambda))$ and $\mathcal{B}(t(\lambda))$ with the replacement $e^{\pm\partial} \mapsto \exp\left(\pm\frac{d}{dx}\right)$,

$$\begin{aligned} \hat{\mathcal{F}}'(\lambda) &\stackrel{\text{def}}{=} B'(0; \lambda)\varphi(x; \lambda)^{-1} \left(1 - \exp\left(\frac{d}{dx}\right)\right), \\ \hat{\mathcal{B}}'(\lambda) &\stackrel{\text{def}}{=} B'(0; \lambda)^{-1} \left(B'(x; \lambda) - D'(x; \lambda) \exp\left(-\frac{d}{dx}\right)\right) \varphi(x; \lambda). \end{aligned} \tag{2.74}$$

Then the relations (2.52) and (2.57) with the replacement $\lambda \mapsto t(\lambda)$ and exchange $n \leftrightarrow v$ give

$$\hat{\mathcal{F}}'(\lambda)\check{\xi}_v(x; \lambda) = \mathcal{E}'_v(\lambda)\check{\xi}_{v-1}(x; \lambda + \tilde{\delta}), \quad \hat{\mathcal{B}}'(\lambda)\check{\xi}_{v-1}(x; \lambda + \tilde{\delta}) = \check{\xi}_v(x; \lambda), \tag{2.75}$$

$$\hat{\mathcal{F}}'(\lambda)(v\check{P}_n)(x; \lambda) = \tilde{\mathcal{E}}'_n(\lambda)(v\check{P}_n)(x; \lambda + \tilde{\delta}), \quad \hat{\mathcal{B}}'(\lambda)(v\check{P}_n)(x; \lambda + \tilde{\delta}) = (v\check{P}_n)(x; \lambda), \tag{2.76}$$

where $(v\check{P}_n)(x; \lambda) \stackrel{\text{def}}{=} v(x; \lambda)\check{P}_n(x; \lambda)$, and $\mathcal{E}'_v(\lambda)$ and $\tilde{\mathcal{E}}'_n(\lambda)$ are

$$\mathcal{E}'_v(\lambda) \stackrel{\text{def}}{=} \mathcal{E}_v(t(\lambda)), \quad \tilde{\mathcal{E}}'_n(\lambda) \stackrel{\text{def}}{=} \tilde{\mathcal{E}}_n(t(\lambda)). \tag{2.77}$$

The relations (2.75)–(2.76) are valid for any $x \in \mathbb{R}$.

By taking $\hat{\mathcal{F}}'$ or $\hat{\mathcal{B}}'$ as \hat{D}_j and using the shape-invariance properties (2.75)–(2.76), the Casoratians $W_C[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}](x; \lambda)$ and $W_C[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}, v\check{P}_n](x; \lambda)$ in Eqs. (2.63)–(2.64) can be rewritten in various ways. We consider two typical cases:

$$A : \hat{D}_j = \hat{\mathcal{F}}'(\lambda + (j - 1)\tilde{\delta}) \quad (j = 1, 2, \dots), \tag{2.78}$$

$$\begin{aligned} B : \hat{D}_{2l-1} &= \exp\left((l - 1)\frac{d}{dx}\right) \circ \hat{\mathcal{F}}'(\lambda) \circ \exp\left(-(l - 1)\frac{d}{dx}\right), \\ \hat{D}_{2l} &= \exp\left(l\frac{d}{dx}\right) \circ \hat{\mathcal{B}}'(\lambda) \circ \exp\left(-(l - 1)\frac{d}{dx}\right) \quad (l = 1, 2, \dots), \end{aligned} \tag{2.79}$$

which correspond to cases A and B in Ref. [42].

2.5.2. Case A

First we consider case A in Eq. (2.78). The functions $q_j(x)$ and $r_j(x)$ are

$$-q_j(x) = r_j(x) = -B'(0; \lambda + (j - 1)\tilde{\delta})\varphi(0; \lambda + (j - 1)\tilde{\delta})^{-1}. \tag{2.80}$$

The shape-invariance properties (2.75)–(2.76) give ($k = 0, 1, \dots$)

$$\begin{aligned} \prod_{l=1}^k \hat{D}_l \cdot \check{\xi}_v(x; \lambda) &= \prod_{m=0}^{k-1} \mathcal{E}'_{v-m}(\lambda + m\tilde{\delta}) \cdot \check{\xi}_{v-k}(x; \lambda + k\tilde{\delta}), \\ \prod_{l=1}^k \hat{D}_l \cdot (v\check{P}_n)(x; \lambda) &= \prod_{m=0}^{k-1} \tilde{\mathcal{E}}'_n(\lambda + m\tilde{\delta}) \cdot (v\check{P}_n)(x; \lambda + k\tilde{\delta}). \end{aligned} \tag{2.81}$$

We rewrite Eqs. (2.63)–(2.64) in the following way. (i) By using Eq. (2.71), rewrite the Casoratians in Eqs. (2.63)–(2.64) as determinants $\det(a_{j,k})_{1 \leq j, k \leq M'}$ ($M' = M$ for $\check{\Xi}_{\mathcal{D}}$ and $M' = M + 1$ for $\check{P}_{\mathcal{D},n}$).

(ii) Rewrite each matrix element $a_{j,k}$ as Eq. (2.81). For $\check{P}_{\mathcal{D},n}$, we do the following (iii) and (iv).
 (iii) Divide the $(M + 1)$ th column of $\det(a_{j,k})$ by $v(x; \lambda + M\tilde{\delta})$, and multiply the determinant by $v(x; \lambda + M\tilde{\delta})$. (iv) Rewrite $v(x; \lambda + (j - 1)\tilde{\delta})/v(x; \lambda + M\tilde{\delta})$ in the $(M + 1)$ th column of $\det(a_{j,k})$ as

$$\frac{v(x; \lambda + (j - 1)\tilde{\delta})}{v(x; \lambda + M\tilde{\delta})} = \begin{cases} 1 & : \text{M,} \\ q^{(M+1-j)x} = (1 - \eta(x))^{M+1-j} & : \text{lqL, lqJ,} \\ \frac{(x + d - a + j, x + d - b + j)_{M+1-j}}{(d - a + j, d - b + j)_{M+1-j}} & : \text{R,} \\ q^{-(M+1-j)x} \frac{(a^{-1}dq^{x+j}, b^{-1}dq^{x+j}; q)_{M+1-j}}{(a^{-1}dq^j, b^{-1}dq^j; q)_{M+1-j}} & : \text{qR.} \end{cases} \quad (2.82)$$

Then $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are expressed in terms of $\check{\xi}_v(x; \lambda')$, $\check{P}_n(x; \lambda')$, $\varphi(x'; \lambda')$, and Eq. (2.82). Straightforward calculation shows that the factors $\varphi(x'; \lambda')$ are canceled out. Thus, for the M, lqL, and lqJ cases, $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are expressed in terms of $\eta(x)$, namely, $\Xi_{\mathcal{D}}(\eta; \lambda)$ and $P_{\mathcal{D},n}(\eta; \lambda)$ are expressed without explicit x -dependence (which is trivial for M, because $\eta(x) = x$). Their final forms are as follows.

o **Meixner:**

The denominator polynomial $\Xi_{\mathcal{D}}(\eta; \lambda)$ is

$$\Xi_{\mathcal{D}}(\eta; \lambda) = \frac{(-c)^{\frac{1}{2}M(M-1)}}{\mathcal{C}_{\mathcal{D}}(\lambda) \prod_{m=1}^{M-1} (\beta)_m} \det(a_{j,k})_{1 \leq j,k \leq M}, \quad (2.83)$$

where $a_{j,k}$ are

$$a_{j,k} = \prod_{m=0}^{j-2} \mathcal{E}'_{d_k-m}(\lambda + m\tilde{\delta}) \cdot \xi_{d_k+1-j}(\eta; \lambda + (j - 1)\tilde{\delta}) \quad (j, k = 1, \dots, M), \quad (2.84)$$

and the multi-indexed orthogonal polynomial $P_{\mathcal{D},n}(\eta; \lambda)$ is

$$P_{\mathcal{D},n}(\eta; \lambda) = \frac{(-c)^{\frac{1}{2}M(M+1)}}{\mathcal{C}_{\mathcal{D},n}(\lambda) \prod_{m=1}^M (\beta)_m} \det(a_{j,k})_{1 \leq j,k \leq M+1}, \quad (2.85)$$

where $a_{j,k}$ are

$$a_{j,k} = \text{Eq. (2.84)} \quad (j = 1, \dots, M + 1; \quad k = 1, \dots, M),$$

$$a_{j,M+1} = \prod_{m=0}^{j-2} \tilde{\mathcal{E}}'_n(\lambda + m\tilde{\delta}) \cdot P_n(\eta; \lambda + (j - 1)\tilde{\delta}) \quad (j = 1, \dots, M + 1). \quad (2.86)$$

o **Little q -Laguerre and little q -Jacobi:**

The denominator polynomial $\Xi_{\mathcal{D}}(\eta; \lambda)$ is

$$\Xi_{\mathcal{D}}(\eta; \lambda) = \frac{(-a)^{\frac{1}{2}M(M-1)}}{q^{\frac{1}{6}M(M-1)(M-2)} \mathcal{C}_{\mathcal{D}}(\lambda)} \det(a_{j,k})_{1 \leq j,k \leq M} \times \begin{cases} 1 & : \text{lqL,} \\ \prod_{m=1}^{M-1} (bq; q)_m^{-1} & : \text{lqJ,} \end{cases} \quad (2.87)$$

where $a_{j,k}$ are given by Eq. (2.84), and the multi-indexed orthogonal polynomial $P_{\mathcal{D},n}(\eta; \lambda)$ is

$$P_{\mathcal{D},n}(\eta; \lambda) = \frac{(-a)^{\frac{1}{2}M(M+1)}}{q^{\frac{1}{6}(M+1)M(M-1)}\mathcal{C}_{\mathcal{D},n}(\lambda)} \det(a_{j,k})_{1 \leq j,k \leq M+1} \times \begin{cases} 1 & : lqL, \\ \prod_{m=1}^M (bq; q)_m^{-1} & : lqJ, \end{cases} \quad (2.88)$$

where $a_{j,k}$ are

$$a_{j,k} = \text{Eq. (2.84)} \quad (j = 1, \dots, M + 1; \quad k = 1, \dots, M),$$

$$a_{j,M+1} = \prod_{m=0}^{j-2} \tilde{\mathcal{E}}'_n(\lambda + m\tilde{\delta}) \cdot (1 - \eta)^{M+1-j} P_n(\eta; \lambda + (j - 1)\tilde{\delta}) \quad (j = 1, \dots, M + 1). \quad (2.89)$$

o **Racah and q -Racah:**

The denominator polynomial $\check{\mathcal{E}}_{\mathcal{D}}(x; \lambda)$ is

$$\check{\mathcal{E}}_{\mathcal{D}}(x; \lambda) = \frac{(-1)^{\frac{1}{2}M(M-1)}}{\mathcal{C}_{\mathcal{D}}(\lambda) \prod_{m=0}^{M-1} B'(0; \lambda + m\tilde{\delta})^{M-1-m}} \det(a_{j,k})_{1 \leq j,k \leq M}, \quad (2.90)$$

where $a_{j,k}$ are

$$a_{j,k} = \prod_{m=0}^{j-2} \mathcal{E}'_{d_k-m}(\lambda + m\tilde{\delta}) \cdot \check{\xi}_{d_k+1-j}(x; \lambda + (j - 1)\tilde{\delta}) \quad (j, k = 1, \dots, M), \quad (2.91)$$

and the multi-indexed orthogonal polynomial $\check{P}_{\mathcal{D},n}(x; \lambda)$ is

$$\check{P}_{\mathcal{D},n}(x; \lambda) = \frac{(-1)^{\frac{1}{2}M(M+1)}}{\mathcal{C}_{\mathcal{D},n}(\lambda) \prod_{m=0}^M B'(0; \lambda + m\tilde{\delta})^{M-m}} \det(a_{j,k})_{1 \leq j,k \leq M+1}, \quad (2.92)$$

where $a_{j,k}$ are

$$a_{j,k} = \text{Eq. (2.91)} \quad (j = 1, \dots, M + 1; \quad k = 1, \dots, M),$$

$$a_{j,M+1} = \prod_{m=0}^{j-2} \tilde{\mathcal{E}}'_n(\lambda + m\tilde{\delta}) \cdot P_n(\eta; \lambda + (j - 1)\tilde{\delta})$$

$$\times \begin{cases} \frac{(x + d - a + j, x + d - b + j)_{M+1-j}}{(d - a + j, d - b + j)_{M+1-j}} & : \mathbb{R}, \\ q^{-(M+1-j)x} \frac{(a^{-1}dq^{x+j}, b^{-1}dq^{x+j}; q)_{M+1-j}}{(a^{-1}dq^j, b^{-1}dq^j; q)_{M+1-j}} & : q\mathbb{R}, \end{cases} \quad (j = 1, \dots, M + 1). \quad (2.93)$$

2.5.3. Case B

Second we consider case B in Eq. (2.79). The functions $q_l(x)$ and $r_l(x)$ are ($l = 1, 2, \dots$)

$$-q_{2l-1}(x) = r_{2l-1}(x) = -B'(0; \lambda)\varphi(x + l - 1; \lambda)^{-1},$$

$$q_{2l}(x) = -B'(0; \lambda)^{-1}D'(x + l; \lambda)\varphi(x + l - 1; \lambda), \quad (2.94)$$

$$r_{2l}(x) = B'(0; \lambda)^{-1}B'(x + l; \lambda)\varphi(x + l; \lambda).$$

The shape-invariance properties (2.75)–(2.76) give ($l = 1, 2, \dots$)

$$\begin{aligned}
 \prod_{m=1}^{\overleftarrow{2l-2}} \hat{D}_m \cdot \check{\xi}_v(x; \lambda) &= \mathcal{E}'_v(\lambda)^{l-1} \check{\xi}_v(x+l-1; \lambda), \\
 \prod_{m=1}^{\overleftarrow{2l-1}} \hat{D}_m \cdot \check{\xi}_v(x; \lambda) &= \mathcal{E}'_v(\lambda)^l \check{\xi}_{v-1}(x+l-1; \lambda + \tilde{\delta}), \\
 \prod_{m=1}^{\overleftarrow{2l-2}} \hat{D}_m \cdot (v\check{P}_n)(x; \lambda) &= \tilde{\mathcal{E}}'_n(\lambda)^{l-1} (v\check{P}_n)(x+l-1; \lambda), \\
 \prod_{m=1}^{\overleftarrow{2l-1}} \hat{D}_m \cdot (v\check{P}_n)(x; \lambda) &= \tilde{\mathcal{E}}'_n(\lambda)^l (v\check{P}_n)(x+l-1; \lambda + \tilde{\delta}).
 \end{aligned} \tag{2.95}$$

