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Multi-indexed (q)-Racah Polynomials

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Abstract

As the second stage of the project *multi-indexed orthogonal polynomials*, we present, in the framework of 'discrete quantum mechanics' with real shifts in one dimension, the multi-indexed (q)-Racah polynomials. They are obtained from the (q)-Racah polynomials by multiple application of the discrete analogue of the Darboux transformations or the Crum-Krein-Adler deletion of 'virtual state' vectors of type I and II, in a similar way to the multi-indexed Laguerre and Jacobi polynomials reported earlier. The virtual state vectors are the 'solutions' of the matrix Schrödinger equation with negative 'eigenvalues', except for one of the two boundary points.

1 Introduction

This is a second report of the project *multi-indexed orthogonal polynomials*. Following the examples of multi-indexed Laguerre and Jacobi polynomials [1], multi-indexed (q)-Racah polynomials are constructed in the framework of discrete quantum mechanics with real shifts [2]. It should be emphasised that the original (q)-Racah polynomials are the most generic members of the Askey scheme of hypergeometric orthogonal polynomials with purely discrete orthogonality measures [3, 4, 5, 6]. They are also called orthogonal polynomials of a discrete variable [7]. These new multi-indexed orthogonal polynomials are specified by a set of indices $\mathcal{D} = \{d_1, \dots, d_M\}$ consisting of distinct natural numbers $d_j \in \mathbb{N}$, on top of n, which counts the nodes as in the ordinary orthogonal polynomials. The simplest examples, $\mathcal{D} = \{\ell\}$, $\ell \geq 1$, $\{P_{\ell,n}(x)\}$ are also called *exceptional orthogonal polynomials* [8]–[27]. They are obtained as the

main part of the eigenfunctions (vectors) of various *exactly solvable* Schrödinger equations in one dimensional quantum mechanics and their 'discrete' generalisations, in which the corresponding Schrödinger equations are second order difference equations [2, 28, 29]. They form a complete set of orthogonal polynomials, although they start at a certain positive degree ($\ell \geq 1$) rather than a degree zero constant term. The latter situation is essential for avoiding the constraints of Bochner's theorem [30]. The exceptional Laguerre polynomials with two extra indices $\mathcal{D} = \{d_1, d_2\}$ were introduced in [31]. We are quite sure that these new orthogonal polynomials will find plenty of novel applications in various branches of science and technology as other orthogonal polynomials. One obvious application is the birth and death processes [32]. These new orthogonal polynomials provide huge stocks of *exactly solvable birth and death processes* [33]. The transition probabilities are given explicitly, not in a general spectral representation form of Karlin-McGregor [34]. An interesting possible application is to one-dimensional spin systems and quantum information theory [35].

The basic logic for constructing multi-indexed orthogonal polynomials is essentially the same for the ordinary Schrödinger equations, *i.e.* those for the Laguerre and Jacobi polynomials and for the difference Schrödinger equations with real shifts, *i.e.* the (q)-Racah polynomials, etc. The main ingredients are the factorised Hamiltonians, the Crum-Krein-Adler formulas [36, 37, 38] for deletion of eigenstates, *that is* the multiple Darboux transformations [39] and the virtual states solutions [1] which are generated by twisting the discrete symmetries of the original Hamiltonians. Most of these methods for discrete Schrödinger equations had been developed [2, 26, 28, 29, 40, 41, 42] and they were used for the exceptional (q)-Racah polynomials [23]. The concept of virtual state 'solutions' requires special explanation in the present case. In the ordinary quantum mechanics cases, the virtual state solutions are the solutions of the Schrödinger equation but they do not belong to the Hilbert space of square integrable functions due to the twisted boundary conditions. In the present case, the Hamiltonians are finite-dimensional real symmetric tri-diagonal matrices. Therefore the eigenvalue equations for a given Hamiltonian matrix cannot have any extra solutions other than the genuine eigenvectors. Thus we will use the term *virtual state vectors*. As will be shown in the text, virtual state vectors are the 'solutions' of the eigenvalue problem for a *virtual* Hamiltonian $\mathcal{H}'$, except for one of the boundaries, $x = x_{\max}$ (2.24) or 0 (2.65). The virtual Hamiltonians are obtained from the original Hamiltonian by twisting the discrete symmetry and they are linearly related to the original Hamiltonian (2.21) and (2.62). Thus

the virtual state vectors 'satisfy' the eigenvalue equation for the original Hamiltonian, except for one of the two boundaries. Corresponding to the two boundary points $x = x_{\max}$ (2.23) and $x = 0$ (2.64), we have type I and II virtual state vectors, as in the ordinary quantum mechanical cases. The polynomial part of the type I virtual state vectors had been used for the exceptional (q)-Racah polynomials. But the type II virtual state vectors are new. One distinctive feature of virtual states deletion in discrete quantum mechanics with real shifts is that the size of the Hamiltonian matrix ($x_{\max}$) remains the same. This is in marked contrast with the eigenstates deletion (Christoffel transformations [3, 42]), in which case the size decreases by the number of deleted eigenstates.

This paper is organised as follows. In section two, the basic logic of virtual states deletion in discrete quantum mechanics with real shifts in general is outlined. Starting from the general setting of discrete quantum mechanics with real shifts in § 2.1, two types of factorisation are introduced. General procedures and formulas of multiple virtual states deletion are explained in § 2.2.1 for the type I and in § 2.2.2 for the type II. In § 2.2.3 it is shown that these two types of virtual state vectors cannot be used simultaneously in contradistinction with the multi-indexed Laguerre and Jacobi cases in [1]. After recapitulating the basic properties of the (q)-Racah systems in § 3.1, the multi-indexed (q)-Racah polynomials are constructed explicitly in § 3.2 for the type I and in § 3.3 for the type II virtual states deletion. Various formulas connecting the type I and II virtual states are collected in § 3.4. The final section is for a summary and comments.

2 Formulation

2.1 Original system

Let us recapitulate the discrete quantum mechanics with real shifts developed in [2]. We restrict ourselves to the finite dimensional matrix case, $x_{\max} = N$.

The Hamiltonian $\mathcal{H} = (\mathcal{H}_{x,y})$ is a tri-diagonal real symmetric (Jacobi) matrix and its rows and columns are indexed by non-negative integers x and y, $x, y = 0, 1, \ldots, x_{\max}$. By adding a scalar matrix to the Hamiltonian, the lowest eigenvalue is assumed to be zero. This makes the Hamiltonian *positive semi-definite*. Since the eigenvector corresponding to the zero eigenvalue has definite sign, i.e., all the components are positive or negative, the

Hamiltonian $\mathcal{H}$ has the following form

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

in which the potential functions $B(x)$ and $D(x)$ are real and positive but vanish at the boundary:

$$\begin{aligned} &B(x) > 0 \quad (x = 0, 1, \ldots, x_{\max} - 1), \quad B(x_{\max}) = 0, \\ &D(x) > 0 \quad (x = 1, 2, \ldots, x_{\max}), \quad D(0) = 0. \end{aligned} \tag{2.2}$$

The Schrödinger equation is the eigenvalue problem for the hermitian matrix $\mathcal{H}$,

$$\mathcal{H}\phi_n(x) = \mathcal{E}_n\phi_n(x) \quad (n = 0, 1, \ldots, n_{\max}), \quad 0 = \mathcal{E}_0 < \mathcal{E}_1 < \cdots < \mathcal{E}_{n_{\max}}, \tag{2.3}$$

where the eigenvector is $\phi_n = (\phi_n(x))_{x=0,1,\ldots,x_{\max}}$ and $n_{\max} = N$. Reflecting the positive semi-definiteness and based on the boundary conditions (2.2), the Hamiltonian (2.1) can be expressed in a factorised form (type-(i) factorisation):

$$\mathcal{H} = \mathcal{A}^\dagger\mathcal{A}, \qquad \mathcal{A} = (\mathcal{A}_{x,y}), \quad \mathcal{A}^\dagger = ((\mathcal{A}^\dagger)_{x,y}) = (\mathcal{A}_{y,x}), \quad (x, y = 0, 1, \ldots, x_{\max}), \tag{2.4}$$

$$\mathcal{A}_{x,y} \stackrel{\text{def}}{=} \sqrt{B(x)}\,\delta_{x,y} - \sqrt{D(x+1)}\,\delta_{x+1,y}, \quad (\mathcal{A}^\dagger)_{x,y} = \sqrt{B(x)}\,\delta_{x,y} - \sqrt{D(x)}\,\delta_{x-1,y}. \tag{2.5}$$

Here $\mathcal{A}$ ($\mathcal{A}^\dagger$) is an upper (lower) triangular matrix with the diagonal and the super(sub)-diagonal entries only. The zero mode equation, $\mathcal{A}\phi_0 = 0$, is

$$\sqrt{B(x)}\,\phi_0(x) - \sqrt{D(x+1)}\,\phi_0(x+1) = 0 \quad (x = 0, 1, \ldots, x_{\max} - 1), \tag{2.6}$$

$$\sqrt{B(x_{\max})}\,\phi_0(x_{\max}) = 0, \tag{2.7}$$

and the second equation is trivially satisfied by the boundary condition $B(x_{\max}) = 0$. The groundstate eigenvector is easily obtained:

$$\phi_0(x) = \sqrt{\prod_{y=0}^{x-1} \frac{B(y)}{D(y+1)}} \quad (x = 0, 1, \ldots, x_{\max}), \tag{2.8}$$

with the normalisation $\phi_0(0) = 1$ (convention: $\prod_{k=n}^{n-1} * = 1$). Needless to say it is positive for $x = 0, 1, \ldots, x_{\max}$. For the explicit examples treated in [2], $\phi_0^2(x)$ can be analytically continued to the entire complex x-plane as a meromorphic function and it vanishes on the

integer points outside the boundary; $\phi_0^2(x) = 0$ ($x \in \mathbb{Z}\backslash\{0, 1, \ldots, x_{\max}\}$). The eigenvectors are mutually orthogonal:

$$(\phi_n, \phi_m) \stackrel{\text{def}}{=} \sum_{x=0}^{x_{\max}} \phi_n(x)\phi_m(x) = \frac{1}{d_n^2}\delta_{nm} \quad (n, m = 0, 1, \ldots, n_{\max}). \tag{2.9}$$

We have another factorisation (type-(ii) factorisation):

$$\mathcal{H} = \mathcal{A}^{(\mathrm{ii})\,\dagger}\mathcal{A}^{(\mathrm{ii})},\ \mathcal{A}^{(\mathrm{ii})} = (\mathcal{A}^{(\mathrm{ii})}_{x,y}),\ \mathcal{A}^{(\mathrm{ii})\,\dagger} = ((\mathcal{A}^{(\mathrm{ii})\,\dagger})_{x,y}) = (\mathcal{A}^{(\mathrm{ii})}_{y,x}),\ (x, y = 0, 1, \ldots, x_{\max}), \tag{2.10}$$

$$\mathcal{A}^{(\mathrm{ii})}_{x,y} \stackrel{\text{def}}{=} \sqrt{D(x)}\,\delta_{x,y} - \sqrt{B(x-1)}\,\delta_{x-1,y}, \quad (\mathcal{A}^{(\mathrm{ii})\,\dagger})_{x,y} = \sqrt{D(x)}\,\delta_{x,y} - \sqrt{B(x)}\,\delta_{x+1,y}. \tag{2.11}$$

Now $\mathcal{A}^{(\mathrm{ii})}$ ($\mathcal{A}^{(\mathrm{ii})\,\dagger}$) is lower (upper) triangular.

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

$$e^{\pm\partial} = ((e^{\pm\partial})_{x,y}) \quad (x, y = 0, 1, \ldots, x_{\max}), \quad (e^{\pm\partial})_{x,y} \stackrel{\text{def}}{=} \delta_{x\pm1,y}, \quad (e^{\partial})^\dagger = e^{-\partial}, \tag{2.12}$$

$$\begin{aligned}\mathcal{H} &= -\sqrt{B(x)}\,e^{\partial}\sqrt{D(x)} - \sqrt{D(x)}\,e^{-\partial}\sqrt{B(x)} + B(x) + D(x) \\ &= -\sqrt{B(x)D(x+1)}\,e^{\partial} - \sqrt{B(x-1)D(x)}\,e^{-\partial} + B(x) + D(x),\end{aligned} \tag{2.13}$$

$$\mathcal{A} = \sqrt{B(x)} - e^{\partial}\sqrt{D(x)}, \quad \mathcal{A}^\dagger = \sqrt{B(x)} - \sqrt{D(x)}\,e^{-\partial}, \tag{2.14}$$

$$\mathcal{A}^{(\mathrm{ii})} = \sqrt{D(x)} - e^{-\partial}\sqrt{B(x)}, \quad \mathcal{A}^{(\mathrm{ii})\,\dagger} = \sqrt{D(x)} - \sqrt{B(x)}\,e^{\partial}. \tag{2.15}$$

For the Schrödinger equation (2.3), it is sufficient that the functions $B(x)$, $D(x)$ and $\phi_n(x)$ are defined only for the integer grid, $x = 0, 1, \ldots, x_{\max}$. In this paper we consider the case that the potential functions $B(x)$ and $D(x)$ are rational functions of x or q^x ($0 < q < 1$). So they are defined for any $x \in \mathbb{C}$ (except for the zeros of their denominators). Also we consider the eigenvectors in a factorised form:

$$\phi_n(x) = \phi_0(x)\check{P}_n(x), \quad \check{P}_n(x) \stackrel{\text{def}}{=} P_n(\eta(x)). \tag{2.16}$$

Here $P_n(\eta)$ is a polynomial of degree n in η and the sinusoidal coordinate $\eta(x)$ is one of the following [2]; $\eta(x) = x, \epsilon' x(x+d), 1-q^x, q^{-x}-1, \epsilon'(q^{-x}-1)(1-dq^x)$, ($\epsilon' = \pm1$). Since P_n is a polynomial, $\check{P}_n(x)$ is defined for any $x \in \mathbb{C}$. The Schrödinger equation (2.3) gives the difference equation for the polynomial eigenvector $\check{P}_n(x)$,

$$B(x)\big(\check{P}_n(x) - \check{P}_n(x+1)\big) + D(x)\big(\check{P}_n(x) - \check{P}_n(x-1)\big) = \mathcal{E}_n\check{P}_n(x) \quad (\forall x \in \mathbb{C}). \tag{2.17}$$

2.2 Deletion of virtual state vectors

In [42] we have presented the Crum-Adler scheme, *i.e,* the deletion of M eigenstates, which corresponds to Christoffel transformations [3]. The index set of the deleted eigenstates $\mathcal{D} \stackrel{\text{def}}{=} \{d_1, d_2, \ldots, d_M\}$ $(0 \le d_j \le n_{\max})$[1] should satisfy the condition $\prod_{j=1}^{M}(m - d_j) \ge 0$ $(\forall m \in \mathbb{Z}_{\ge 0})$, eq. (4.1) in [42] and the size of the Hamiltonian matrix changes from $x_{\max}$ to $x_{\max}^M = x_{\max} - M$.

We apply the Crum-Adler scheme to virtual state vectors instead of eigenvectors. Since all the eigenvalues remain the same, *i.e.* the process is *exactly iso-spectral deformation*, the size of the Hamiltonian is unchanged and the above condition eq. (4.1) in [42] is unnecessary.

We present two kinds of virtual states, the type I and type II and construct the corresponding multi-indexed orthogonal polynomials. As shown in §2.2.3 the type I and II virtual states cannot be used simultaneously.