Like case A, we rewrite Eqs. (2.63)–(2.64) using steps (i)–(iv). In (iv) we use

$$\begin{aligned}
 \frac{v(x+l-1; \lambda)}{v(x; \lambda + M\tilde{\delta})} &= \begin{cases} c^{l-1} & : \text{M}, \\ a^{l-1} q^{Mx} & : lqL, lqJ, \\ \frac{(x+d-a+l, x+d-b+l)_{M+1-l}(x+a, x+b)_{l-1}}{(d-a+1, d-b+1)_M} & : \text{R}, \\ \frac{(a^{-1}dq^{x+l}, b^{-1}dq^{x+l}; q)_{M+1-l}(aq^x, bq^x; q)_{l-1}}{(abd^{-1}q^{-1})^{l-1}q^{Mx}(a^{-1}dq, b^{-1}dq; q)_M} & : qR, \end{cases} \\
 \frac{v(x+l-1; \lambda + \tilde{\delta})}{v(x; \lambda + M\tilde{\delta})} &= \begin{cases} c^{l-1} & : \text{M}, \\ (aq^{-1})^{l-1}q^{(M-1)x} & : lqL, lqJ, \\ \frac{(x+d-a+l+1, x+d-b+l+1)_{M-l}(x+a, x+b)_{l-1}}{(d-a+2, d-b+2)_{M-1}} & : \text{R}, \\ \frac{(a^{-1}dq^{x+l+1}, b^{-1}dq^{x+l+1}; q)_{M-l}(aq^x, bq^x; q)_{l-1}}{(abd^{-1}q^{-2})^{l-1}q^{(M-1)x}(a^{-1}dq^2, b^{-1}dq^2; q)_{M-1}} & : qR. \end{cases}
 \end{aligned} \tag{2.96}$$

In contrast to case A, the determinants contain $\check{\xi}_v(x'; \lambda')$ and $\check{P}_n(x'; \lambda')$ at various points x' , and the factors $\varphi(x'; \lambda')$ are not canceled out. Their final forms are as follows. The denominator polynomial $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ is

$$\begin{aligned}
 \check{\Xi}_{\mathcal{D}}(x; \lambda) &= \frac{(-1)^{\frac{1}{2}(1+(-1)^M)\frac{M}{2}} \prod_{m=0}^{\lfloor \frac{M-2}{2} \rfloor} \varphi(x+m; \lambda) \cdot \varphi_M(x; \lambda)^{-1}}{\mathcal{C}_{\mathcal{D}}(\lambda) B'(0; \lambda)^{\lfloor \frac{M}{2} \rfloor}} \\
 &\quad \times \left(\prod_{m=0}^{\lfloor \frac{M-2}{2} \rfloor} \prod_{l=1}^{M-2-2m} B'(x+l+m; \lambda) \right)^{-1} \det(a_{j,k})_{1 \leq j, k \leq M},
 \end{aligned} \tag{2.97}$$

where $a_{j,k}$ are

$$\begin{aligned}
 a_{2l-1,k} &= \mathcal{E}'_{d_k}(\boldsymbol{\lambda})^{l-1} \check{\xi}_{d_k}(x+l-1; \boldsymbol{\lambda}) \quad (l = 1, \dots, [\frac{M+1}{2}]; k = 1, \dots, M), \\
 a_{2l,k} &= \mathcal{E}'_{d_k}(\boldsymbol{\lambda})^l \check{\xi}_{d_k-1}(x+l-1; \boldsymbol{\lambda} + \tilde{\boldsymbol{\delta}}) \quad (l = 1, \dots, [\frac{M}{2}]; k = 1, \dots, M),
 \end{aligned}
 \tag{2.98}$$

and the multi-indexed orthogonal polynomial $\check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda})$ is

$$\begin{aligned}
 \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) &= \frac{(-1)^{\frac{1}{2}(1-(-1)^M) \frac{M+1}{2}}}{\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda}) B'(0; \boldsymbol{\lambda})^{[\frac{M+1}{2}]}} \prod_{m=0}^{[\frac{M-1}{2}]} \varphi(x+m; \boldsymbol{\lambda}) \cdot \varphi_{M+1}(x; \boldsymbol{\lambda})^{-1} \\
 &\quad \times \left(\prod_{m=0}^{[\frac{M-1}{2}] M-1-2m} \prod_{l=1} B'(x+l+m; \boldsymbol{\lambda}) \right)^{-1} \det(a_{j,k})_{1 \leq j,k \leq M+1},
 \end{aligned}
 \tag{2.99}$$

where $a_{j,k}$ are

$$\begin{aligned}
 a_{2l-1,k} &= \mathcal{E}'_{d_k}(\boldsymbol{\lambda})^{l-1} \check{\xi}_{d_k}(x+l-1; \boldsymbol{\lambda}) \quad (l = 1, \dots, [\frac{M+2}{2}]; k = 1, \dots, M), \\
 a_{2l,k} &= \mathcal{E}'_{d_k}(\boldsymbol{\lambda})^l \check{\xi}_{d_k-1}(x+l-1; \boldsymbol{\lambda} + \tilde{\boldsymbol{\delta}}) \quad (l = 1, \dots, [\frac{M+1}{2}]; k = 1, \dots, M), \\
 a_{2l-1,M+1} &= \tilde{\mathcal{E}}'_n(\boldsymbol{\lambda})^{l-1} \check{P}_n(x+l-1; \boldsymbol{\lambda}) \quad (l = 1, \dots, [\frac{M+2}{2}]) \\
 &\quad \times \begin{cases} c^{l-1} & : \text{M}, \\ a^{l-1} q^{Mx} & : lqL, lqJ, \\ \frac{(x+d-a+l, x+d-b+l)_{M+1-l}(x+a, x+b)_{l-1}}{(d-a+1, d-b+1)_M} & : \text{R}, \\ \frac{(a^{-1}dq^{x+l}, b^{-1}dq^{x+l}; q)_{M+1-l}(aq^x, bq^x; q)_{l-1}}{(abd^{-1}q^{-1})^{l-1} q^{Mx}(a^{-1}dq, b^{-1}dq; q)_M} & : q\text{R}, \end{cases} \\
 a_{2l,M+1} &= \tilde{\mathcal{E}}'_n(\boldsymbol{\lambda})^l \check{P}_n(x+l-1; \boldsymbol{\lambda} + \tilde{\boldsymbol{\delta}}) \quad (l = 1, \dots, [\frac{M+1}{2}])
 \end{aligned}
 \tag{2.100}$$

$$\times \begin{cases} c^{l-1} & : \text{M}, \\ (aq^{-1})^{l-1} q^{(M-1)x} & : lqL, lqJ, \\ \frac{(x+d-a+l+1, x+d-b+l+1)_{M-l}(x+a, x+b)_{l-1}}{(d-a+2, d-b+2)_{M-1}} & : \text{R}, \\ \frac{(a^{-1}dq^{x+l+1}, b^{-1}dq^{x+l+1}; q)_{M-l}(aq^x, bq^x; q)_{l-1}}{(abd^{-1}q^{-2})^{l-1} q^{(M-1)x}(a^{-1}dq^2, b^{-1}dq^2; q)_{M-1}} & : q\text{R}. \end{cases}$$

3. Multi-indexed orthogonal polynomials in idQM

In this section we derive various equivalent expressions for the multi-indexed Wilson and Askey–Wilson polynomials in the framework of discrete quantum mechanics with pure imaginary shifts.

3.1. Original systems

The Hamiltonian of discrete quantum mechanics with pure imaginary shifts (idQM) (Refs. [46,47]), whose dynamical variables are the real coordinate x ($x_1 \leq x \leq x_2$) and the conjugate momentum

$p = -i \frac{d}{dx}$, is

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

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

Here the potential function $V(x)$ is an analytic function of x , and γ 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 . Since the momentum operator appears in exponentiated forms, the Schrödinger equation

$$\mathcal{H}\phi_n(x) = \mathcal{E}_n \phi_n(x) \quad (n = 0, 1, 2, \dots), \quad 0 = \mathcal{E}_0 < \mathcal{E}_1 < \mathcal{E}_2 < \dots \tag{3.3}$$

is an analytic difference equation with pure imaginary shifts.

We consider idQM described by the Wilson and Askey–Wilson polynomials. The various parameters are

$$W : x_1 = 0, \quad x_2 = \infty, \quad \gamma = 1, \quad \lambda = (a_1, a_2, a_3, a_4), \quad \delta = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \quad \kappa = 1, \tag{3.4}$$

$$AW : x_1 = 0, \quad x_2 = \pi, \quad \gamma = \log q, \quad q^\lambda = (a_1, a_2, a_3, a_4), \quad \delta = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}), \quad \kappa = q^{-1}, \tag{3.5}$$

where $0 < q < 1$. The parameters are restricted by

$$\{a_1^*, a_2^*, a_3^*, a_4^*\} = \{a_1, a_2, a_3, a_4\} \quad (\text{as a set}); \quad W : \text{Re } a_i > 0, \quad AW : |a_i| < 1. \tag{3.6}$$

Here are the fundamental data (Ref. [46]):

$$V(x; \lambda) = \begin{cases} (2ix(2ix + 1))^{-1} \prod_{j=1}^4 (a_j + ix) & : W, \\ ((1 - e^{2ix})(1 - qe^{2ix}))^{-1} \prod_{j=1}^4 (1 - a_j e^{ix}) & : AW, \end{cases} \tag{3.7}$$

$$\eta(x) = \begin{cases} x^2 & : W, \\ \cos x & : AW, \end{cases} \quad \varphi(x) = \begin{cases} 2x & : W, \\ 2 \sin x & : AW, \end{cases} \tag{3.8}$$

$$\mathcal{E}_n(\lambda) = \begin{cases} n(n + b_1 - 1) & : W, & b_1 \stackrel{\text{def}}{=} a_1 + a_2 + a_3 + a_4, \\ (q^{-n} - 1)(1 - b_4 q^{n-1}) & : AW, & b_4 \stackrel{\text{def}}{=} a_1 a_2 a_3 a_4, \end{cases} \tag{3.9}$$

$$\phi_n(x; \lambda) = \phi_0(x; \lambda) \check{P}_n(x; \lambda), \tag{3.10}$$

$$\check{P}_n(x; \lambda) = P_n(\eta(x); \lambda) = \begin{cases} W_n(\eta(x); a_1, a_2, a_3, a_4) & : W, \\ p_n(\eta(x); a_1, a_2, a_3, a_4 | q) & : AW, \end{cases}$$

$$= \begin{cases} (a_1 + a_2, a_1 + a_3, a_1 + a_4)_n \\ \times {}_4F_3 \left(\begin{matrix} -n, n + b_1 - 1, a_1 + ix, a_1 - ix \\ a_1 + a_2, a_1 + a_3, a_1 + a_4 \end{matrix} \middle| 1 \right) & : W, \\ a_1^{-n} (a_1 a_2, a_1 a_3, a_1 a_4; q)_n \\ \times {}_4\phi_3 \left(\begin{matrix} q^{-n}, b_4 q^{n-1}, a_1 e^{ix}, a_1 e^{-ix} \\ a_1 a_2, a_1 a_3, a_1 a_4 \end{matrix} \middle| q; q \right) & : AW, \end{cases} \tag{3.11}$$

$$\phi_0(x; \lambda) = \begin{cases} \left((\Gamma(2ix)\Gamma(-2ix))^{-1} \prod_{j=1}^4 \Gamma(a_j + ix)\Gamma(a_j - ix) \right)^{1/2} & : \text{W}, \\ \left((e^{2ix}, e^{-2ix}; q)_\infty \prod_{j=1}^4 (a_j e^{ix}, a_j e^{-ix}; q)_\infty^{-1} \right)^{1/2} & : \text{AW}, \end{cases} \tag{3.12}$$

where $W_n(\eta; a_1, a_2, a_3, a_4)$ and $p_n(\eta; a_1, a_2, a_3, a_4|q)$ are the Wilson and Askey–Wilson polynomials (Ref. [45]), respectively. Note that

$$\phi_0(x; \lambda + \delta) = \varphi(x) \left(V(x + i\frac{\gamma}{2}; \lambda) \right)^{1/2} \phi_0(x + i\frac{\gamma}{2}; \lambda), \tag{3.13}$$

$$V(x; \lambda + \delta) = \kappa^{-1} \frac{\varphi(x - i\gamma)}{\varphi(x)} V(x - i\frac{\gamma}{2}; \lambda). \tag{3.14}$$

3.2. Virtual states

The virtual state wave functions are obtained by using the discrete symmetries of the Hamiltonian (Ref. [10]). In the following we restrict the parameters as follows:

$$a_1, a_2 \in \mathbb{R} \quad \text{or} \quad a_2^* = a_1; \quad a_3, a_4 \in \mathbb{R} \quad \text{or} \quad a_4^* = a_3. \tag{3.15}$$

We define two twist operations t , type I and type II:

$$t^I(\lambda) \stackrel{\text{def}}{=} (1 - \lambda_1, 1 - \lambda_2, \lambda_3, \lambda_4), \quad t^{II}(\lambda) \stackrel{\text{def}}{=} (\lambda_1, \lambda_2, 1 - \lambda_3, 1 - \lambda_4), \tag{3.16}$$

which are involutions $t^2 = \text{id}$ and satisfy

$$t(\lambda) + u\delta = t(\lambda + u\tilde{\delta}) \quad (\forall u \in \mathbb{R}), \quad \tilde{\delta}^I \stackrel{\text{def}}{=} \left(-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right), \quad \tilde{\delta}^{II} \stackrel{\text{def}}{=} \left(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right). \tag{3.17}$$

By using these two types of twist operations, two types of virtual state wave functions, $\tilde{\phi}_v^I(x; \lambda)$ and $\tilde{\phi}_v^{II}(x; \lambda)$, are introduced:

$$\begin{aligned} \tilde{\phi}_v(x; \lambda) &\stackrel{\text{def}}{=} \phi_v(x; t(\lambda)) = \tilde{\phi}_0(x; \lambda) \check{\xi}_v(x; \lambda), & \tilde{\phi}_0(x; \lambda) &\stackrel{\text{def}}{=} \phi_0(x; t(\lambda)), \\ \check{\xi}_v(x; \lambda) &\stackrel{\text{def}}{=} \xi_v(\eta(x); \lambda) \stackrel{\text{def}}{=} \check{P}_v(x; t(\lambda)) = P_v(\eta(x); t(\lambda)). \end{aligned} \tag{3.18}$$

The virtual state polynomials $\xi_v(\eta; \lambda)$ (two types ξ_v^I and ξ_v^{II}) are polynomials of degree v in η . The virtual state wave functions satisfy the Schrödinger equation $\mathcal{H}(\lambda)\tilde{\phi}_v(x; \lambda) = \tilde{\mathcal{E}}_v(\lambda)\tilde{\phi}_v(x; \lambda)$ with the virtual energies $\tilde{\mathcal{E}}_v(\lambda)$,

$$\begin{aligned} \tilde{\mathcal{E}}_v^I(\lambda) &= \begin{cases} -(a_1 + a_2 - v - 1)(a_3 + a_4 + v) & : \text{W}, \\ -(1 - a_1 a_2 q^{-v-1})(1 - a_3 a_4 q^v) & : \text{AW}, \end{cases} \\ \tilde{\mathcal{E}}_v^{II}(\lambda) &= \begin{cases} -(a_3 + a_4 - v - 1)(a_1 + a_2 + v) & : \text{W}, \\ -(1 - a_3 a_4 q^{-v-1})(1 - a_1 a_2 q^v) & : \text{AW}. \end{cases} \end{aligned} \tag{3.19}$$

The other data $\alpha(\lambda)$ and $\alpha'(\lambda)$ (see Ref. [10] for details) are

$$\begin{aligned} \alpha^I(\lambda) &= \begin{cases} 1 & : \text{W}, \\ a_1 a_2 q^{-1} & : \text{AW}, \end{cases} & \alpha'^I(\lambda) &= \begin{cases} -(a_1 + a_2 - 1)(a_3 + a_4) & : \text{W}, \\ -(1 - a_1 a_2 q^{-1})(1 - a_3 a_4) & : \text{AW}, \end{cases} \\ \alpha^{II}(\lambda) &= \begin{cases} 1 & : \text{W}, \\ a_3 a_4 q^{-1} & : \text{AW}, \end{cases} & \alpha'^{II}(\lambda) &= \begin{cases} -(a_3 + a_4 - 1)(a_1 + a_2) & : \text{W}, \\ -(1 - a_3 a_4 q^{-1})(1 - a_1 a_2) & : \text{AW}. \end{cases} \end{aligned} \tag{3.20}$$

In order to obtain well-defined quantum systems, we have to restrict the degree ν and the parameters a_i so that the conditions, $\tilde{\mathcal{E}}_\nu(\boldsymbol{\lambda}) < 0$, $\alpha(\boldsymbol{\lambda}) > 0$, $\alpha'(\boldsymbol{\lambda}) < 0$, no zeros of $\xi_\nu(\eta; \boldsymbol{\lambda})$ in the domain, etc., are satisfied; see Ref. [10]. In this paper, however, we consider algebraic properties only and we do not bother about the ranges of ν and a_i .

The functions $\nu(x; \boldsymbol{\lambda})$ (two types ν^I and ν^{II}) are defined as the ratio of ϕ_0 and $\tilde{\phi}_0$:

$$\nu(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{\phi_0(x; \boldsymbol{\lambda})}{\tilde{\phi}_0(x; \boldsymbol{\lambda})}. \tag{3.21}$$

The functions $r_j(x_j^{(M)}; \boldsymbol{\lambda}, M)$ (two types r_j^I and r_j^{II}) are defined as the ratio of ν 's:

$$r_j(x_j^{(M)}; \boldsymbol{\lambda}, M) \stackrel{\text{def}}{=} \frac{\nu(x_j^{(M)}; \boldsymbol{\lambda})}{\nu(x; \boldsymbol{\lambda} + (M-1)\boldsymbol{\delta})} \quad (1 \leq j \leq M), \tag{3.22}$$

where $x_j^{(M)} \stackrel{\text{def}}{=} x + i(\frac{M+1}{2} - j)\gamma$. Their explicit forms are

$$r_j^I(x_j^{(M)}; \boldsymbol{\lambda}, M) = \alpha^I(\boldsymbol{\lambda} + (M-1)\tilde{\boldsymbol{\delta}}^I)^{-\frac{1}{2}(M-1)} \kappa^{\frac{1}{2}(M-1)^2 - (j-1)(M-j)} \tag{3.23}$$

$$\times \begin{cases} \prod_{k=1,2} (a_k - \frac{M-1}{2} + ix)_{j-1} (a_k - \frac{M-1}{2} - ix)_{M-j} & : W, \\ e^{ix(M+1-2j)} \prod_{k=1,2} (a_k q^{-\frac{M-1}{2}} e^{ix}; q)_{j-1} (a_k q^{-\frac{M-1}{2}} e^{-ix}; q)_{M-j} & : AW, \end{cases}$$

$$r_j^{II}(x_j^{(M)}; \boldsymbol{\lambda}, M) = \alpha^{II}(\boldsymbol{\lambda} + (M-1)\tilde{\boldsymbol{\delta}}^{II})^{-\frac{1}{2}(M-1)} \kappa^{\frac{1}{2}(M-1)^2 - (j-1)(M-j)} \tag{3.24}$$

$$\times \begin{cases} \prod_{k=3,4} (a_k - \frac{M-1}{2} + ix)_{j-1} (a_k - \frac{M-1}{2} - ix)_{M-j} & : W, \\ e^{ix(M+1-2j)} \prod_{k=3,4} (a_k q^{-\frac{M-1}{2}} e^{ix}; q)_{j-1} (a_k q^{-\frac{M-1}{2}} e^{-ix}; q)_{M-j} & : AW. \end{cases}$$

The auxiliary function $\varphi_M(x)$ (Ref. [34]) is defined by

$$\begin{aligned} \varphi_M(x) &\stackrel{\text{def}}{=} \varphi(x)^{\lfloor \frac{M}{2} \rfloor} \prod_{k=1}^{M-2} (\varphi(x - i\frac{k}{2}\gamma)\varphi(x + i\frac{k}{2}\gamma))^{\lfloor \frac{M-k}{2} \rfloor} \\ &= \prod_{1 \leq j < k \leq M} \frac{\eta(x_j^{(M)}) - \eta(x_k^{(M)})}{\varphi(i\frac{j}{2}\gamma)} \times \begin{cases} 1 & : W, \\ (-2)^{\frac{1}{2}M(M-1)} & : AW, \end{cases} \end{aligned} \tag{3.25}$$

and $\varphi_0(x) = \varphi_1(x) = 1$.

For $-M \leq k \leq M$ and $k \equiv M \pmod{2}$, we can show that

$$\frac{\nu(x; \boldsymbol{\lambda} + M\boldsymbol{\delta})}{\nu(x; \boldsymbol{\lambda} + k\boldsymbol{\delta})} = \prod_{l=0}^{\frac{M-k}{2}-1} \check{U}(x; \boldsymbol{\lambda} + (k+2l)\boldsymbol{\delta}), \tag{3.26}$$

where the functions $\check{U}(x; \lambda)$ (two types \check{U}^I and \check{U}^{II}) are

$$\begin{aligned} \check{U}^I(x; \lambda) &\stackrel{\text{def}}{=} \begin{cases} \prod_{k=1}^2 (a_k + ix)(a_k - ix) & : W, \\ (a_1 a_2)^{-1} \prod_{k=1}^2 (1 - a_k e^{ix})(1 - a_k e^{-ix}) & : AW, \end{cases} \\ \check{U}^{II}(x; \lambda) &\stackrel{\text{def}}{=} \begin{cases} \prod_{k=3}^4 (a_k + ix)(a_k - ix) & : W, \\ (a_3 a_4)^{-1} \prod_{k=3}^4 (1 - a_k e^{ix})(1 - a_k e^{-ix}) & : AW. \end{cases} \end{aligned} \tag{3.27}$$

In fact, these functions $\check{U}(x; \lambda)$ are polynomials $U(\eta; \lambda)$ in η as defined by

$$U(\eta(x); \lambda) \stackrel{\text{def}}{=} \check{U}(x; \lambda), \tag{3.28}$$

$$U^I(\eta; \lambda) = \begin{cases} \prod_{k=1}^2 (a_k^2 + \eta) & : W, \\ \prod_{k=1}^2 (a_k + a_k^{-1} - 2\eta) & : AW, \end{cases} \quad U^{II}(\eta; \lambda) = \begin{cases} \prod_{k=3}^4 (a_k^2 + \eta) & : W, \\ \prod_{k=3}^4 (a_k + a_k^{-1} - 2\eta) & : AW. \end{cases}$$

Since $v(x; \lambda)$ satisfies $v(x; \lambda + k\tilde{\delta}) = v(x; \lambda - k\delta)$ ($k \in \mathbb{Z}$), Eq. (3.26) gives

$$\frac{v(x; \lambda + M\tilde{\delta})}{v(x; \lambda + M\delta)} = \prod_{l=0}^{M-1} \check{U}(x; \lambda + (-M + 2l)\delta)^{-1}. \tag{3.29}$$

In the following we adopt the convention

$$\check{P}_n(x; \lambda) \stackrel{\text{def}}{=} 0 \quad (n \in \mathbb{Z}_{<0}), \quad \check{\xi}_v(x; \lambda) \stackrel{\text{def}}{=} 0 \quad (v \in \mathbb{Z}_{<0}). \tag{3.30}$$

3.3. Shape invariance

The original systems in Sect. 3.1 are shape invariant (Refs. [46,47]) and they satisfy the relation

$$\mathcal{A}(\lambda)\mathcal{A}(\lambda)^\dagger = \kappa \mathcal{A}(\lambda + \delta)^\dagger \mathcal{A}(\lambda + \delta) + \mathcal{E}_1(\lambda), \tag{3.31}$$

which is a sufficient condition for exact solvability. As a consequence of the shape invariance, the action of the operators $\mathcal{A}(\lambda)$ and $\mathcal{A}(\lambda)^\dagger$ on the eigenfunctions is

$$\mathcal{A}(\lambda)\phi_n(x; \lambda) = f_n(\lambda)\phi_{n-1}(x; \lambda + \delta), \quad \mathcal{A}(\lambda)^\dagger\phi_{n-1}(x; \lambda + \delta) = b_{n-1}(\lambda)\phi_n(x; \lambda), \tag{3.32}$$

where the factors of the energy eigenvalue, $f_n(\lambda)$ and $b_{n-1}(\lambda)$, $\mathcal{E}_n(\lambda) = f_n(\lambda)b_{n-1}(\lambda)$, are given by

$$f_n(\lambda) \stackrel{\text{def}}{=} \begin{cases} -n(n + b_1 - 1) & : W, \\ q^{n/2}(q^n - 1)(1 - b_4 q^{n-1}) & : AW, \end{cases} \quad b_{n-1}(\lambda) \stackrel{\text{def}}{=} \begin{cases} -1 & : W, \\ q^{-n/2} & : AW. \end{cases} \tag{3.33}$$

The relations (3.32) are equivalent to the forward and backward shift relations of the orthogonal polynomials P_n (Ref. [45]),

$$\mathcal{F}(\lambda)\check{P}_n(x; \lambda) = f_n(\lambda)\check{P}_{n-1}(x; \lambda + \delta), \quad \mathcal{B}(\lambda)\check{P}_{n-1}(x; \lambda + \delta) = b_{n-1}(\lambda)\check{P}_n(x; \lambda), \tag{3.34}$$

where the forward and backward shift operators $\mathcal{F}(\lambda)$ and $\mathcal{B}(\lambda)$ are defined by

$$\mathcal{F}(\lambda) \stackrel{\text{def}}{=} \phi_0(x; \lambda + \delta)^{-1} \circ \mathcal{A}(\lambda) \circ \phi_0(x; \lambda) = i\varphi(x)^{-1}(e^{\frac{\gamma}{2}p} - e^{-\frac{\gamma}{2}p}), \tag{3.35}$$

$$\mathcal{B}(\lambda) \stackrel{\text{def}}{=} \phi_0(x; \lambda)^{-1} \circ \mathcal{A}(\lambda)^\dagger \circ \phi_0(x; \lambda + \delta) = -i(V(x; \lambda)e^{\frac{\gamma}{2}p} - V^*(x; \lambda)e^{-\frac{\gamma}{2}p})\varphi(x). \tag{3.36}$$

Note that the forward shift operator $\mathcal{F}(\lambda)$ is parameter independent. The second-order difference operator $\tilde{\mathcal{H}}(\lambda)$ acting on the polynomial eigenfunctions is square-root-free. It is defined by

$$\begin{aligned} \tilde{\mathcal{H}}(\lambda) &\stackrel{\text{def}}{=} \phi_0(x; \lambda)^{-1} \circ \mathcal{H}(\lambda) \circ \phi_0(x; \lambda) = \mathcal{B}(\lambda)\mathcal{F}(\lambda) \\ &= V(x; \lambda)(e^{\gamma p} - 1) + V^*(x; \lambda)(e^{-\gamma p} - 1), \end{aligned} \tag{3.37}$$

$$\tilde{\mathcal{H}}(\lambda)\check{P}_n(x; \lambda) = \mathcal{E}_n(\lambda)\check{P}_n(x; \lambda). \tag{3.38}$$

The action of the operators $\mathcal{A}(\lambda)$ and $\mathcal{A}(\lambda)^\dagger$ on the virtual state wave functions $\tilde{\phi}_v(x; \lambda)$ ($\tilde{\phi}_v^{\text{I}}$ and $\tilde{\phi}_v^{\text{II}}$) is

$$\mathcal{A}(\lambda)\tilde{\phi}_v(x; \lambda) = \tilde{f}_v(\lambda)\tilde{\phi}_v(x; \lambda + \delta), \quad \mathcal{A}(\lambda)^\dagger\tilde{\phi}_v(x; \lambda + \delta) = \tilde{b}_v(\lambda)\tilde{\phi}_v(x; \lambda), \tag{3.39}$$

where the factors of the virtual energy eigenvalue, $\tilde{f}_v(\lambda)$ and $\tilde{b}_v(\lambda)$, $\tilde{\mathcal{E}}_v(\lambda) = \tilde{f}_v(\lambda)\tilde{b}_v(\lambda)$, are given by

$$\begin{aligned} \tilde{f}_v^{\text{I}}(\lambda) &\stackrel{\text{def}}{=} \alpha^{\text{I}}(\lambda)^{-1/2} \times \begin{cases} a_1 + a_2 - v - 1 & : \text{W}, \\ -q^{v/2}(1 - a_1 a_2 q^{-v-1}) & : \text{AW}, \end{cases} \\ \tilde{b}_v^{\text{I}}(\lambda) &\stackrel{\text{def}}{=} \alpha^{\text{I}}(\lambda)^{1/2} \times \begin{cases} -(a_3 + a_4 + v) & : \text{W}, \\ q^{-v/2}(1 - a_3 a_4 q^v) & : \text{AW}, \end{cases} \\ \tilde{f}_v^{\text{II}}(\lambda) &\stackrel{\text{def}}{=} \alpha^{\text{II}}(\lambda)^{-1/2} \times \begin{cases} a_3 + a_4 - v - 1 & : \text{W}, \\ -q^{v/2}(1 - a_3 a_4 q^{-v-1}) & : \text{AW}, \end{cases} \\ \tilde{b}_v^{\text{II}}(\lambda) &\stackrel{\text{def}}{=} \alpha^{\text{II}}(\lambda)^{1/2} \times \begin{cases} -(a_1 + a_2 + v) & : \text{W}, \\ q^{-v/2}(1 - a_1 a_2 q^v) & : \text{AW}. \end{cases} \end{aligned} \tag{3.40}$$