2.2.1 type I

In this subsection we use the type-(i) factorisation. The Casorati determinant of a set of n functions $\{f_j(x)\}$ is defined by

$$\mathrm{W}[f_1, \ldots, f_n](x) \stackrel{\text{def}}{=} \det\Big(f_k(x+j-1)\Big)_{1\le j,k\le n},$$

(for $n = 0$, we set $\mathrm{W}[\cdot](x) = 1$), which satisfies identities

$$\begin{aligned}
&\mathrm{W}[gf_1, gf_2, \ldots, gf_n](x) = \prod_{k=0}^{n-1} g(x+k) \cdot \mathrm{W}[f_1, f_2, \ldots, f_n](x),\\
&\mathrm{W}\big[\mathrm{W}[f_1, f_2, \ldots, f_n, g], \mathrm{W}[f_1, f_2, \ldots, f_n, h]\,\big](x)\\
&= \mathrm{W}[f_1, f_2, \ldots, f_n](x+1)\,\mathrm{W}[f_1, f_2, \ldots, f_n, g, h](x) \quad (n \ge 0).
\end{aligned}$$

Let us assume the existence of two rational functions $B'(x)$ and $D'(x)$ of x or q^x satisfying

$$B(x)D(x+1) = \alpha^2 B'(x)D'(x+1), \qquad \alpha > 0, \tag{2.18}$$

$$B(x) + D(x) = \alpha\big(B'(x) + D'(x)\big) + \alpha', \qquad \alpha' < 0, \tag{2.19}$$

$$\begin{aligned}
&B'(x) > 0 \quad (x = 0, 1, \ldots, x_{\max} + L - 1),\\
&D'(x) > 0 \quad (x = 1, 2, \ldots, x_{\max}), \quad D'(0) = D'(x_{\max}+1) = 0,
\end{aligned} \tag{2.20}$$

[1] Although this notation d_j conflicts with the notation of the normalisation constant d_n in (2.9), we think this does not cause any confusion because the latter appears as $\frac{1}{d_n^2}\,\delta_{nm}$.

where α and α' are constants and L is a certain positive integer to be specified later. This type of identities appear repeatedly in the text and they allow to rewrite one Hamiltonian into another form. Here we obtain a linear relation between two Hamiltonians:

$$\mathcal{H} = \alpha\mathcal{H}' + \alpha', \tag{2.21}$$

$$\mathcal{H}' \stackrel{\text{def}}{=} -\sqrt{B'(x)}\, e^{\partial}\sqrt{D'(x)} - \sqrt{D'(x)}\, e^{-\partial}\sqrt{B'(x)} + B'(x) + D'(x). \tag{2.22}$$

Let us also assume the existence of *virtual state vectors* $\tilde{\phi}_{\mathrm{v}}(x)$ $(x = 0, 1, \ldots, x_{\max};\ \mathrm{v} \in \mathcal{V})$, which are polynomial 'solutions' of the Schrödinger equation *except for one end-point*:

$$\mathcal{H}\tilde{\phi}_{\mathrm{v}}(x) = \tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\phi}_{\mathrm{v}}(x) \quad (x = 0, 1, \ldots, x_{\max} - 1), \quad \mathcal{H}\tilde{\phi}_{\mathrm{v}}(x_{\max}) \neq \tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\phi}_{\mathrm{v}}(x_{\max}), \tag{2.23}$$

or equivalently,

$$\mathcal{H}'\tilde{\phi}_{\mathrm{v}}(x) = \mathcal{E}'_{\mathrm{v}}\tilde{\phi}_{\mathrm{v}}(x) \quad (x = 0, 1, \ldots, x_{\max} - 1), \quad \mathcal{H}'\tilde{\phi}_{\mathrm{v}}(x_{\max}) \neq \mathcal{E}'_{\mathrm{v}}\tilde{\phi}_{\mathrm{v}}(x_{\max}), \tag{2.24}$$

$$\tilde{\mathcal{E}}_{\mathrm{v}} \stackrel{\text{def}}{=} \alpha\mathcal{E}'_{\mathrm{v}} + \alpha'. \tag{2.25}$$

Here $\mathcal{V}$ is the index set of the virtual state vectors. They have a factorised form

$$\tilde{\phi}_{\mathrm{v}}(x) = \tilde{\phi}_0(x)\check{\xi}_{\mathrm{v}}(x), \quad \check{\xi}_{\mathrm{v}}(x) \stackrel{\text{def}}{=} \xi_{\mathrm{v}}(\eta(x)) \quad (x = 0, 1, \ldots, x_{\max}; \mathrm{v} \in \mathcal{V}), \tag{2.26}$$

in which $\xi_{\mathrm{v}}(\eta)$ is a polynomial in the sinusoidal coordinate η. The function $\tilde{\phi}_0(x)$ is defined by

$$\tilde{\phi}_0(x) \stackrel{\text{def}}{=} \sqrt{\prod_{y=0}^{x-1} \frac{B'(y)}{D'(y+1)}} \quad (x = 0, 1, \ldots, x_{\max}). \tag{2.27}$$

We introduce a function $\nu(x)$ by the ratio $\phi_0(x)/\tilde{\phi}_0(x)$:

$$\nu(x) \stackrel{\text{def}}{=} \frac{\phi_0(x)}{\tilde{\phi}_0(x)} = \prod_{y=0}^{x-1} \frac{B(y)}{\alpha B'(y)} = \prod_{y=0}^{x-1} \frac{\alpha D'(y+1)}{D(y+1)} \quad (x = 0, 1, \ldots, x_{\max}). \tag{2.28}$$

It can be analytically continued into a meromorphic function of x or q^x through the functional relations:

$$\nu(x+1) = \frac{B(x)}{\alpha B'(x)}\nu(x), \quad \nu(x-1) = \frac{D(x)}{\alpha D'(x)}\nu(x). \tag{2.29}$$

By $B(x_{\max}) = 0$, it vanishes for integer $x > x_{\max}$, $\nu(x) = 0$ $(x = x_{\max} + 1, x_{\max} + 2, \ldots)$, and at negative integer points it takes nonzero finite values in general. The difference equation

for the virtual state polynomial $\check{\xi}_{\rm v}(x)$, (2.24) is rewritten in the same form as that for the polynomial eigenvector $\check{P}_n(x)$ (2.17):

$$B'(x)\bigl(\check{\xi}_{\rm v}(x)-\check{\xi}_{\rm v}(x+1)\bigr)+D'(x)\bigl(\check{\xi}_{\rm v}(x)-\check{\xi}_{\rm v}(x-1)\bigr)=\mathcal{E}'_{\rm v}\check{\xi}_{\rm v}(x). \tag{2.30}$$

On top of the standard normalisation condition $\check{\xi}_{\rm v}(0)=1$ (v $\in\mathcal{V}$), we require the following conditions:

$$\check{\xi}_{\rm v}(x)>0 \quad (x=0,1,\ldots,x_{\max},x_{\max}+1;{\rm v}\in\mathcal{V}), \tag{2.31}$$

$$\tilde{\mathcal{E}}_{\rm v}<0 \quad ({\rm v}\in\mathcal{V}). \tag{2.32}$$

<u>one virtual state vector deletion</u>

First we rewrite the original Hamiltonian by introducing potential functions $\hat{B}_{d_1}(x)$ and $\hat{D}_{d_1}(x)$ determined by one of the virtual state polynomials $\check{\xi}_{d_1}(x)$ ($d_1\in\mathcal{V}$):

$$\hat{B}_{d_1}(x)\stackrel{\rm def}{=}\alpha B'(x)\frac{\check{\xi}_{d_1}(x+1)}{\check{\xi}_{d_1}(x)},\quad \hat{D}_{d_1}(x)\stackrel{\rm def}{=}\alpha D'(x)\frac{\check{\xi}_{d_1}(x-1)}{\check{\xi}_{d_1}(x)}. \tag{2.33}$$