The relations (3.39) are equivalent to the forward and backward shift relations of $(v^{-1}\check{\xi}_v)(x; \lambda) \stackrel{\text{def}}{=} v(x; \lambda)^{-1}\check{\xi}_v(x; \lambda)$ ($v^{\text{I}-1}\check{\xi}_v^{\text{I}}$ and $v^{\text{II}-1}\check{\xi}_v^{\text{II}}$),

$$\begin{aligned} \mathcal{F}(\lambda)(v^{-1}\check{\xi}_v)(x; \lambda) &= \tilde{f}_v(\lambda)(v^{-1}\check{\xi}_v)(x; \lambda + \delta), \\ \mathcal{B}(\lambda)(v^{-1}\check{\xi}_v)(x; \lambda + \delta) &= \tilde{b}_v(\lambda)(v^{-1}\check{\xi}_v)(x; \lambda). \end{aligned} \tag{3.41}$$

Explicitly they give square-root-free relations: forward and backward shift relations of the virtual polynomials ξ_v (ξ_v^{I} and ξ_v^{II} ; Ref. [10]),

$$\begin{aligned} i\varphi(x)^{-1}(v_1^*(x; \lambda + \tilde{\delta})e^{\frac{\gamma}{2}p} - v_1(x; \lambda + \tilde{\delta})e^{-\frac{\gamma}{2}p})\check{\xi}_v(x; \lambda) &= \alpha(\lambda)^{1/2}\tilde{f}_v(\lambda)\check{\xi}_v(x; \lambda + \delta), \\ i\varphi(x)^{-1}(v_2(x; \lambda)e^{\frac{\gamma}{2}p} - v_2^*(x; \lambda)e^{-\frac{\gamma}{2}p})\check{\xi}_v(x; \lambda + \delta) &= \alpha(\lambda)^{-1/2}\tilde{b}_v(\lambda)\check{\xi}_v(x; \lambda), \end{aligned} \tag{3.42}$$

where the functions $v_1(x; \lambda)$ and $v_2(x; \lambda)$ are

$$v_1(x; \lambda) \stackrel{\text{def}}{=} \begin{cases} \prod_{j=1}^2 (a_j + ix) & : \text{W}, \\ e^{-ix} \prod_{j=1}^2 (1 - a_j e^{ix}) & : \text{AW}, \end{cases} \quad v_2(x; \lambda) \stackrel{\text{def}}{=} \begin{cases} \prod_{j=3}^4 (a_j + ix) & : \text{W}, \\ e^{-ix} \prod_{j=3}^4 (1 - a_j e^{ix}) & : \text{AW}. \end{cases} \tag{3.43}$$

3.4. Multi-indexed orthogonal polynomials

The original systems in Sect. 3.1 are iso-spectrally deformed by applying multiple Darboux transformations with virtual state wave functions $\{\tilde{\phi}_v(x)\}$ as seed solutions. The virtual state wave functions are labeled (v, t) , where v is the degree of the polynomial part ξ_v and t stands for type I or II. We take M virtual state wave functions specified by the multi-index set $\mathcal{D} = \{(d_1, t_1), \dots, (d_M, t_M)\}$ (or in short $\mathcal{D} = \{d_1, \dots, d_M\}$) (ordered set), $M = M_I + M_{II}$, $M_I \stackrel{\text{def}}{=} \#\{d_j | (d_j, I) \in \mathcal{D}\}$, $M_{II} \stackrel{\text{def}}{=} \#\{d_j | (d_j, II) \in \mathcal{D}\}$. The deformed Hamiltonian is denoted $\mathcal{H}_{\mathcal{D}}(\lambda)$.

The multi-indexed orthogonal polynomials $\{\check{P}_{\mathcal{D},n}(x; \lambda)\}$ are the main parts of the eigenfunctions $\{\phi_{\mathcal{D},n}(x; \lambda)\}$ of the deformed system $\mathcal{H}_{\mathcal{D}}(\lambda)\phi_{\mathcal{D},n}(x; \lambda) = \mathcal{E}_n(\lambda)\phi_{\mathcal{D},n}(x; \lambda)$ (Ref. [10]):

$$\begin{aligned} \phi_{\mathcal{D},n}(x; \lambda) &= \left(\frac{\left(\prod_{j=0}^{M-1} V(x + i(\frac{M}{2} - j)\gamma; \lambda) V^*(x - i(\frac{M}{2} - j)\gamma; \lambda) \right)^{1/2}}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}](x - i\frac{\gamma}{2}; \lambda) W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}](x + i\frac{\gamma}{2}; \lambda)} \right)^{1/2} \\ &\quad \times W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \phi_n](x; \lambda) \\ &= \alpha^I (\lambda^{[M_I, M_{II}]})^{\frac{1}{2}M_I} \alpha^{II} (\lambda^{[M_I, M_{II}]})^{\frac{1}{2}M_{II}} \kappa^{-\frac{1}{4}M_I(M_I+1) - \frac{1}{4}M_{II}(M_{II}+1) + \frac{5}{2}M_I M_{II}} \\ &\quad \times \psi_{\mathcal{D}}(x; \lambda) \check{P}_{\mathcal{D},n}(x; \lambda), \end{aligned} \tag{3.44}$$

$$\psi_{\mathcal{D}}(x; \lambda) \stackrel{\text{def}}{=} \frac{\phi_0(x; \lambda^{[M_I, M_{II}]})}{\left(\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \lambda) \check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \lambda) \right)^{1/2}}, \quad \lambda^{[M_I, M_{II}]} \stackrel{\text{def}}{=} \lambda + M_I \delta^I + M_{II} \delta^{II}, \tag{3.45}$$

$$\check{P}_{\mathcal{D},n}(x; \lambda) \stackrel{\text{def}}{=} P_{\mathcal{D},n}(\eta(x); \lambda), \quad \check{\Xi}_{\mathcal{D}}(x; \lambda) \stackrel{\text{def}}{=} \Xi_{\mathcal{D}}(\eta(x); \lambda). \tag{3.46}$$

Here $W_\gamma[f_1, \dots, f_n](x)$ is the Casoratian (3.52), and $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are the main polynomial part of the Casoratians $W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}](x; \lambda)$ and $W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_M}, \phi_n](x; \lambda)$, respectively. The denominator polynomial $\Xi_{\mathcal{D}}(\eta; \lambda)$ and the multi-indexed orthogonal polynomial $P_{\mathcal{D},n}(\eta; \lambda)$ are polynomials in η and their degrees are generically $\ell_{\mathcal{D}}$ and $\ell_{\mathcal{D}} + n$, respectively. Here $\ell_{\mathcal{D}} \stackrel{\text{def}}{=} \sum_{j=1}^M d_j - \frac{1}{2}M(M-1) + 2M_I M_{II}$.

In Ref. [10], the denominator polynomials and the multi-indexed orthogonal polynomials for the Wilson and Askey–Wilson types are expressed as

$$\begin{aligned} \check{\Xi}_{\mathcal{D}}(x; \lambda) &\stackrel{\text{def}}{=} i^{\frac{1}{2}M(M-1)} \left| \begin{array}{ccc} \vec{X}_{d_1}^{(M)} & \dots & \vec{X}_{d_M}^{(M)} \end{array} \right| \times \varphi_M(x)^{-1} \kappa^{-\frac{1}{2}M_I M_{II}(M-2)} \\ &\quad \times \left(\prod_{l=0}^{M_I-1} \check{U}^{II}(x; \lambda + (1 - M + 2l)\delta)^{M_I-1-l} \cdot \prod_{l=0}^{M_{II}-1} \check{U}^I(x; \lambda + (1 - M + 2l)\delta)^{M_{II}-1-l} \right)^{-1}, \end{aligned} \tag{3.47}$$

$$\begin{aligned} \check{P}_{\mathcal{D},n}(x; \lambda) &\stackrel{\text{def}}{=} i^{\frac{1}{2}M(M+1)} \left| \begin{array}{ccc} \vec{X}_{d_1}^{(M+1)} & \dots & \vec{X}_{d_M}^{(M+1)} \quad \vec{Z}_n^{(M+1)} \end{array} \right| \times \varphi_{M+1}(x)^{-1} \kappa^{-\frac{1}{2}M_I M_{II}(M+2)} \\ &\quad \times \left(\prod_{l=0}^{M_I-1} \check{U}^{II}(x; \lambda + (-M + 2l)\delta)^{M_I-1-l} \cdot \prod_{l=0}^{M_{II}-1} \check{U}^I(x; \lambda + (-M + 2l)\delta)^{M_{II}-1-l} \right)^{-1}, \end{aligned} \tag{3.48}$$

where $\vec{X}_v^{(M)}$ ($\vec{X}_v^{(M)I}$ or $\vec{X}_v^{(M)II}$) and $\vec{Z}_n^{(M)}$ are

$$\begin{aligned} (\vec{X}_v^{(M)t})_j &= r_j^{\bar{t}}(x_j^{(M)}; \lambda, M) \check{\xi}_v^t(x_j^{(M)}; \lambda), \quad \bar{t} \stackrel{\text{def}}{=} \begin{cases} \text{II} & : t = \text{I}, \\ \text{I} & : t = \text{II}, \end{cases} \\ (\vec{Z}_n^{(M)})_j &= r_j^{\text{II}}(x_j^{(M)}; \lambda, M) r_j^{\text{I}}(x_j^{(M)}; \lambda, M) \check{P}_n(x_j^{(M)}; \lambda) \quad (1 \leq j \leq M). \end{aligned} \tag{3.49}$$

By using the properties of the determinant, Eqs. (3.53), (3.22), (3.26), and (3.29), we can rewrite these as

$$\begin{aligned} \check{\Xi}_{\mathcal{D}}(x; \lambda) &= W_\gamma[v^{-1}\check{\xi}_{d_1}, \dots, v^{-1}\check{\xi}_{d_M}](x; \lambda) \times \varphi_M(x)^{-1} \kappa^{-\frac{1}{2}M_1 M_{\text{II}}(M-2)} \\ &\quad \times v^{\text{I}}(x; \lambda + (M-1)\delta)^{M_1} v^{\text{II}}(x; \lambda + (M-1)\delta)^{M_{\text{II}}} \\ &\quad \times \left(\prod_{m=1}^{M_1} \check{U}^{\text{I}}(x; \lambda + (M-1-2m)\delta)^{M_1-m} \cdot \prod_{m=1}^{M_{\text{II}}} \check{U}^{\text{II}}(x; \lambda + (M-1-2m)\delta)^{M_{\text{II}}-m} \right)^{-1}, \end{aligned} \tag{3.50}$$

$$\begin{aligned} \check{P}_{\mathcal{D},n}(x; \lambda) &= W_\gamma[v^{-1}\check{\xi}_{d_1}, \dots, v^{-1}\check{\xi}_{d_M}, \check{P}_n](x; \lambda) \times \varphi_{M+1}(x)^{-1} \kappa^{-\frac{1}{2}M_1 M_{\text{II}}(M+2)} \\ &\quad \times v^{\text{I}}(x; \lambda + M\delta)^{M_1} v^{\text{II}}(x; \lambda + M\delta)^{M_{\text{II}}} \\ &\quad \times \left(\prod_{m=1}^{M_1} \check{U}^{\text{I}}(x; \lambda + (M-2m)\delta)^{M_1-m} \cdot \prod_{m=1}^{M_{\text{II}}} \check{U}^{\text{II}}(x; \lambda + (M-2m)\delta)^{M_{\text{II}}-m} \right)^{-1}. \end{aligned} \tag{3.51}$$

For the special situations when the index set \mathcal{D} consists of type I indices only (or type II indices only), the above Casoratians can be simplified to

$$\begin{aligned} W_\gamma[v^{-1}\check{\xi}_{d_1}, \dots, v^{-1}\check{\xi}_{d_M}](x; \lambda) &= \prod_{j=1}^M v(x_j^{(M)}; \lambda)^{-1} \cdot W_\gamma[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}](x; \lambda), \\ W_\gamma[v^{-1}\check{\xi}_{d_1}, \dots, v^{-1}\check{\xi}_{d_M}, \check{P}_n](x; \lambda) &= \prod_{j=1}^{M+1} v(x_j^{(M+1)}; \lambda)^{-1} \cdot W_\gamma[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}, v\check{P}_n](x; \lambda), \end{aligned}$$

by Eq. (3.53). However, when \mathcal{D} contains both I and II types, such rewriting is impossible since $v^{\text{I}}(x; \lambda) \neq v^{\text{II}}(x; \lambda)$.

In the next subsection we will rewrite Eqs. (3.50)–(3.51) using the identities obtained from the shape invariance and the Casoratian.

3.5. New determinant expressions

3.5.1. Casoratian

The Casorati determinant of a set of n functions $\{f_j(x)\}$ is defined by

$$W_\gamma[f_1, f_2, \dots, f_n](x) \stackrel{\text{def}}{=} i^{\frac{1}{2}n(n-1)} \det\left(f_k(x_j^{(n)})\right)_{1 \leq j, k \leq n}, \quad x_j^{(n)} \stackrel{\text{def}}{=} x + i\left(\frac{n+1}{2} - j\right)\gamma \tag{3.52}$$

(for $n = 0$, we set $W_\gamma[\cdot](x) = 1$), which satisfies

$$W_\gamma[gf_1, gf_2, \dots, gf_n] = \prod_{j=1}^n g(x_j^{(n)}) \cdot W_\gamma[f_1, f_2, \dots, f_n](x). \tag{3.53}$$

The following determinant formula holds for any analytic functions $q_j(x)$, $r_j(x)$, $q'_j(x)$ and $r'_j(x)$ ($j = 1, 2, \dots$):

$$i^{\frac{1}{2}n(n-1)} \det(a_{j,k})_{1 \leq j,k \leq n} = \prod_{m=1}^{\lfloor \frac{n}{2} \rfloor} D_{n+1-2m}(x) \cdot \prod_{m=0}^{n-2} \prod_{l=0}^{\lfloor \frac{m-1}{2} \rfloor} r_{n-1-m}(x + i(\frac{m}{2} - l)\gamma) q_{n-1-m}(x - i(\frac{m}{2} - l)\gamma) \times W_\gamma[f_1, \dots, f_n](x), \tag{3.54}$$

$$\begin{cases} a_{j,k} = \prod_{l=1}^{\overleftarrow{n+1-2j}} \hat{D}_l \cdot f_k(x) & (j = 1, \dots, \lfloor \frac{n+1}{2} \rfloor), \\ & (k = 1, \dots, n), \\ a_{j,k} = \hat{D}'_{2j-n-1} \prod_{l=1}^{\overleftarrow{2j-n-2}} \hat{D}_l \cdot f_k(x) & (j = \lfloor \frac{n+3}{2} \rfloor, \dots, n), \end{cases} \tag{3.55}$$

where the operators \hat{D}_j , \hat{D}'_j and functions $D_j(x)$ ($j = 1, 2, \dots$) are

$$\hat{D}_j = q_j(x)e^{\frac{\gamma}{2}j} + r_j(x)e^{-\frac{\gamma}{2}j}, \quad \hat{D}'_j = q'_j(x)e^{\frac{\gamma}{2}j} + r'_j(x)e^{-\frac{\gamma}{2}j}, \tag{3.56}$$

$$D_j(x) = r_j(x)q'_j(x) - r'_j(x)q_j(x). \tag{3.57}$$

This formula can be proven by using the properties of the determinant (row properties) and induction on n (even $n \rightarrow$ odd $n + 1$, odd $n \rightarrow$ even $n + 1$).