We have $\hat{B}_{d_1}(x)>0$ ($x=0,1,\ldots,x_{\max}$), $\hat{D}_{d_1}(0)=\hat{D}_{d_1}(x_{\max}+1)=0$, $\hat{D}_{d_1}(x)>0$ ($x=1,2,\ldots,x_{\max}$) and

$$\begin{aligned}&B(x)D(x+1)=\hat{B}_{d_1}(x)\hat{D}_{d_1}(x+1),\\&B(x)+D(x)=\hat{B}_{d_1}(x)+\hat{D}_{d_1}(x)+\tilde{\mathcal{E}}_{d_1},\end{aligned}$$

where use is made of (2.30) in the second equation. The original Hamiltonian reads:

$$\begin{aligned}&\mathcal{H}=\hat{\mathcal{A}}^{\dagger}_{d_1}\hat{\mathcal{A}}_{d_1}+\tilde{\mathcal{E}}_{d_1},\\&\hat{\mathcal{A}}_{d_1}\stackrel{\rm def}{=}\sqrt{\hat{B}_{d_1}(x)}-e^{\partial}\sqrt{\hat{D}_{d_1}(x)},\quad \hat{\mathcal{A}}^{\dagger}_{d_1}=\sqrt{\hat{B}_{d_1}(x)}-\sqrt{\hat{D}_{d_1}(x)}\,e^{-\partial}.\end{aligned}$$

The virtual state vector $\tilde{\phi}_{d_1}(x)$ is almost annihilated by $\hat{\mathcal{A}}_{d_1}$, except for the upper end point:

$$\hat{\mathcal{A}}_{d_1}\tilde{\phi}_{d_1}(x)=0 \quad (x=0,1,\ldots,x_{\max}-1),\quad \hat{\mathcal{A}}_{d_1}\tilde{\phi}_{d_1}(x_{\max})\neq 0.$$

Next let us define a new Hamiltonian $\mathcal{H}_{d_1}$ by changing the order of the two matrices $\hat{\mathcal{A}}^{\dagger}_{d_1}$ and $\hat{\mathcal{A}}_{d_1}$ together with the sets of new eigenvectors $\phi_{d_1 n}(x)$ and new virtual state vectors $\tilde{\phi}_{d_1{\rm v}}(x)$:

$$\mathcal{H}_{d_1}\stackrel{\rm def}{=}\hat{\mathcal{A}}_{d_1}\hat{\mathcal{A}}^{\dagger}_{d_1}+\tilde{\mathcal{E}}_{d_1},\quad \mathcal{H}_{d_1}=(\mathcal{H}_{d_1\,x,y}) \quad (x,y=0,1,\ldots,x_{\max}), \tag{2.34}$$

$$\phi_{d_1 n}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1}\phi_n(x) \quad (x=0,1,\ldots,x_{\max}; n=0,1,\ldots,n_{\max}), \tag{2.35}$$

$$\tilde{\phi}_{d_1\mathrm{v}}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1}\tilde{\phi}_{\mathrm{v}}(x) + \delta_{x,x_{\max}}\varphi_{d_1\mathrm{v}} \quad (x=0,1,\ldots,x_{\max}; \mathrm{v}\in\mathcal{V}\backslash\{d_1\}),$$

$$\varphi_{d_1\mathrm{v}} \stackrel{\text{def}}{=} -\frac{\sqrt{\alpha B'(x_{\max})}\,\tilde{\phi}_0(x_{\max})}{\sqrt{\check{\xi}_{d_1}(x_{\max})\check{\xi}_{d_1}(x_{\max}+1)}}\,\check{\xi}_{d_1}(x_{\max})\check{\xi}_{\mathrm{v}}(x_{\max}+1). \tag{2.36}$$

It is easy to verify that $\phi_{d_1 n}(x)$ is an eigenvector and that $\tilde{\phi}_{d_1\mathrm{v}}(x)$ is a virtual state vector

$$\mathcal{H}_{d_1}\phi_{d_1 n}(x) = \mathcal{E}_n\phi_{d_1 n}(x) \quad (x=0,1,\ldots,x_{\max}; n=0,1,\ldots,n_{\max}),$$
$$\mathcal{H}_{d_1}\tilde{\phi}_{d_1\mathrm{v}}(x) = \tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\phi}_{d_1\mathrm{v}}(x) \quad (x=0,1,\ldots,x_{\max}-1; \mathrm{v}\in\mathcal{V}\backslash\{d_1\}),$$
$$\mathcal{H}_{d_1}\tilde{\phi}_{d_1\mathrm{v}}(x_{\max}) \neq \tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\phi}_{d_1\mathrm{v}}(x_{\max}).$$

For example,

$$\mathcal{H}_{d_1}\phi_{d_1 n} = (\hat{\mathcal{A}}_{d_1}\hat{\mathcal{A}}_{d_1}^{\dagger} + \tilde{\mathcal{E}}_{d_1})\hat{\mathcal{A}}_{d_1}\phi_n = \hat{\mathcal{A}}_{d_1}(\hat{\mathcal{A}}_{d_1}^{\dagger}\hat{\mathcal{A}}_{d_1} + \tilde{\mathcal{E}}_{d_1})\phi_n$$
$$= \hat{\mathcal{A}}_{d_1}\mathcal{H}\phi_n = \hat{\mathcal{A}}_{d_1}\mathcal{E}_n\phi_n = \mathcal{E}_n\hat{\mathcal{A}}_{d_1}\phi_n = \mathcal{E}_n\phi_{d_1 n}.$$

The two Hamiltonians $\mathcal{H}$ and $\mathcal{H}_{d_1}$ are exactly iso-spectral. If the original system is exactly solvable, this new system is also exactly solvable. The orthogonality relation for the new eigenvectors is

$$(\phi_{d_1 n}, \phi_{d_1 m}) = \sum_{x=0}^{x_{\max}} \phi_{d_1 n}(x)\phi_{d_1 m}(x)$$
$$= (\hat{\mathcal{A}}_{d_1}\phi_n, \hat{\mathcal{A}}_{d_1}\phi_m) = (\hat{\mathcal{A}}_{d_1}^{\dagger}\hat{\mathcal{A}}_{d_1}\phi_n, \phi_m) = \big((\mathcal{H}-\tilde{\mathcal{E}}_{d_1})\phi_n, \phi_m\big)$$
$$= (\mathcal{E}_n - \tilde{\mathcal{E}}_{d_1})(\phi_n, \phi_m) = (\mathcal{E}_n - \tilde{\mathcal{E}}_{d_1})\frac{1}{d_n^2}\delta_{nm} \quad (n,m=0,1,\ldots,n_{\max}).$$

This shows clearly that the *negative* virtual state energy ($\tilde{\mathcal{E}}_{\mathrm{v}} < 0$) is necessary for the positivity of the inner products.

The new eigenvector $\phi_{d_1 n}(x)$ (2.35) and the virtual state vector $\tilde{\phi}_{d_1\mathrm{v}}(x)$ (2.36) are expressed neatly in terms of the Casoratian ($x=0,1,\ldots,x_{\max}$)

$$\phi_{d_1 n}(x) = \frac{-\sqrt{\alpha B'(x)}\,\tilde{\phi}_0(x)}{\sqrt{\check{\xi}_{d_1}(x)\check{\xi}_{d_1}(x+1)}}\,\mathrm{W}\big[\check{\xi}_{d_1}, \nu\check{P}_n\big](x), \quad \tilde{\phi}_{d_1\mathrm{v}}(x) = \frac{-\sqrt{\alpha B'(x)}\,\tilde{\phi}_0(x)}{\sqrt{\check{\xi}_{d_1}(x)\check{\xi}_{d_1}(x+1)}}\,\mathrm{W}[\check{\xi}_{d_1}, \check{\xi}_{\mathrm{v}}](x). \tag{2.37}$$

The positivity of the virtual state vector is inherited by the new virtual state vector $\tilde{\phi}_{d_1\mathrm{v}}(x)$ (2.36). The Casoratian $\mathrm{W}[\check{\xi}_{d_1}, \check{\xi}_{\mathrm{v}}](x)$ has definite sign for $x=0,1,\ldots,x_{\max}+1$, namely all positive or all negative. By using (2.30) we have

$$\alpha B'(x)\mathrm{W}[\check{\xi}_{d_1}, \check{\xi}_{\mathrm{v}}](x) = \alpha D'(x)\mathrm{W}[\check{\xi}_{d_1}, \check{\xi}_{\mathrm{v}}](x-1) + (\tilde{\mathcal{E}}_{d_1} - \tilde{\mathcal{E}}_{\mathrm{v}})\check{\xi}_{d_1}(x)\check{\xi}_{\mathrm{v}}(x).$$

By setting $x = 0, 1, \ldots, x_{\max} + 1$ in turn, we obtain

$$\pm(\tilde{\mathcal{E}}_{d_1} - \tilde{\mathcal{E}}_{\mathrm{v}}) > 0 \Rightarrow \pm \mathrm{W}[\check{\xi}_{d_1}, \check{\xi}_{\mathrm{v}}](x) > 0 \quad (x = 0, 1, \ldots, x_{\max} + 1).$$

The new groundstate eigenvector $\phi_{d_1 0}(x)$ is of definite sign as the original one $\phi_0(x)$ (2.8). We show that the Casoratian $\mathrm{W}[\check{\xi}_{d_1}, \nu](x)$ has definite sign for $x = 0, 1, \ldots, x_{\max}$. By writing down the equation $\mathcal{H}\phi_n(x) = \mathcal{E}_n \phi_n(x)$ $(x = 0, 1, \ldots, x_{\max})$ with $\mathcal{H} = \hat{A}_{d_1}^{\dagger} \hat{A}_{d_1} + \tilde{\mathcal{E}}_{d_1}$, we have

$$\alpha B'(x)\nu(x+1)\check{P}_n(x+1) + \alpha D'(x)\nu(x-1)\check{P}_n(x-1) = \big(B(x) + D(x) - \mathcal{E}_n\big)\nu(x)\check{P}_n(x).$$

In terms of the functional relations of $\nu(x)$ (2.29), it is reduced to the original difference equation for $\check{P}_n(x)$ and it is valid any $x \in \mathbb{C}$. By using this, we can show

$$\alpha B'(x)\mathrm{W}[\check{\xi}_{d_1}, \nu\check{P}_n](x) = \alpha D'(x)\mathrm{W}[\check{\xi}_{d_1}, \nu\check{P}_n](x-1) + (\tilde{\mathcal{E}}_{d_1} - \mathcal{E}_n)\check{\xi}_{d_1}(x)\nu(x)\check{P}_n(x).$$

By setting $n = 0$ and $x = 0, 1, \ldots, x_{\max}$ in turn, we obtain

$$-\mathrm{W}[\check{\xi}_{d_1}, \nu](x) > 0 \quad (x = 0, 1, \ldots, x_{\max}).$$

Let us rewrite the deformed Hamiltonian $\mathcal{H}_{d_1}$ in the standard form. The potential functions $B_{d_1}(x)$ and $D_{d_1}(x)$ are introduced:

$$B_{d_1}(x) \stackrel{\mathrm{def}}{=} \alpha B'(x+1) \frac{\check{\xi}_{d_1}(x)}{\check{\xi}_{d_1}(x+1)} \frac{\mathrm{W}[\check{\xi}_{d_1}, \nu](x+1)}{\mathrm{W}[\check{\xi}_{d_1}, \nu](x)}, \tag{2.38}$$

$$D_{d_1}(x) \stackrel{\mathrm{def}}{=} \alpha D'(x) \frac{\check{\xi}_{d_1}(x+1)}{\check{\xi}_{d_1}(x)} \frac{\mathrm{W}[\check{\xi}_{d_1}, \nu](x-1)}{\mathrm{W}[\check{\xi}_{d_1}, \nu](x)}. \tag{2.39}$$

The positivity of $B_{d_1}(x)$ and $D_{d_1}(x)$ is shown above and the boundary conditions $B_{d_1}(x_{\max}) = 0$ and $D_{d_1}(0) = 0$ are satisfied. They satisfy the relations

$$B_{d_1}(x)D_{d_1}(x+1) = \hat{B}_{d_1}(x+1)\hat{D}_{d_1}(x+1),$$
$$B_{d_1}(x) + D_{d_1}(x) = \hat{B}_{d_1}(x) + \hat{D}_{d_1}(x+1) + \tilde{\mathcal{E}}_{d_1}.$$

The standard form Hamiltonian is obtained:

$$\mathcal{H}_{d_1} = \mathcal{A}_{d_1}^{\dagger} \mathcal{A}_{d_1}, \tag{2.40}$$

$$\mathcal{A}_{d_1} \stackrel{\mathrm{def}}{=} \sqrt{B_{d_1}(x)} - e^{\partial}\sqrt{D_{d_1}(x)}, \quad \mathcal{A}_{d_1}^{\dagger} = \sqrt{B_{d_1}(x)} - \sqrt{D_{d_1}(x)}\, e^{-\partial}, \tag{2.41}$$

in which $\mathcal{A}_{d_1}$ annihilates the groundstate eigenvector

$$\mathcal{A}_{d_1}\phi_{d_1 0}(x) = 0 \quad (x = 0, 1, \ldots, x_{\max}). \tag{2.42}$$

This one virtual state vector deletion is essentially the same procedure as that developed for the exceptional orthogonal polynomials in [23]. See § 3 for the explicit expressions.

<u>multi virtual state vector deletion</u>

We repeat the above procedure and obtain the modified systems. The number of deleted virtual state vectors should be less than or equal $|\mathcal{V}|$ and L.

Let us assume that we have already deleted s virtual state vectors ($s \geq 1$), which are labeled by $\{d_1, \ldots, d_s\}$ ($d_j \in \mathcal{V}$: mutually distinct). Namely we have

$$\mathcal{H}_{d_1\ldots d_s} \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1\ldots d_s}\hat{\mathcal{A}}^{\dagger}_{d_1\ldots d_s} + \tilde{\mathcal{E}}_{d_s}, \quad \mathcal{H}_{d_1\ldots d_s} = (\mathcal{H}_{d_1\ldots d_s\, x,y}) \quad (x, y = 0, 1, \ldots, x_{\max}), \tag{2.43}$$

$$\hat{\mathcal{A}}_{d_1\ldots d_s} \stackrel{\text{def}}{=} \sqrt{\hat{B}_{d_1\ldots d_s}(x)} - e^{\partial}\sqrt{\hat{D}_{d_1\ldots d_s}(x)}, \quad \hat{\mathcal{A}}^{\dagger}_{d_1\ldots d_s} = \sqrt{\hat{B}_{d_1\ldots d_s}(x)} - \sqrt{\hat{D}_{d_1\ldots d_s}(x)}\, e^{-\partial}, \tag{2.44}$$

$$\hat{B}_{d_1\ldots d_s}(x) \stackrel{\text{def}}{=} \alpha B'(x+s-1)\frac{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}](x)}{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}](x+1)}\,\frac{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x+1)}{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)}, \tag{2.45}$$

$$\hat{D}_{d_1\ldots d_s}(x) \stackrel{\text{def}}{=} \alpha D'(x)\frac{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}](x+1)}{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}](x)}\,\frac{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x-1)}{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)}, \tag{2.46}$$

$$\phi_{d_1\ldots d_s\, n}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1\ldots d_s}\phi_{d_1\ldots d_{s-1}\, n}(x) \quad (x = 0, 1, \ldots, x_{\max}; n = 0, 1, \ldots, n_{\max}), \tag{2.47}$$

$$\tilde{\phi}_{d_1\ldots d_s\, \mathrm{v}}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1\ldots d_s}\tilde{\phi}_{d_1\ldots d_{s-1}\, \mathrm{v}}(x) + \delta_{x,x_{\max}}\varphi_{d_1\ldots d_s\, \mathrm{v}}, \quad (x = 0, 1, \ldots, x_{\max}; \mathrm{v} \in \mathcal{V}\backslash\{d_1, \ldots, d_s\}),$$