By taking \mathcal{F} or \mathcal{B} as \hat{D}_j and \hat{D}'_j and using the shape-invariance properties (3.34) and (3.41), the Casoratians $W_\gamma[v^{-1}\check{\xi}_{d_1}, \dots, v^{-1}\check{\xi}_{d_M}](x; \lambda)$ and $W_\gamma[v^{-1}\check{\xi}_{d_1}, \dots, v^{-1}\check{\xi}_{d_M}, \check{P}_n](x; \lambda)$ in Eqs. (3.50)–(3.51) can be rewritten in various ways. We consider two typical cases:

$$A : \hat{D}_j = \mathcal{F}(\lambda + (j - 1)\delta), \quad \hat{D}'_j = \mathcal{B}(\lambda + (j - 2)\delta) \quad (j = 1, 2, \dots), \tag{3.58}$$

$$B : \hat{D}_{2l-1} = \mathcal{F}(\lambda), \quad \hat{D}_{2l} = \mathcal{B}(\lambda), \quad \hat{D}'_{2l-1} = \mathcal{B}(\lambda - \delta), \quad \hat{D}'_{2l} = \mathcal{F}(\lambda + \delta) \quad (l = 1, 2, \dots), \tag{3.59}$$

which correspond to cases A and B in Ref. [42]. For the function $D_j(x)$ in Eq. (3.57), we define a function $\check{S}(x; \lambda)$ and a polynomial $S(\eta; \lambda)$:

$$\check{S}(x; \lambda) \stackrel{\text{def}}{=} -i(V(x; \lambda)\varphi(x - i\frac{\gamma}{2}) - V^*(x; \lambda)\varphi(x + i\frac{\gamma}{2})),$$

$$S(\eta; \lambda) \stackrel{\text{def}}{=} \begin{cases} b_1\eta - b_3 & : W, \\ q^{-1/2}(2(1 - b_4)\eta + b_3 - b_1) & : AW, \end{cases} \quad \check{S}(x; \lambda) = S(\eta(x); \lambda), \tag{3.60}$$

where b_3 is $b_3 \stackrel{\text{def}}{=} a_1a_2a_3 + a_1a_2a_4 + a_1a_3a_4 + a_2a_3a_4$.

3.5.2. Case A

First we consider case A in Eq. (3.58). The functions $q_j(x)$, $r_j(x)$, $q'_j(x)$, $r'_j(x)$, and $D_j(x)$ are

$$\begin{aligned} q_j(x) &= i\varphi(x)^{-1}, & r_j(x) &= -i\varphi(x)^{-1}, \\ q'_j(x) &= -iV(x; \lambda + (j-2)\delta)\varphi(x - i\frac{\gamma}{2}), & r'_j(x) &= iV^*(x; \lambda + (j-2)\delta)\varphi(x + i\frac{\gamma}{2}), \\ D_j(x) &= -i\varphi(x)^{-1}\check{S}(x; \lambda + (j-2)\delta). \end{aligned} \tag{3.61}$$

The shape-invariance properties (3.34) and (3.41) give ($k = 0, 1, \dots$)

$$\begin{aligned} \prod_{l=1}^{\leftarrow k} \hat{D}_l \cdot \check{P}_n(x; \lambda) &= \prod_{m=0}^{k-1} f_{n-m}(\lambda + m\delta) \cdot \check{P}_{n-k}(x; \lambda + k\delta), \\ \prod_{l=1}^{\leftarrow k} \hat{D}_l \cdot (v^{-1}\check{\xi}_v)(x; \lambda) &= \prod_{m=0}^{k-1} \check{f}_v(\lambda + m\delta) \cdot (v^{-1}\check{\xi}_v)(x; \lambda + k\delta), \\ \hat{D}'_{k+1} \prod_{l=1}^{\leftarrow k} \hat{D}_l \cdot \check{P}_n(x; \lambda) &= b_{n-k}(\lambda + (k-1)\delta) \prod_{m=0}^{k-1} f_{n-m}(\lambda + m\delta) \cdot \check{P}_{n+1-k}(x; \lambda + (k-1)\delta), \\ \hat{D}'_{k+1} \prod_{l=1}^{\leftarrow k} \hat{D}_l \cdot (v^{-1}\check{\xi}_v)(x; \lambda) &= \check{b}_v(\lambda + (k-1)\delta) \prod_{m=0}^{k-1} \check{f}_v(\lambda + m\delta) \cdot (v^{-1}\check{\xi}_v)(x; \lambda + (k-1)\delta). \end{aligned} \tag{3.62}$$

We rewrite Eqs. (3.50)–(3.51) in the following way. (i) By using Eqs. (3.54)–(3.55), rewrite the Casoratians in Eqs. (3.50)–(3.51) as determinants $\det(a_{j,k})_{1 \leq j,k \leq M'}$ ($M' = M$ for $\check{\Xi}_{\mathcal{D}}$ and $M' = M+1$ for $\check{P}_{\mathcal{D},n}$). (ii) Rewrite each matrix element $a_{j,k}$ using Eq. (3.62). (iii) Multiply the k th column ($1 \leq k \leq M$) of $\det(a_{j,k})$ by $v(x; \lambda + (M'-1)\delta)$ (v^I or v^{II} depending on d_k), and divide the determinant by $v^I(x; \lambda + (M'-1)\delta)^{M_I} v^{II}(x; \lambda + (M'-1)\delta)^{M_{II}}$. (iv) Rewrite $v(x; \lambda + (M'-1)\delta)/v(x; \lambda + l\delta)$ in $a_{j,k}$ by Eq. (3.26). Then $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are expressed in terms of $\check{\xi}_{d_k}(x; \lambda')$, $\check{P}_{n'}(x; \lambda')$, $\check{U}(x; \lambda')$, $\check{S}(x; \lambda')$, and $\varphi(x')$. Straightforward calculation shows that the factors $\varphi(x')$ are canceled out. Thus $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are expressed in terms of $\eta(x)$, namely, $\Xi_{\mathcal{D}}(\eta; \lambda)$ and $P_{\mathcal{D},n}(\eta; \lambda)$ are expressed without explicit x -dependence. Their final forms are as follows. The denominator polynomial $\Xi_{\mathcal{D}}(\eta; \lambda)$ is

$$\begin{aligned} \Xi_{\mathcal{D}}(\eta; \lambda) &= (-1)^{\frac{1}{6}(M-1)M(M+1)} \kappa^{-\frac{1}{2}M_I M_{II}(M-2)} \det(a_{j,k})_{1 \leq j,k \leq M} \\ &\quad \times \left(\prod_{l=0}^{M_I-1} U^I(\eta; \lambda + (M_{II} - M_I - 1 + 2l)\delta)^l \cdot \prod_{l=0}^{M_{II}-1} U^{II}(\eta; \lambda + (M_I - M_{II} - 1 + 2l)\delta)^l \right. \\ &\quad \left. \times \prod_{m=1}^{\lfloor \frac{M}{2} \rfloor} S(\eta; \lambda + (M-1-2m)\delta) \right)^{-1}, \end{aligned} \tag{3.63}$$

where $a_{j,k}$ are

$$a_{j,k} = \prod_{m=0}^{M-2j} \check{f}_{d_k}(\lambda + m\delta) \cdot \prod_{l=1}^{j-1} U(\eta; \lambda + (M-1-2l)\delta) \cdot \xi_{d_k}(\eta; \lambda + (M+1-2j)\delta)$$

$$\begin{aligned}
 & (j = 1, \dots, [\frac{M+1}{2}]; k = 1, \dots, M), \\
 a_{j,k} &= \tilde{b}_{d_k}(\lambda + (2j - M - 3)\delta) \prod_{m=0}^{2j-M-3} \tilde{f}_{d_k}(\lambda + m\delta) \cdot \prod_{l=1}^{M+1-j} U(\eta; \lambda + (M - 1 - 2l)\delta) \\
 & \times \xi_{d_k}(\eta; \lambda + (2j - M - 3)\delta) \quad (j = [\frac{M+3}{2}], \dots, M; k = 1, \dots, M). \tag{3.64}
 \end{aligned}$$

The multi-indexed orthogonal polynomial $P_{\mathcal{D},n}(\eta; \lambda)$ is

$$\begin{aligned}
 & P_{\mathcal{D},n}(\eta; \lambda) \\
 &= (-1)^{\frac{1}{6}M(M+1)(M+2)} \kappa^{-\frac{1}{2}M_{\text{I}}M_{\text{II}}(M+2)} \det(a_{j,k})_{1 \leq j,k \leq M+1} \\
 & \times \left(\prod_{l=0}^{M_{\text{I}}-1} U^{\text{I}}(\eta; \lambda + (M_{\text{II}} - M_{\text{I}} + 2l)\delta)^l \cdot \prod_{l=0}^{M_{\text{II}}-1} U^{\text{II}}(\eta; \lambda + (M_{\text{I}} - M_{\text{II}} + 2l)\delta)^l \right. \\
 & \left. \times \prod_{m=1}^{[\frac{M+1}{2}]} S(\eta; \lambda + (M - 2m)\delta) \right)^{-1}, \tag{3.65}
 \end{aligned}$$

where $a_{j,k}$ are

$$\begin{aligned}
 a_{j,k} &= \prod_{m=0}^{M+1-2j} \tilde{f}_{d_k}(\lambda + m\delta) \cdot \prod_{l=1}^{j-1} U(\eta; \lambda + (M - 2l)\delta) \cdot \xi_{d_k}(\eta; \lambda + (M + 2 - 2j)\delta) \\
 & (j = 1, \dots, [\frac{M+2}{2}]; k = 1, \dots, M), \\
 a_{j,k} &= \tilde{b}_{d_k}(\lambda + (2j - M - 4)\delta) \prod_{m=0}^{2j-M-4} \tilde{f}_{d_k}(\lambda + m\delta) \cdot \prod_{l=1}^{M+2-j} U(\eta; \lambda + (M - 2l)\delta) \\
 & \times \xi_{d_k}(\eta; \lambda + (2j - M - 4)\delta) \quad (j = [\frac{M+4}{2}], \dots, M + 1; k = 1, \dots, M), \\
 a_{j,M+1} &= \prod_{m=0}^{M+1-2j} f_{n-m}(\lambda + m\delta) \cdot P_{n-M-2+2j}(\eta; \lambda + (M + 2 - 2j)\delta) \quad (j = 1, \dots, [\frac{M+2}{2}]), \\
 a_{j,M+1} &= b_{n-2j+M+3}(\lambda + (2j - M - 4)\delta) \prod_{m=0}^{2j-M-4} f_{n-m}(\lambda + m\delta) \\
 & \times P_{n-2j+M+4}(\eta; \lambda + (2j - M - 4)\delta) \quad (j = [\frac{M+4}{2}], \dots, M + 1). \tag{3.66}
 \end{aligned}$$

3.5.3. Case B

Second we consider case B in Eq. (3.59). The functions $q_j(x)$, $r_j(x)$, $q'_j(x)$, $r'_j(x)$, and $D_j(x)$ are ($l = 1, 2, \dots$)

$$\begin{aligned}
 q_{2l-1}(x) &= i\varphi(x)^{-1}, & r_{2l-1}(x) &= -i\varphi(x)^{-1}, \\
 q_{2l}(x) &= -iV(x; \lambda)\varphi(x - i\frac{\gamma}{2}), & r_{2l}(x) &= iV^*(x; \lambda)\varphi(x + i\frac{\gamma}{2}), \\
 q'_{2l-1}(x) &= -iV(x; \lambda - \delta)\varphi(x - i\frac{\gamma}{2}), & r'_{2l-1}(x) &= iV^*(x; \lambda - \delta)\varphi(x + i\frac{\gamma}{2}), \\
 q'_{2l}(x) &= i\varphi(x)^{-1}, & r'_{2l}(x) &= -i\varphi(x)^{-1}, \\
 D_{2l-1}(x) &= -i\varphi(x)^{-1}\check{S}(x; \lambda - \delta), & D_{2l}(x) &= i\varphi(x)^{-1}\check{S}(x; \lambda).
 \end{aligned} \tag{3.67}$$