$$\varphi_{d_1\ldots d_s\, \mathrm{v}} \stackrel{\text{def}}{=} \phi_{d_1\ldots d_s\, 0}(x_{\max})\frac{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x_{\max})\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}, \check{\xi}_{\mathrm{v}}](x_{\max}+1)}{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}](x_{\max}+1)\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x_{\max})}, \tag{2.48}$$

$$\mathcal{H}_{d_1\ldots d_s}\phi_{d_1\ldots d_s\, n}(x) = \mathcal{E}_n\phi_{d_1\ldots d_s\, n}(x) \quad (x = 0, 1, \ldots, x_{\max}; n = 0, 1, \ldots, n_{\max}), \tag{2.49}$$

$$\mathcal{H}_{d_1\ldots d_s}\tilde{\phi}_{d_1\ldots d_s\, \mathrm{v}}(x) = \tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\phi}_{d_1\ldots d_s\, \mathrm{v}}(x) \quad (x = 0, 1, \ldots, x_{\max} - 1; \mathrm{v} \in \mathcal{V}\backslash\{d_1, \ldots, d_s\}), \tag{2.50}$$

$$(\phi_{d_1\ldots d_s\, n}, \phi_{d_1\ldots d_s\, m}) \stackrel{\text{def}}{=} \sum_{x=0}^{x_{\max}} \phi_{d_1\ldots d_s\, n}(x)\phi_{d_1\ldots d_s\, m}(x) = \prod_{j=1}^{s}(\mathcal{E}_n - \tilde{\mathcal{E}}_{d_j}) \cdot \frac{1}{d_n^2}\delta_{nm}$$
$$(n, m = 0, 1, \ldots, n_{\max}). \tag{2.51}$$

The eigenvectors and the virtual state vectors have Casoratian expressions ($x = 0, 1, \ldots, x_{\max}$):

$$\phi_{d_1\ldots d_s\, n}(x) = \frac{(-1)^s\sqrt{\prod_{j=1}^{s}\alpha B'(x+j-1)}\,\tilde{\phi}_0(x)\,\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu\check{P}_n](x)}{\sqrt{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)\,\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x+1)}}, \tag{2.52}$$

$$\tilde{\phi}_{d_1\ldots d_s\, \mathrm{v}}(x) = \frac{(-1)^s\sqrt{\prod_{j=1}^{s}\alpha B'(x+j-1)}\,\tilde{\phi}_0(x)\,\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \check{\xi}_{\mathrm{v}}](x)}{\sqrt{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)\,\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x+1)}}. \tag{2.53}$$

The Casoratian in the virtual state vectors $\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \check{\xi}_{\mathrm{v}}](x)$ has definite sign for $x = 0, 1, \ldots, x_{\max}+1$, and that appearing in the groundstate eigenvector $\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x)$ has definite sign for $x = 0, 1, \ldots, x_{\max}$, too.

The next step begins with rewriting the Hamiltonian $\mathcal{H}_{d_1\dots d_s}$ by choosing the next virtual state to be deleted $d_{s+1} \in \mathcal{V}\backslash\{d_1,\dots,d_s\}$. The potential functions $\hat{B}_{d_1\dots d_{s+1}}(x)$ and $\hat{D}_{d_1\dots d_{s+1}}(x)$ are defined as in (2.45)–(2.46) by $s \to s+1$. We have $\hat{B}_{d_1\dots d_{s+1}}(x) > 0$ $(x = 0,1,\dots,x_{\max})$, $\hat{D}_{d_1\dots d_{s+1}}(0) = \hat{D}_{d_1\dots d_{s+1}}(x_{\max}+1) = 0$, $\hat{D}_{d_1\dots d_{s+1}}(x) > 0$ $(x = 1,2,\dots,x_{\max})$. These functions satisfy the relations

$$\hat{B}_{d_1\dots d_{s+1}}(x)\hat{D}_{d_1\dots d_{s+1}}(x+1) = \hat{B}_{d_1\dots d_s}(x+1)\hat{D}_{d_1\dots d_s}(x+1),$$
$$\hat{B}_{d_1\dots d_{s+1}}(x) + \hat{D}_{d_1\dots d_{s+1}}(x) + \tilde{\mathcal{E}}_{d_{s+1}} = \hat{B}_{d_1\dots d_s}(x) + \hat{D}_{d_1\dots d_s}(x+1) + \tilde{\mathcal{E}}_{d_s}.$$

The Hamiltonian $\mathcal{H}_{d_1\dots d_s}$ is rewritten as:

$$\mathcal{H}_{d_1\dots d_s} = \hat{\mathcal{A}}^{\dagger}_{d_1\dots d_{s+1}}\hat{\mathcal{A}}_{d_1\dots d_{s+1}} + \tilde{\mathcal{E}}_{d_{s+1}},$$
$$\hat{\mathcal{A}}_{d_1\dots d_{s+1}} \stackrel{\text{def}}{=} \sqrt{\hat{B}_{d_1\dots d_{s+1}}(x)} - e^{\partial}\sqrt{\hat{D}_{d_1\dots d_{s+1}}(x)},\ \hat{\mathcal{A}}^{\dagger}_{d_1\dots d_{s+1}} = \sqrt{\hat{B}_{d_1\dots d_{s+1}}(x)} - \sqrt{\hat{D}_{d_1\dots d_{s+1}}(x)}\, e^{-\partial}.$$

Now let us define a new Hamiltonian $\mathcal{H}_{d_1\dots d_{s+1}}$ by changing the orders of $\hat{\mathcal{A}}^{\dagger}_{d_1\dots d_{s+1}}$ and $\hat{\mathcal{A}}_{d_1\dots d_{s+1}}$ together with the eigenvectors $\phi_{d_1\dots d_{s+1}\,n}(x)$ and the virtual state vectors $\tilde{\phi}_{d_1\dots d_{s+1}\,\mathrm{v}}(x)$:

$$\mathcal{H}_{d_1\dots d_{s+1}} \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1\dots d_{s+1}}\hat{\mathcal{A}}^{\dagger}_{d_1\dots d_{s+1}} + \tilde{\mathcal{E}}_{d_{s+1}}, \quad \mathcal{H}_{d_1\dots d_{s+1}} = (\mathcal{H}_{d_1\dots d_{s+1}\,x,y}) \ \ (x,y = 0,1,\dots,x_{\max}),$$
$$\phi_{d_1\dots d_{s+1}\,n}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1\dots d_{s+1}}\phi_{d_1\dots d_s\,n}(x) \ \ (x = 0,1,\dots,x_{\max}; n = 0,1,\dots,n_{\max}),$$
$$\tilde{\phi}_{d_1\dots d_{s+1}\,\mathrm{v}}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1\dots d_{s+1}}\tilde{\phi}_{d_1\dots d_s\,\mathrm{v}}(x) + \delta_{x,x_{\max}}\varphi_{d_1\dots d_{s+1}\,\mathrm{v}},$$
$$(x = 0,1,\dots,x_{\max}; \mathrm{v} \in \mathcal{V}\backslash\{d_1,\dots,d_{s+1}\}),$$
$$\varphi_{d_1\dots d_{s+1}\,\mathrm{v}} \stackrel{\text{def}}{=} \phi_{d_1\dots d_{s+1}\,0}(x_{\max})\frac{\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_{s+1}}](x_{\max})\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_s},\check{\xi}_{\mathrm{v}}](x_{\max}+1)}{\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_s}](x_{\max}+1)\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_{s+1}},\nu](x_{\max})}.$$

The orthogonality relation reads

$$(\phi_{d_1\dots d_{s+1}\,n}, \phi_{d_1\dots d_{s+1}\,m}) = \prod_{j=1}^{s+1}(\mathcal{E}_n - \tilde{\mathcal{E}}_{d_j}) \cdot \frac{1}{d_n^2}\delta_{nm} \ \ (n,m = 0,1,\dots,n_{\max}).$$