The shape-invariance properties (3.34) and (3.41) give ($l = 1, 2, \dots$)

$$\begin{aligned}
 & \prod_{m=1}^{\overleftarrow{2l-2}} \hat{D}_m \cdot \check{P}_n(x; \lambda) = \mathcal{E}_n(\lambda)^{l-1} \check{P}_n(x; \lambda), \\
 & \prod_{m=1}^{\overleftarrow{2l-1}} \hat{D}_m \cdot \check{P}_n(x; \lambda) = f_n(\lambda) \mathcal{E}_n(\lambda)^{l-1} \check{P}_{n-1}(x; \lambda + \delta), \\
 & \prod_{m=1}^{\overleftarrow{2l-2}} \hat{D}_m \cdot (v^{-1} \check{\xi}_v)(x; \lambda) = \tilde{\mathcal{E}}_v(\lambda)^{l-1} (v^{-1} \check{\xi}_v)(x; \lambda), \\
 & \prod_{m=1}^{\overleftarrow{2l-1}} \hat{D}_m \cdot (v^{-1} \check{\xi}_v)(x; \lambda) = \tilde{f}_v(\lambda) \tilde{\mathcal{E}}_v(\lambda)^{l-1} (v^{-1} \check{\xi}_v)(x; \lambda + \delta), \\
 & \hat{D}'_{2l-1} \prod_{m=1}^{\overleftarrow{2l-2}} \hat{D}_m \cdot \check{P}_n(x; \lambda) = b_n(\lambda - \delta) \mathcal{E}_n(\lambda)^{l-1} \check{P}_{n+1}(x; \lambda - \delta), \\
 & \hat{D}'_{2l} \prod_{m=1}^{\overleftarrow{2l-1}} \hat{D}_m \cdot \check{P}_n(x; \lambda) = f_{n-1}(\lambda + \delta) f_n(\lambda) \mathcal{E}_n(\lambda)^{l-1} \check{P}_{n-2}(x; \lambda + 2\delta), \\
 & \hat{D}'_{2l-1} \prod_{m=1}^{\overleftarrow{2l-2}} \hat{D}_m \cdot (v^{-1} \check{\xi}_v)(x; \lambda) = \tilde{b}_v(\lambda - \delta) \tilde{\mathcal{E}}_v(\lambda)^{l-1} (v^{-1} \check{\xi}_v)(x; \lambda - \delta), \\
 & \hat{D}'_{2l} \prod_{m=1}^{\overleftarrow{2l-1}} \hat{D}_m \cdot (v^{-1} \check{\xi}_v)(x; \lambda) = \tilde{f}_v(\lambda + \delta) \tilde{f}_v(\lambda) \tilde{\mathcal{E}}_v(\lambda)^{l-1} (v^{-1} \check{\xi}_v)(x; \lambda + 2\delta).
 \end{aligned} \tag{3.68}$$

Like case A, we rewrite Eqs. (3.50)–(3.51) using steps (i)–(iv). By using Eq. (3.14) and

$$V(x; \lambda) V^*(x; \lambda) = \alpha^I(\lambda) \alpha^{II}(\lambda) \kappa^{-1} \frac{\check{U}^I(x; \lambda) \check{U}^{II}(x; \lambda)}{\varphi(x - i\frac{\nu}{2}) \varphi(x)^2 \varphi(x + i\frac{\nu}{2})}, \tag{3.69}$$

$\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are expressed in terms of $\check{\xi}_{d_k}(x; \lambda')$, $\check{P}_{n'}(x; \lambda')$, $\check{U}(x; \lambda')$, $\check{S}(x; \lambda')$, and $\varphi(x')$. Straightforward calculation shows that the factors $\varphi(x')$ are canceled out. Thus $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are expressed in terms of $\eta(x)$, namely, $\Xi_{\mathcal{D}}(\eta; \lambda)$ and $P_{\mathcal{D},n}(\eta; \lambda)$ are expressed without explicit x -dependence. Their final forms are as follows. The denominator polynomial $\Xi_{\mathcal{D}}(\eta; \lambda)$ is

$$\begin{aligned}
 & \Xi_{\mathcal{D}}(\eta; \lambda) \\
 & = (-1)^{\lfloor \frac{M}{2} \rfloor} \kappa^{-\frac{1}{2} M_I M_{II} (M-2)} (\alpha^I(\lambda) \alpha^{II}(\lambda) \kappa^{-1})^{-\frac{1}{2} \lfloor \frac{M-2}{2} \rfloor \lfloor \frac{M}{2} \rfloor} \det(a_{j,k})_{1 \leq j,k \leq M} \\
 & \times \left(\prod_{m=1}^{M_I} U^I(\eta; \lambda + (M-1-2m)\delta) \delta \right)^{M_I - m} \cdot \prod_{m=1}^{M_{II}} U^{II}(\eta; \lambda + (M-1-2m)\delta) \delta)^{M_{II} - m} \\
 & \times \prod_{m=0}^{\lfloor \frac{M-2}{2} \rfloor} U^I(\eta; \lambda + (M-1-2m)\delta)^m \cdot \prod_{m=0}^{\lfloor \frac{M-2}{2} \rfloor} U^{II}(\eta; \lambda + (M-1-2m)\delta)^m \\
 & \times S(\eta; \lambda - \frac{1}{2}(1 + (-1)^M)\delta)^{\lfloor \frac{M}{2} \rfloor} \Big)^{-1}, \tag{3.70}
 \end{aligned}$$

where $a_{j,k}$ are

$$\begin{aligned}
 a_{j,k} &= \tilde{\mathcal{E}}_{d_k}(\boldsymbol{\lambda})^{\frac{M+1}{2}-j} \prod_{l=0}^{\frac{M-3}{2}} U(\eta; \boldsymbol{\lambda} + 2l\boldsymbol{\delta}) \cdot \xi_{d_k}(\eta; \boldsymbol{\lambda}) \quad (j = 1, \dots, \frac{M+1}{2}; k = 1, \dots, M), \\
 a_{j,k} &= \tilde{f}_{d_k}(\boldsymbol{\lambda} + \boldsymbol{\delta}) \tilde{f}_{d_k}(\boldsymbol{\lambda}) \tilde{\mathcal{E}}_{d_k}(\boldsymbol{\lambda})^{j-\frac{M+3}{2}} \prod_{l=1}^{\frac{M-3}{2}} U(\eta; \boldsymbol{\lambda} + 2l\boldsymbol{\delta}) \cdot \xi_{d_k}(\eta; \boldsymbol{\lambda} + 2\boldsymbol{\delta}) \\
 &\quad (j = \frac{M+3}{2}, \dots, M; k = 1, \dots, M)
 \end{aligned} \tag{3.71}$$

for odd M and

$$\begin{aligned}
 a_{j,k} &= \tilde{f}_{d_k}(\boldsymbol{\lambda}) \tilde{\mathcal{E}}_{d_k}(\boldsymbol{\lambda})^{\frac{M}{2}-j} \prod_{l=1}^{\frac{M-2}{2}} U(\eta; \boldsymbol{\lambda} + (2l-1)\boldsymbol{\delta}) \cdot \xi_{d_k}(\eta; \boldsymbol{\lambda} + \boldsymbol{\delta}) \\
 &\quad (j = 1, \dots, \frac{M}{2}; k = 1, \dots, M), \\
 a_{j,k} &= \tilde{b}_{d_k}(\boldsymbol{\lambda} - \boldsymbol{\delta}) \tilde{\mathcal{E}}_{d_k}(\boldsymbol{\lambda})^{j-\frac{M+2}{2}} \prod_{l=0}^{\frac{M-2}{2}} U(\eta; \boldsymbol{\lambda} + (2l-1)\boldsymbol{\delta}) \cdot \xi_{d_k}(\eta; \boldsymbol{\lambda} - \boldsymbol{\delta}) \quad (j = \frac{M+2}{2}, \dots, M)
 \end{aligned} \tag{3.72}$$

for even M . The multi-indexed orthogonal polynomial $P_{\mathcal{D},n}(\eta; \boldsymbol{\lambda})$ is

$$\begin{aligned}
 &P_{\mathcal{D},n}(\eta; \boldsymbol{\lambda}) \\
 &= (-1)^{[\frac{M+1}{2}]_{\kappa} - \frac{1}{2}M_{\text{I}}M_{\text{II}}(M+2)} (\alpha^{\text{I}}(\boldsymbol{\lambda})\alpha^{\text{II}}(\boldsymbol{\lambda})\kappa^{-1})^{-\frac{1}{2}[\frac{M-1}{2}][\frac{M+1}{2}]} \det(a_{j,k})_{1 \leq j,k \leq M+1} \\
 &\quad \times \left(\prod_{m=1}^{M_{\text{I}}} U^{\text{I}}(\eta; \boldsymbol{\lambda} + (M-2m)\boldsymbol{\delta})^{M_{\text{I}}-m} \cdot \prod_{m=1}^{M_{\text{II}}} U^{\text{II}}(\eta; \boldsymbol{\lambda} + (M-2m)\boldsymbol{\delta})^{M_{\text{II}}-m} \right. \\
 &\quad \times \prod_{m=0}^{[\frac{M-1}{2}]} U^{\text{I}}(\eta; \boldsymbol{\lambda} + (M-2m)\boldsymbol{\delta})^m \cdot \prod_{m=0}^{[\frac{M-1}{2}]} U^{\text{II}}(\eta; \boldsymbol{\lambda} + (M-2m)\boldsymbol{\delta})^m \\
 &\quad \left. \times S(\eta; \boldsymbol{\lambda} - \frac{1}{2}(1 - (-1)^M)\boldsymbol{\delta})^{[\frac{M+1}{2}]} \right)^{-1},
 \end{aligned} \tag{3.73}$$

where $a_{j,k}$ are

$$\begin{aligned}
 a_{j,k} &= \tilde{\mathcal{E}}_{d_k}(\boldsymbol{\lambda})^{\frac{M+2}{2}-j} \prod_{l=0}^{\frac{M}{2}-1} U(\eta; \boldsymbol{\lambda} + 2l\boldsymbol{\delta}) \cdot \xi_{d_k}(\eta; \boldsymbol{\lambda}) \quad (j = 1, \dots, \frac{M+2}{2}; k = 1, \dots, M), \\
 a_{j,k} &= \tilde{f}_{d_k}(\boldsymbol{\lambda} + \boldsymbol{\delta}) \tilde{f}_{d_k}(\boldsymbol{\lambda}) \tilde{\mathcal{E}}_{d_k}(\boldsymbol{\lambda})^{j-\frac{M+4}{2}} \prod_{l=1}^{\frac{M}{2}-1} U(\eta; \boldsymbol{\lambda} + 2l\boldsymbol{\delta}) \cdot \xi_{d_k}(\eta; \boldsymbol{\lambda} + 2\boldsymbol{\delta}) \\
 &\quad (j = \frac{M+4}{2}, \dots, M+1; k = 1, \dots, M), \\
 a_{j,M+1} &= \mathcal{E}_n(\boldsymbol{\lambda})^{\frac{M+2}{2}-j} P_n(\eta; \boldsymbol{\lambda}) \quad (j = 1, \dots, \frac{M+2}{2}), \\
 a_{j,M+1} &= f_{n-1}(\boldsymbol{\lambda} + \boldsymbol{\delta}) f_n(\boldsymbol{\lambda}) \mathcal{E}_n(\boldsymbol{\lambda})^{j-\frac{M+4}{2}} P_{n-2}(\eta; \boldsymbol{\lambda} + 2\boldsymbol{\delta}) \quad (j = \frac{M+4}{2}, \dots, M+1)
 \end{aligned} \tag{3.74}$$

for even M and

$$\begin{aligned}
 a_{j,k} &= \tilde{f}_{d_k}(\lambda) \tilde{\mathcal{E}}_{d_k}(\lambda)^{\frac{M+1}{2}-j} \prod_{l=1}^{\frac{M-1}{2}} U(\eta; \lambda + (2l-1)\delta) \cdot \xi_{d_k}(\eta; \lambda + \delta), \\
 &\quad (j = 1, \dots, \frac{M+1}{2}; \quad k = 1, \dots, M), \\
 a_{j,k} &= \tilde{b}_{d_k}(\lambda - \delta) \tilde{\mathcal{E}}_{d_k}(\lambda)^{j-\frac{M+3}{2}} \prod_{l=0}^{\frac{M-1}{2}} U(\eta; \lambda + (2l-1)\delta) \cdot \xi_{d_k}(\eta; \lambda - \delta) \\
 &\quad (j = \frac{M+3}{2}, \dots, M+1; \quad k = 1, \dots, M), \\
 a_{j,M+1} &= f_n(\lambda) \mathcal{E}_n(\lambda)^{\frac{M+1}{2}-j} P_{n-1}(\eta; \lambda + \delta) \quad (j = 1, \dots, \frac{M+1}{2}), \\
 a_{j,M+1} &= b_n(\lambda - \delta) \mathcal{E}_n(\lambda)^{j-\frac{M+3}{2}} P_{n+1}(\eta; \lambda - \delta) \quad (j = \frac{M+3}{2}, \dots, M+1)
 \end{aligned} \tag{3.75}$$

for odd M .

3.5.4. Single type

As remarked after Eq. (3.51), when the index set \mathcal{D} consists of type I indices only (or type II indices only), simplifications occur. We consider such a single-type index set here. As shown in Refs. [48,49], the multi-indexed polynomials with both types of indices can always be recovered from those with single-type indices \mathcal{D}' (type I only or type II only) with shifted parameters λ' , namely,

$$P_{\mathcal{D},n}(\eta; \lambda) = \frac{c_{\mathcal{D},n}^P(\lambda)}{c_{\mathcal{D}',n}^P(\lambda')} P_{\mathcal{D}',n}(\eta; \lambda'), \tag{3.76}$$

where $c_{\mathcal{D},n}^P(\lambda)$ is the coefficient of the highest-degree term of $P_{\mathcal{D},n}(\eta; \lambda)$ (Ref. [10]), and \mathcal{D}' and λ' are determined by \mathcal{D} and λ (Ref. [48]).

Let us define $\mathcal{F}'(\lambda)$, $\mathcal{B}'(\lambda)$, $f'_n(\lambda)$, $\mathcal{E}'_n(\lambda)$, etc. as

$$\begin{aligned}
 \mathcal{F}'(\lambda) &\stackrel{\text{def}}{=} \mathcal{F}(\mathfrak{t}(\lambda)), & \mathcal{B}'(\lambda) &\stackrel{\text{def}}{=} \mathcal{B}(\mathfrak{t}(\lambda)), \\
 f'_n(\lambda) &\stackrel{\text{def}}{=} f_n(\mathfrak{t}(\lambda)), & b'_n(\lambda) &\stackrel{\text{def}}{=} b_n(\mathfrak{t}(\lambda)), & \tilde{f}'_v(\lambda) &\stackrel{\text{def}}{=} \tilde{f}_v(\mathfrak{t}(\lambda)), & \tilde{b}'_v(\lambda) &\stackrel{\text{def}}{=} \tilde{b}_v(\mathfrak{t}(\lambda)), \\
 \mathcal{E}'_n(\lambda) &\stackrel{\text{def}}{=} \mathcal{E}_n(\mathfrak{t}(\lambda)) = f'_n(\lambda) b'_{n-1}(\lambda), & \tilde{\mathcal{E}}'_v(\lambda) &\stackrel{\text{def}}{=} \tilde{\mathcal{E}}_v(\mathfrak{t}(\lambda)) = \tilde{f}'_v(\lambda) \tilde{b}'_v(\lambda).
 \end{aligned} \tag{3.77}$$

For $\mathcal{F}'(\lambda)$, $\mathcal{B}'(\lambda)$, $f'_n(\lambda)$, $b'_n(\lambda)$, and $\mathcal{E}'_n(\lambda)$, the type of \mathfrak{t} is I or II, e.g., $\mathcal{F}'^I(\lambda) = \mathcal{F}(\mathfrak{t}^I(\lambda))$ and $\mathcal{F}'^{II}(\lambda) = \mathcal{F}(\mathfrak{t}^{II}(\lambda))$. For $\tilde{f}'_v(\lambda)$, $\tilde{b}'_v(\lambda)$, and $\tilde{\mathcal{E}}'_v(\lambda)$, the type of \mathfrak{t} is matched to that of them, e.g., $\tilde{f}'^{I'}_v(\lambda) = \tilde{f}'_v(\mathfrak{t}^I(\lambda))$ and $\tilde{f}'^{II'}_v(\lambda) = \tilde{f}'_v(\mathfrak{t}^{II}(\lambda))$. Then the relations (3.34) and (3.41) with the replacement $\lambda \mapsto \mathfrak{t}(\lambda)$ (the type of \mathfrak{t} is I or II for Eq. (3.34), and matched to $\nu^{-1}\check{\xi}_v$ for Eq. (3.41)) and exchange $n \leftrightarrow v$ give

$$\hat{\mathcal{F}}'(\lambda) \check{\xi}_v(x; \lambda) = f'_v(\lambda) \check{\xi}_{v-1}(x; \lambda + \tilde{\delta}), \quad \hat{\mathcal{B}}'(\lambda) \check{\xi}_{v-1}(x; \lambda + \tilde{\delta}) = b'_{v-1}(\lambda) \check{\xi}_v(x; \lambda), \tag{3.78}$$

$$\hat{\mathcal{F}}'(\lambda) (\nu \check{P}_n)(x; \lambda) = \tilde{f}'_n(\lambda) (\nu \check{P}_n)(x; \lambda + \tilde{\delta}), \quad \hat{\mathcal{B}}'(\lambda) (\nu \check{P}_n)(x; \lambda + \tilde{\delta}) = \tilde{b}'_n(\lambda) (\nu \check{P}_n)(x; \lambda), \tag{3.79}$$

where $(\nu \check{P}_n)(x; \lambda) \stackrel{\text{def}}{=} \nu(x; \lambda) \check{P}_n(x; \lambda)$.

In the following we consider the index set \mathcal{D} with single-type twists. The type of unspecified t , $v(x; \lambda)$, $\check{U}(x; \lambda)$, $\mathcal{F}'(\lambda)$, $\mathcal{B}'(\lambda)$, $f'_n(\lambda)$, $\mathcal{E}'_n(\lambda)$, $\tilde{\delta}$, etc. is the same as the type of the indices of \mathcal{D} . The expressions (3.50)–(3.51) are simplified to

$$\check{\Xi}_{\mathcal{D}}(x; \lambda) = W_{\gamma}[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}](x; \lambda) \times \varphi_M(x)^{-1} \prod_{j=1}^M \frac{v(x; \lambda + (M - 1)\delta)}{v(x_j^{(M)}; \lambda)} \times \left(\prod_{m=1}^M \check{U}(x; \lambda + (M - 1 - 2m)\delta)^{M-m} \right)^{-1}, \tag{3.80}$$

$$\check{P}_{\mathcal{D},n}(x; \lambda) = W_{\gamma}[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}, v\check{P}_n](x; \lambda) \times \varphi_{M+1}(x)^{-1} \prod_{j=1}^{M+1} \frac{v(x; \lambda + M\delta)}{v(x_j^{(M+1)}; \lambda)} \times v(x; \lambda + M\delta)^{-1} \left(\prod_{m=1}^M \check{U}(x; \lambda + (M - 2m)\delta)^{M-m} \right)^{-1}. \tag{3.81}$$

By taking \mathcal{F}' or \mathcal{B}' as \hat{D}_j and \hat{D}'_j and using the shape-invariance properties (3.78)–(3.79), the Casoratians $W_{\gamma}[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}](x; \lambda)$ and $W_{\gamma}[\check{\xi}_{d_1}, \dots, \check{\xi}_{d_M}, v\check{P}_n](x; \lambda)$ in Eqs. (3.80)–(3.81) can be rewritten in various ways. We consider two typical cases:

$$A : \hat{D}_j = \mathcal{F}'(\lambda + (j - 1)\tilde{\delta}), \quad \hat{D}'_j = \mathcal{B}'(\lambda + (j - 2)\tilde{\delta}) \quad (j = 1, 2, \dots), \tag{3.82}$$

$$B : \hat{D}_{2l-1} = \mathcal{F}'(\lambda), \quad \hat{D}_{2l} = \mathcal{B}'(\lambda), \\ \hat{D}'_{2l-1} = \mathcal{B}'(\lambda - \tilde{\delta}), \quad \hat{D}'_{2l} = \mathcal{F}'(\lambda + \tilde{\delta}) \quad (l = 1, 2, \dots), \tag{3.83}$$

which correspond to cases A and B in Ref. [42].

Case A

First we consider case A in Eq. (3.82). The functions $q_j(x)$, $r_j(x)$, $q'_j(x)$, $r'_j(x)$, and $D_j(x)$ are

$$q_j(x) = i\varphi(x)^{-1}, \quad r_j(x) = -i\varphi(x)^{-1}, \\ q'_j(x) = -iV(x; t(\lambda) + (j - 2)\delta)\varphi(x - i\frac{\gamma}{2}), \quad r'_j(x) = iV^*(x; t(\lambda) + (j - 2)\delta)\varphi(x + i\frac{\gamma}{2}), \\ D_j(x) = -i\varphi(x)^{-1}\check{S}(x; t(\lambda) + (j - 2)\delta). \tag{3.84}$$

The shape-invariance properties (3.78)–(3.79) give ($k = 0, 1, \dots$)

$$\prod_{l=1}^k \hat{D}_l \cdot \check{\xi}_v(x; \lambda) = \prod_{m=0}^{k-1} f'_{v-m}(\lambda + m\tilde{\delta}) \cdot \check{\xi}_{v-k}(x; \lambda + k\tilde{\delta}), \\ \prod_{l=1}^k \hat{D}_l \cdot (v\check{P}_n)(x; \lambda) = \prod_{m=0}^{k-1} \check{f}'_n(\lambda + m\tilde{\delta}) \cdot (v\check{P}_n)(x; \lambda + k\tilde{\delta}), \tag{3.85} \\ \hat{D}'_{k+1} \prod_{l=1}^k \hat{D}_l \cdot \check{\xi}_v(x; \lambda) = b'_{v-k}(\lambda + (k - 1)\tilde{\delta}) \prod_{m=0}^{k-1} f'_{v-m}(\lambda + m\tilde{\delta}) \cdot \check{\xi}_{v+1-k}(x; \lambda + (k - 1)\tilde{\delta}), \\ \hat{D}'_{k+1} \prod_{l=1}^k \hat{D}_l \cdot (v\check{P}_n)(x; \lambda) = \tilde{b}'_n(\lambda + (k - 1)\tilde{\delta}) \prod_{m=0}^{k-1} \check{f}'_n(\lambda + m\tilde{\delta}) \cdot (v\check{P}_n)(x; \lambda + (k - 1)\tilde{\delta}).$$

We rewrite Eqs. (3.80)–(3.81) in the following way. (i) Using Eqs. (3.54)–(3.55), rewrite the Casoratians in Eqs. (3.80)–(3.81) as determinants $\det(a_{j,k})_{1 \leq j,k \leq M'}$ ($M' = M$ for $\check{\Xi}_{\mathcal{D}}$ and $M' = M + 1$ for $\check{P}_{\mathcal{D},n}$). (ii) Rewrite each matrix element $a_{j,k}$ using Eq. (3.85). For $\check{P}_{\mathcal{D},n}$, we do the following (iii)–(v). (iii) Divide the $(M + 1)$ th column of $\det(a_{j,k})$ by $v(x; \lambda + M\delta)$, and multiply the determinant by $v(x; \lambda + M\delta)$. (iv) Rewrite $v(x; \lambda')/v(x; \lambda + M\delta)$ in the $(M + 1)$ th column of $\det(a_{j,k})$ using Eq. (3.26). (v) Multiply the $(M + 1)$ th column of $\det(a_{j,k})$ by $\prod_{m=1}^M \check{U}(x; \lambda + (M - 2m)\delta)$, and divide the determinant by $\prod_{m=1}^M \check{U}(x; \lambda + (M - 2m)\delta)$. Then $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are expressed in terms of $\check{\xi}_v(x; \lambda')$, $\check{P}_n(x; \lambda')$, $\check{U}(x; \lambda')$, $\check{S}(x; \lambda')$, and $\varphi(x')$. Straightforward calculation shows that the factors $\varphi(x')$ are canceled out. Thus $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are expressed in terms of $\eta(x)$, namely, $\Xi_{\mathcal{D}}(\eta; \lambda)$ and $P_{\mathcal{D},n}(\eta; \lambda)$ are expressed without explicit x -dependence. Their final forms are as follows. The denominator polynomial $\Xi_{\mathcal{D}}(\eta; \lambda)$ is

$$\begin{aligned} \Xi_{\mathcal{D}}(\eta; \lambda) &= (-1)^{\frac{1}{6}(M-1)M(M+1)} \left(\prod_{m=1}^{\lfloor \frac{M}{2} \rfloor} S(\eta; t(\lambda) + (M - 1 - 2m)\delta) \right)^{-1} \\ &\quad \times \det(a_{j,k})_{1 \leq j,k \leq M}, \end{aligned} \tag{3.86}$$

where $a_{j,k}$ are

$$\begin{aligned} a_{j,k} &= \prod_{m=0}^{M-2j} f'_{d_k-m}(\lambda + m\tilde{\delta}) \cdot \xi_{d_k-M-1+2j}(\eta; \lambda + (M + 1 - 2j)\tilde{\delta}) \\ &\quad (j = 1, \dots, \lfloor \frac{M+1}{2} \rfloor; k = 1, \dots, M), \\ a_{j,k} &= b'_{d_k-2j+M+2}(\lambda + (2j - M - 3)\tilde{\delta}) \prod_{m=0}^{2j-M-3} f'_{d_k-m}(\lambda + m\tilde{\delta}) \\ &\quad \times \xi_{d_k-2j+M+3}(\eta; \lambda + (2j - M - 3)\tilde{\delta}) \quad (j = \lfloor \frac{M+3}{2} \rfloor, \dots, M; k = 1, \dots, M). \end{aligned} \tag{3.87}$$

The multi-indexed orthogonal polynomial $P_{\mathcal{D},n}(\eta; \lambda)$ is

$$\begin{aligned} P_{\mathcal{D},n}(\eta; \lambda) &= (-1)^{\frac{1}{6}M(M+1)(M+2)} \left(\prod_{m=1}^{\lfloor \frac{M+1}{2} \rfloor} S(\eta; t(\lambda) + (M - 2m)\delta) \right)^{-1} \\ &\quad \times \det(a_{j,k})_{1 \leq j,k \leq M+1}, \end{aligned} \tag{3.88}$$

where $a_{j,k}$ are

$$\begin{aligned} a_{j,k} &= \prod_{m=0}^{M+1-2j} f'_{d_k-m}(\lambda + m\tilde{\delta}) \cdot \xi_{d_k-M-2+2j}(\eta; \lambda + (M + 2 - 2j)\tilde{\delta}) \\ &\quad (j = 1, \dots, \lfloor \frac{M+2}{2} \rfloor; k = 1, \dots, M), \\ a_{j,k} &= b'_{d_k-2j+M+3}(\lambda + (2j - M - 4)\tilde{\delta}) \prod_{m=0}^{2j-M-4} f'_{d_k-m}(\lambda + m\tilde{\delta}) \\ &\quad \times \xi_{d_k-2j+M+4}(\eta; \lambda + (2j - M - 4)\tilde{\delta}) \quad (j = \lfloor \frac{M+4}{2} \rfloor, \dots, M + 1; k = 1, \dots, M), \\ a_{j,M+1} &= \prod_{m=0}^{M+1-2j} \tilde{f}'_n(\lambda + m\tilde{\delta}) \cdot \prod_{l=M+2-j}^M U(\eta; \lambda + (M - 2l)\delta) \cdot P_n(\eta; \lambda + (M + 2 - 2j)\tilde{\delta}) \end{aligned}$$

$$(j = 1, \dots, \lceil \frac{M+2}{2} \rceil), \tag{3.89}$$

$$a_{j,M+1} = \tilde{b}'_n(\lambda + (2j - M - 4)\tilde{\delta}) \prod_{m=0}^{2j-M-4} \tilde{f}'_n(\lambda + m\tilde{\delta}) \cdot \prod_{l=j-1}^M U(\eta; \lambda + (M - 2l)\delta) \\ \times P_n(\eta; \lambda + (2j - M - 4)\tilde{\delta}) \quad (j = \lceil \frac{M+4}{2} \rceil, \dots, M + 1).$$

Case B

Second we consider case B in Eq. (3.83). The functions $q_j(x)$, $r_j(x)$, $q'_j(x)$, $r'_j(x)$, and $D_j(x)$ are ($l = 1, 2, \dots$)

$$q_{2l-1}(x) = i\varphi(x)^{-1}, \quad r_{2l-1}(x) = -i\varphi(x)^{-1}, \\ q_{2l}(x) = -iV(x; t(\lambda))\varphi(x - i\frac{\gamma}{2}), \quad r_{2l}(x) = iV^*(x; t(\lambda))\varphi(x + i\frac{\gamma}{2}), \\ q'_{2l-1}(x) = -iV(x; t(\lambda) - \delta)\varphi(x - i\frac{\gamma}{2}), \quad r'_{2l-1} = iV^*(x; t(\lambda) - \delta)\varphi(x + i\frac{\gamma}{2}), \tag{3.90} \\ q'_{2l}(x) = i\varphi(x)^{-1}, \quad r'_{2l}(x) = -i\varphi(x)^{-1}, \\ D_{2l-1}(x) = -i\varphi(x)^{-1}\check{S}(x; t(\lambda) - \delta), \quad D_{2l}(x) = i\varphi(x)^{-1}\check{S}(x; t(\lambda)).$$