The functions $\phi_{d_1\dots d_{s+1}\,n}(x)$ and $\tilde{\phi}_{d_1\dots d_{s+1}\,\mathrm{v}}(x)$ are expressed as Casoratians as in (2.52)–(2.53). The Casoratian $\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_{s+1}},\check{\xi}_{\mathrm{v}}](x)$ has definite sign

$$\pm\frac{\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_s}](0)(\tilde{\mathcal{E}}_{d_{s+1}} - \tilde{\mathcal{E}}_{\mathrm{v}})}{\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_{s+1}}](0)\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_s},\check{\xi}_{\mathrm{v}}](0)} > 0$$
$$\Rightarrow \pm\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_{s+1}},\check{\xi}_{\mathrm{v}}](x) > 0 \ \ (x = 0,1,\dots,x_{\max}+1).$$

Likewise $\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_{s+1}},\nu](x)$ and the lowest eigenvector $\phi_{d_1\dots d_{s+1}\,0}(x)$ have definite sign

$$\mp\frac{\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_s}](0)}{\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_{s+1}}](0)\mathrm{W}[\check{\xi}_{d_1},\dots,\check{\xi}_{d_s},\nu](0)} > 0$$

$$\Rightarrow \pm \mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s+1}}, \nu](x) > 0 \quad (x = 0, 1, \ldots, x_{\max}).$$

These establish the $s+1$ case.

At the end of this subsection we present this deformed Hamiltonian $\mathcal{H}_{d_1 \ldots d_s}$ in the standard form, in which the $\mathcal{A}$ operator annihilates the groundstate eigenvector:

$$\mathcal{H}_{d_1 \ldots d_s} = \mathcal{A}^{\dagger}_{d_1 \ldots d_s} \mathcal{A}_{d_1 \ldots d_s}, \tag{2.54}$$

$$\mathcal{A}_{d_1 \ldots d_s} \stackrel{\text{def}}{=} \sqrt{B_{d_1 \ldots d_s}(x)} - e^{\partial} \sqrt{D_{d_1 \ldots d_s}(x)}, \quad \mathcal{A}^{\dagger}_{d_1 \ldots d_s} = \sqrt{B_{d_1 \ldots d_s}(x)} - \sqrt{D_{d_1 \ldots d_s}(x)}\, e^{-\partial}, \tag{2.55}$$

which satisfies

$$\mathcal{A}_{d_1 \ldots d_s} \phi_{d_1 \ldots d_s\, 0}(x) = 0 \quad (x = 0, 1, \ldots, x_{\max}). \tag{2.56}$$

The potential functions $B_{d_1 \ldots d_s}(x)$ and $D_{d_1 \ldots d_s}(x)$ are:

$$B_{d_1 \ldots d_s}(x) \stackrel{\text{def}}{=} \alpha B'(x+s) \frac{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)}{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x+1)} \frac{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x+1)}{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x)}, \tag{2.57}$$

$$D_{d_1 \ldots d_s}(x) \stackrel{\text{def}}{=} \alpha D'(x) \frac{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x+1)}{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)} \frac{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x-1)}{\mathrm{W}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x)}. \tag{2.58}$$

The positivity of $B_{d_1 \ldots d_s}(x)$ and $D_{d_1 \ldots d_s}(x)$ is shown above and the boundary conditions $B_{d_1 \ldots d_s}(x_{\max}) = 0$ and $D_{d_1 \ldots d_s}(0) = 0$ are satisfied. They satisfy the relations

$$B_{d_1 \ldots d_s}(x) D_{d_1 \ldots d_s}(x+1) = \hat{B}_{d_1 \ldots d_s}(x+1) \hat{D}_{d_1 \ldots d_s}(x+1),$$
$$B_{d_1 \ldots d_s}(x) + D_{d_1 \ldots d_s}(x) = \hat{B}_{d_1 \ldots d_s}(x) + \hat{D}_{d_1 \ldots d_s}(x+1) + \tilde{\mathcal{E}}_{d_s}.$$

It should be stressed that the above results after s-deletions are independent of the orders of deletions ($\phi_{d_1 \ldots d_s\, n}(x)$ and $\tilde{\phi}_{d_1 \ldots d_s\, \mathrm{v}}(x)$ may change sign).

2.2.2 type II

In this subsection we use the type-(ii) factorisation. A slightly modified Casorati determinant of a set of n functions $\{f_j(x)\}$ is defined by

$$\mathrm{W}^{(-)}[f_1, \ldots, f_n](x) \stackrel{\text{def}}{=} \det\Big(f_k(x-j+1)\Big)_{1 \le j,k \le n} = (-1)^{\frac{1}{2}n(n-1)} \mathrm{W}[f_1, \ldots, f_n](x-n+1),$$

(for $n = 0$, we set $\mathrm{W}^{(-)}[\cdot](x) = 1$), which satisfies identities

$$\mathrm{W}^{(-)}[g f_1, g f_2, \ldots, g f_n](x) = \prod_{k=0}^{n-1} g(x-k) \cdot \mathrm{W}^{(-)}[f_1, f_2, \ldots, f_n](x),$$

$$
\begin{aligned}
&\mathrm{W}^{(-)}\big[\mathrm{W}^{(-)}[f_1,f_2,\ldots,f_n,g],\mathrm{W}^{(-)}[f_1,f_2,\ldots,f_n,h]\,\big](x)\\
&=\mathrm{W}^{(-)}[f_1,f_2,\ldots,f_n](x-1)\,\mathrm{W}^{(-)}[f_1,f_2,\ldots,f_n,g,h](x)\quad(n\geq 0).
\end{aligned}
$$

Let us assume the existence of two rational functions $B'(x)$ and $D'(x)$ of x or q^x satisfying

$$
B(x)D(x+1)=\alpha^2B'(x)D'(x+1),\qquad \alpha>0, \tag{2.59}
$$

$$
B(x)+D(x)=\alpha\big(B'(x)+D'(x)\big)+\alpha',\qquad \alpha'<0, \tag{2.60}
$$

$$
\begin{aligned}
&D'(x)>0\ \ (x=-L+1,\ldots,-1,0,1,\ldots,x_{\max}),\\
&B'(x)>0\ \ (x=0,1,\ldots,x_{\max}-1),\quad B'(x_{\max})=B'(-1)=0,
\end{aligned} \tag{2.61}
$$

where α and α' are constants and L is a certain positive integer. The first two equations are the same as in the type I case (2.18)-(2.19). The positive ranges (2.61) are different. We obtain

$$
\mathcal{H}=\alpha\mathcal{H}'+\alpha', \tag{2.62}
$$

$$
\mathcal{H}'\stackrel{\mathrm{def}}{=}-\sqrt{B'(x)}\,e^{\partial}\sqrt{D'(x)}-\sqrt{D'(x)}\,e^{-\partial}\sqrt{B'(x)}+B'(x)+D'(x). \tag{2.63}
$$

The virtual state vectors $\tilde{\phi}_{\mathrm{v}}(x)$ $(x=0,1,\ldots,x_{\max};\ \mathrm{v}\in\mathcal{V})$ are assumed to satisfy

$$
\mathcal{H}\tilde{\phi}_{\mathrm{v}}(x)=\tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\phi}_{\mathrm{v}}(x)\ \ (x=1,2,\ldots,x_{\max}),\quad \mathcal{H}\tilde{\phi}_{\mathrm{v}}(0)\neq\tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\phi}_{\mathrm{v}}(0), \tag{2.64}
$$

or equivalently,

$$
\mathcal{H}'\tilde{\phi}_{\mathrm{v}}(x)=\mathcal{E}'_{\mathrm{v}}\tilde{\phi}_{\mathrm{v}}(x)\ \ (x=1,2,\ldots,x_{\max}),\quad \mathcal{H}'\tilde{\phi}_{\mathrm{v}}(0)\neq\mathcal{E}'_{\mathrm{v}}\tilde{\phi}_{\mathrm{v}}(0),\quad \tilde{\mathcal{E}}_{\mathrm{v}}\stackrel{\mathrm{def}}{=}\alpha\mathcal{E}'_{\mathrm{v}}+\alpha'. \tag{2.65}
$$