The shape-invariance properties (3.78)–(3.79) give ($l = 1, 2, \dots$)

$$\prod_{m=1}^{\overleftarrow{2l-2}} \hat{D}_m \cdot \check{\xi}_v(x; \lambda) = \mathcal{E}'_v(\lambda)^{l-1} \check{\xi}_v(x; \lambda), \\ \prod_{m=1}^{\overleftarrow{2l-1}} \hat{D}_m \cdot \check{\xi}_v(x; \lambda) = f'_v(\lambda) \mathcal{E}'_v(\lambda)^{l-1} \check{\xi}_{v-1}(x; \lambda + \tilde{\delta}), \\ \prod_{m=1}^{\overleftarrow{2l-2}} \hat{D}_m \cdot (v\check{P}_n)(x; \lambda) = \tilde{\mathcal{E}}'_n(\lambda)^{l-1} (v\check{P}_n)(x; \lambda), \\ \prod_{m=1}^{\overleftarrow{2l-1}} \hat{D}_m \cdot (v\check{P}_n)(x; \lambda) = \tilde{f}'_n(\lambda) \tilde{\mathcal{E}}'_n(\lambda)^{l-1} (v\check{P}_n)(x; \lambda + \tilde{\delta}), \tag{3.91} \\ \hat{D}'_{2l-1} \prod_{m=1}^{\overleftarrow{2l-2}} \hat{D}_m \cdot \check{\xi}_v(x; \lambda) = b'_v(\lambda - \tilde{\delta}) \mathcal{E}'_v(\lambda)^{l-1} \check{\xi}_{v+1}(x; \lambda - \tilde{\delta}), \\ \hat{D}'_{2l} \prod_{m=1}^{\overleftarrow{2l-1}} \hat{D}_m \cdot \check{\xi}_v(x; \lambda) = f'_{v-1}(\lambda + \tilde{\delta}) f'_v(\lambda) \mathcal{E}'_v(\lambda)^{l-1} \check{\xi}_{v-2}(x; \lambda + 2\tilde{\delta}), \\ \hat{D}'_{2l-1} \prod_{m=1}^{\overleftarrow{2l-2}} \hat{D}_m \cdot (v\check{P}_n)(x; \lambda) = \tilde{b}'_n(\lambda - \tilde{\delta}) \tilde{\mathcal{E}}'_n(\lambda)^{l-1} (v\check{P}_n)(x; \lambda - \tilde{\delta}), \\ \hat{D}'_{2l} \prod_{m=1}^{\overleftarrow{2l-1}} \hat{D}_m \cdot (v\check{P}_n)(x; \lambda) = \tilde{f}'_n(\lambda + \tilde{\delta}) \tilde{f}'_n(\lambda) \tilde{\mathcal{E}}'_n(\lambda)^{l-1} (v\check{P}_n)(x; \lambda + 2\tilde{\delta}).$$

Like case A, we rewrite Eqs. (3.80)–(3.81) using steps (i)–(v). In (v), multiply and divide by $\prod_{l=1}^{\lceil \frac{M+2}{2} \rceil} \check{U}(x; \lambda + (M - 2l)\delta)$. Using Eqs. (3.14) and (3.69), $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are expressed

in terms of $\check{\xi}_v(x; \lambda')$, $\check{P}_n(x; \lambda')$, $\check{U}(x; \lambda')$, $\check{S}(x; \lambda')$, and $\varphi(x')$. Straightforward calculation shows that the factors $\varphi(x')$ are canceled out. Thus $\check{\Xi}_{\mathcal{D}}(x; \lambda)$ and $\check{P}_{\mathcal{D},n}(x; \lambda)$ are expressed in terms of $\eta(x)$, namely, $\Xi_{\mathcal{D}}(\eta; \lambda)$ and $P_{\mathcal{D},n}(\eta; \lambda)$ are expressed without explicit x -dependence. Their final forms are as follows. The denominator polynomial $\Xi_{\mathcal{D}}(\eta; \lambda)$ is

$$\begin{aligned} \Xi_{\mathcal{D}}(\eta; \lambda) &= (-1)^{\lfloor \frac{M}{2} \rfloor} (\alpha^t(\lambda) \alpha^{\bar{t}}(\lambda)^{-1} \kappa)^{\frac{1}{2} \lfloor \frac{M-2}{2} \rfloor \lfloor \frac{M}{2} \rfloor} \det(a_{j,k})_{1 \leq j,k \leq M} \\ &\quad \times \left(\prod_{m=\lfloor \frac{M+3}{2} \rfloor}^M U(\eta; \lambda + (M-1-2m)\delta)^{M-m} \cdot \prod_{m=0}^{\lfloor \frac{M-2}{2} \rfloor} U^{\bar{t}}(\eta; \lambda + (M-1-2m)\delta)^m \right. \\ &\quad \left. \times S(\eta; \mathfrak{t}(\lambda) - \frac{1}{2}(1 + (-1)^M)\delta)^{\lfloor \frac{M}{2} \rfloor} \right)^{-1}, \end{aligned} \tag{3.92}$$

where \mathfrak{t} is the type of the indices of \mathcal{D} , and $a_{j,k}$ are

$$\begin{aligned} a_{j,k} &= \mathcal{E}'_{d_k}(\lambda)^{\frac{M+1}{2}-j} \xi_{d_k}(\eta; \lambda) \quad (j = 1, \dots, \frac{M+1}{2}; k = 1, \dots, M), \\ a_{j,k} &= f'_{d_{k-1}}(\lambda + \tilde{\delta}) f'_{d_k}(\lambda) \mathcal{E}'_{d_k}(\lambda)^{j-\frac{M+3}{2}} \xi_{d_{k-2}}(\eta; \lambda + 2\tilde{\delta}) \quad (j = \frac{M+3}{2}, \dots, M; k = 1, \dots, M) \end{aligned} \tag{3.93}$$

for odd M , and

$$\begin{aligned} a_{j,k} &= f'_{d_k}(\lambda) \mathcal{E}'_{d_k}(\lambda)^{\frac{M}{2}-j} \xi_{d_{k-1}}(\eta; \lambda + \tilde{\delta}) \quad (j = 1, \dots, \frac{M}{2}; k = 1, \dots, M), \\ a_{j,k} &= b'_{d_k}(\lambda - \tilde{\delta}) \mathcal{E}'_{d_k}(\lambda)^{j-\frac{M+2}{2}} \xi_{d_{k+1}}(\eta; \lambda - \tilde{\delta}) \quad (j = \frac{M+2}{2}, \dots, M; k = 1, \dots, M) \end{aligned} \tag{3.94}$$

for even M . The multi-indexed orthogonal polynomial $P_{\mathcal{D},n}(\eta; \lambda)$ is

$$\begin{aligned} P_{\mathcal{D},n}(\eta; \lambda) &= (-1)^{\lfloor \frac{M+1}{2} \rfloor} (\alpha^t(\lambda) \alpha^{\bar{t}}(\lambda)^{-1} \kappa)^{\frac{1}{2} \lfloor \frac{M-1}{2} \rfloor \lfloor \frac{M+1}{2} \rfloor} \det(a_{j,k})_{1 \leq j,k \leq M+1} \\ &\quad \times \left(\prod_{m=\lfloor \frac{M+4}{2} \rfloor}^M U(\eta; \lambda + (M-2m)\delta)^{M-m} \cdot \prod_{m=0}^{\lfloor \frac{M-1}{2} \rfloor} U^{\bar{t}}(\eta; \lambda + (M-2m)\delta)^m \right. \\ &\quad \left. \times S(\eta; \mathfrak{t}(\lambda) - \frac{1}{2}(1 - (-1)^M)\delta)^{\lfloor \frac{M+1}{2} \rfloor} \right)^{-1}, \end{aligned} \tag{3.95}$$

where \mathfrak{t} is the type of the indices of \mathcal{D} , and $a_{j,k}$ are

$$\begin{aligned} a_{j,k} &= \mathcal{E}'_{d_k}(\lambda)^{\frac{M+2}{2}-j} \xi_{d_k}(\eta; \lambda) \quad (j = 1, \dots, \frac{M+2}{2}; k = 1, \dots, M), \\ a_{j,k} &= f'_{d_{k-1}}(\lambda + \tilde{\delta}) f'_{d_k}(\lambda) \mathcal{E}'_{d_k}(\lambda)^{j-\frac{M+4}{2}} \xi_{d_{k-2}}(\eta; \lambda + 2\tilde{\delta}) \\ &\quad (j = \frac{M+4}{2}, \dots, M+1; k = 1, \dots, M), \\ a_{j,M+1} &= \tilde{\mathcal{E}}'_n(\lambda)^{\frac{M+2}{2}-j} U(\eta; \lambda - 2\tilde{\delta}) P_n(\eta; \lambda) \quad (j = 1, \dots, \frac{M+2}{2}), \\ a_{j,M+1} &= \tilde{f}'_n(\lambda + \tilde{\delta}) \tilde{f}'_n(\lambda) \tilde{\mathcal{E}}'_n(\lambda)^{j-\frac{M+4}{2}} P_n(\eta; \lambda + 2\tilde{\delta}) \quad (j = \frac{M+4}{2}, \dots, M+1) \end{aligned} \tag{3.96}$$

for even M , and

$$\begin{aligned} a_{j,k} &= f'_{d_k}(\lambda) \mathcal{E}'_{d_k}(\lambda)^{\frac{M+1}{2}-j} \xi_{d_{k-1}}(\eta; \lambda + \tilde{\delta}) \quad (j = 1, \dots, \frac{M+1}{2}; k = 1, \dots, M), \\ a_{j,k} &= b'_{d_k}(\lambda - \tilde{\delta}) \mathcal{E}'_{d_k}(\lambda)^{j-\frac{M+3}{2}} \xi_{d_{k+1}}(\eta; \lambda - \tilde{\delta}) \quad (j = \frac{M+3}{2}, \dots, M+1; k = 1, \dots, M), \end{aligned}$$

$$\begin{aligned}
 a_{j,M+1} &= \tilde{f}'_n(\lambda) \tilde{\mathcal{E}}'_n(\lambda)^{\frac{M+1}{2}-j} P_n(\eta; \lambda + \tilde{\delta}) \quad (j = 1, \dots, \frac{M+1}{2}), \\
 a_{j,M+1} &= \tilde{b}'_n(\lambda - \tilde{\delta}) \tilde{\mathcal{E}}'_n(\lambda)^{j-\frac{M+3}{2}} U(\eta; \lambda - \delta) P_n(\eta; \lambda - \tilde{\delta}) \quad (j = \frac{M+3}{2}, \dots, M+1)
 \end{aligned}
 \tag{3.97}$$

for odd M .

4. Summary and comments

Multi-indexed orthogonal polynomials (the Meixner, little q -Laguerre, little q -Jacobi, Racah, q -Racah, Wilson, and Askey–Wilson types) introduced in the framework of discrete quantum mechanics are expressed in terms of Casoratians. Various new determinant expressions of the multi-indexed orthogonal polynomials are derived by using the properties of the Casoratians and shape invariance. Two typical cases are presented explicitly. For the Meixner, little q -Laguerre, little q -Jacobi, Wilson, and Askey–Wilson cases, the new expressions for the multi-indexed polynomials $P_{\mathcal{D},n}(\eta)$ do not have explicit dependence on x , which is the coordinate of the quantum system. We hope that these new expressions are helpful in achieving a deeper understanding of multi-indexed orthogonal polynomials.

In Ref. [42], simplified expressions of the multi-indexed Laguerre and Jacobi polynomials are derived. From the viewpoint adopted in this paper, the calculation in Ref. [42] is regarded as follows. The eigenfunctions of the deformed systems, namely the multi-indexed orthogonal polynomials, are expressed in terms of the Wronskian. The Wronskian of a set of n functions $\{f_j(x)\}$ is defined by

$$W[f_1, f_2, \dots, f_n](x) \stackrel{\text{def}}{=} \det\left(\frac{d^{j-1}f_k(x)}{dx^{j-1}}\right)_{1 \leq j, k \leq n}
 \tag{4.1}$$

(for $n = 0$, we set $W[\cdot](x) = 1$), and the following formula holds for any smooth functions $q_j(x)$ ($j = 1, 2, \dots$):

$$\det\left(\prod_{l=1}^{j-1} \hat{D}_l \cdot f_k(x)\right)_{1 \leq j, k \leq n} = W[f_1, \dots, f_n](x), \quad \hat{D}_j = \frac{d}{dx} - q_j(x).
 \tag{4.2}$$

The original systems have shape invariance $\mathcal{A}(\lambda)\mathcal{A}(\lambda)^\dagger = \mathcal{A}(\lambda + \delta)^\dagger\mathcal{A}(\lambda + \delta) + \mathcal{E}_1(\lambda)$, where $\mathcal{A}(\lambda) = \frac{d}{dx} - \frac{d}{dx} \log \phi_0(x; \lambda)$ and $\mathcal{A}(\lambda)^\dagger = -\frac{d}{dx} - \frac{d}{dx} \log \phi_0(x; \lambda)$. These operators act on the eigenstates and virtual states as

$$\mathcal{A}(\lambda)\phi_n(x; \lambda) = f_n(\lambda)\phi_{n-1}(x; \lambda + \delta), \quad \mathcal{A}(\lambda)^\dagger\phi_{n-1}(x; \lambda + \delta) = b_{n-1}(\lambda)\phi_n(x; \lambda),
 \tag{4.3}$$

$$\mathcal{A}(\lambda)\tilde{\phi}_v(x; \lambda) = \tilde{f}_v(\lambda)\tilde{\phi}_v(x; \lambda + \delta), \quad \mathcal{A}(\lambda)^\dagger\tilde{\phi}_v(x; \lambda + \delta) = \tilde{b}_v(\lambda)\tilde{\phi}_v(x; \lambda),
 \tag{4.4}$$

where

$$f_n(\lambda) = \begin{cases} -2 & : \text{L}, \\ -2(n + g + h) & : \text{J}, \end{cases} \quad b_{n-1}(\lambda) = -2n : \text{L, J},
 \tag{4.5}$$

$$\tilde{f}_v(\lambda) = \begin{cases} 2 & : \text{L, I}, \\ -2(g - \frac{1}{2} - v) & : \text{L, II}, \\ 2(h - \frac{1}{2} - v) & : \text{J, I}, \\ -2(g - \frac{1}{2} - v) & : \text{J, II}, \end{cases} \quad \tilde{b}_v(\lambda) = \begin{cases} -2(g + \frac{1}{2} + v) & : \text{L, I}, \\ 2 & : \text{L, II}, \\ -2(g + \frac{1}{2} + v) & : \text{J, I}, \\ 2(h + \frac{1}{2} + v) & : \text{J, II}. \end{cases}
 \tag{4.6}$$

By taking \mathcal{A} or \mathcal{A}^\dagger as \hat{D}_j in Eq. (4.2) and using the shape-invariant properties (4.3)–(4.4), the Wronskians can be rewritten in various ways. Two typical cases are studied in Ref. [42]:

$$A : \hat{D}_j = \mathcal{A}(\lambda + (j - 1)\delta) \quad (j = 1, 2, \dots), \quad (4.7)$$

$$B : \hat{D}_{2l-1} = \mathcal{A}(\lambda), \quad \hat{D}_{2l} = -\mathcal{A}(\lambda)^\dagger \quad (l = 1, 2, \dots). \quad (4.8)$$

Like Sect. 3.5.4, the equivalence property (3.76) holds (Refs. [48,49]) and simplifications occur for the index set with a single type. This calculation is left to readers as an exercise.

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