They also have a factorised form

$$
\tilde{\phi}_{\mathrm{v}}(x)=\tilde{\phi}_0(x)\check{\xi}_{\mathrm{v}}(x),\quad \check{\xi}_{\mathrm{v}}(x)\stackrel{\mathrm{def}}{=}\xi_{\mathrm{v}}(\eta(x))\ \ (x=0,1,\ldots,x_{\max};\mathrm{v}\in\mathcal{V}). \tag{2.66}
$$

The function $\tilde{\phi}_0(x)$ and the ratio $\nu(x)\stackrel{\mathrm{def}}{=}\phi_0(x)/\tilde{\phi}_0(x)$ have the same expressions as in the type I case (2.27)–(2.28). After analytic continuation $\nu(x)$ vanishes at negative integer points, $\nu(x)=0$ $(x=-1,-2,\ldots)$, and at positive integer points outside the boundary $(x\in\mathbb{Z}_{>x_{\max}})$, it takes nonzero finite values in general. The difference equation for the virtual state polynomials takes the same form as before (2.30). On top of the different normalisation condition $\check{\xi}_{\mathrm{v}}(x_{\max})=1$ $(\mathrm{v}\in\mathcal{V})$, we require the following conditions:

$$
\check{\xi}_{\mathrm{v}}(x)>0\ \ (x=-1,0,1,\ldots,x_{\max};\mathrm{v}\in\mathcal{V}),\quad \tilde{\mathcal{E}}_{\mathrm{v}}<0\ \ (\mathrm{v}\in\mathcal{V}). \tag{2.67}
$$

Note the positivity requirement at $x=-1$ instead of $x_{\max}+1$ in the type I case (2.31).

<u>one virtual state vector deletion</u>

First we rewrite the original Hamiltonian by introducing $\hat{B}_{d_1}(x)$ and $\hat{D}_{d_1}(x)$:

$$\hat{B}_{d_1}(x) \stackrel{\text{def}}{=} \alpha B'(x)\frac{\check{\xi}_{d_1}(x+1)}{\check{\xi}_{d_1}(x)}, \quad \hat{D}_{d_1}(x) \stackrel{\text{def}}{=} \alpha D'(x)\frac{\check{\xi}_{d_1}(x-1)}{\check{\xi}_{d_1}(x)}. \tag{2.68}$$

We have $\hat{D}_{d_1}(x) > 0$ $(x=0,1,\ldots,x_{\max})$, $\hat{B}_{d_1}(x_{\max}) = \hat{B}_{d_1}(-1) = 0$, $\hat{B}_{d_1}(x) > 0$ $(x = 0,1,\ldots,x_{\max}-1)$ and

$$\begin{aligned} B(x)D(x+1) &= \hat{B}_{d_1}(x)\hat{D}_{d_1}(x+1), \\ B(x)+D(x) &= \hat{B}_{d_1}(x)+\hat{D}_{d_1}(x)+\tilde{\mathcal{E}}_{d_1}. \end{aligned}$$

The original Hamiltonian is expressed by a different factorisation:

$$\begin{aligned} &\mathcal{H} = \hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})\,\dagger}\hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})} + \tilde{\mathcal{E}}_{d_1}, \\ &\hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})} \stackrel{\text{def}}{=} \sqrt{\hat{D}_{d_1}(x)} - e^{-\partial}\sqrt{\hat{B}_{d_1}(x)}, \quad \hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})\,\dagger} = \sqrt{\hat{D}_{d_1}(x)} - \sqrt{\hat{B}_{d_1}(x)}\,e^{\partial}. \end{aligned}$$

The virtual state vector $\tilde{\phi}_{d_1}(x)$ is almost annihilated by $\hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})}$:

$$\hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})}\tilde{\phi}_{d_1}(x) = 0 \quad (x=1,2,\ldots,x_{\max}), \quad \hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})}\tilde{\phi}_{d_1}(0) \neq 0.$$

Next let us define a new Hamiltonian $\mathcal{H}_{d_1}$ together with the sets of new eigenvectors $\phi_{d_1 n}(x)$ and the virtual state vectors $\tilde{\phi}_{d_1\mathrm{v}}(x)$:

$$\mathcal{H}_{d_1} \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})}\hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})\,\dagger} + \tilde{\mathcal{E}}_{d_1}, \quad \mathcal{H}_{d_1} = (\mathcal{H}_{d_1\,x,y}) \quad (x,y=0,1,\ldots,x_{\max}), \tag{2.69}$$

$$\phi_{d_1 n}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})}\phi_n(x) \quad (x=0,1,\ldots,x_{\max}; n=0,1,\ldots,n_{\max}), \tag{2.70}$$

$$\begin{aligned} &\tilde{\phi}_{d_1\mathrm{v}}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1}^{(\mathrm{ii})}\tilde{\phi}_{\mathrm{v}}(x) + \delta_{x,0}\varphi_{d_1\mathrm{v}} \quad (x=0,1,\ldots,x_{\max}; \mathrm{v}\in\mathcal{V}\backslash\{d_1\}), \\ &\qquad \varphi_{d_1\mathrm{v}} \stackrel{\text{def}}{=} -\frac{\sqrt{\alpha D'(0)}\,\tilde{\phi}_0(0)}{\sqrt{\check{\xi}_{d_1}(0)\check{\xi}_{d_1}(-1)}}\,\check{\xi}_{d_1}(0)\check{\xi}_{\mathrm{v}}(-1), \end{aligned} \tag{2.71}$$

$$\mathcal{H}_{d_1}\phi_{d_1 n}(x) = \mathcal{E}_n\phi_{d_1 n}(x) \quad (x=0,1,\ldots,x_{\max}; n=0,1,\ldots,n_{\max}), \tag{2.72}$$

$$\mathcal{H}_{d_1}\tilde{\phi}_{d_1\mathrm{v}}(x) = \tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\phi}_{d_1\mathrm{v}}(x) \quad (x=1,2,\ldots,x_{\max}; \mathrm{v}\in\mathcal{V}\backslash\{d_1\}), \quad \mathcal{H}_{d_1}\tilde{\phi}_{d_1\mathrm{v}}(0) \neq \tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\phi}_{d_1\mathrm{v}}(0). \tag{2.73}$$

The two Hamiltonians $\mathcal{H}$ and $\mathcal{H}_{d_1}$ are exactly iso-spectral. The orthogonality relation reads

$$(\phi_{d_1 n},\phi_{d_1 m}) = (\mathcal{E}_n - \tilde{\mathcal{E}}_{d_1})(\phi_n,\phi_m) = (\mathcal{E}_n - \tilde{\mathcal{E}}_{d_1})\frac{1}{d_n^2}\delta_{nm} \quad (n,m=0,1,\ldots,n_{\max}).$$

The functions (2.70) and (2.71) are expressed in terms of the Casoratian

$$\left.\begin{array}{l}\phi_{d_1 n}(x)\\ \tilde{\phi}_{d_1 \mathrm{v}}(x)\end{array}\right\} = \frac{-\sqrt{\alpha D'(x)}\,\tilde{\phi}_0(x)}{\sqrt{\check{\xi}_{d_1}(x)\check{\xi}_{d_1}(x-1)}} \times \left\{\begin{array}{l}\mathrm{W}^{(-)}\big[\check{\xi}_{d_1}, \nu\check{P}_n\big](x)\\ \mathrm{W}^{(-)}[\check{\xi}_{d_1}, \check{\xi}_{\mathrm{v}}](x)\end{array}\right. \quad (x = 0, 1, \ldots, x_{\max}). \tag{2.74}$$

The Casoratian $\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \check{\xi}_{\mathrm{v}}](x)$ and the virtual state vector $\tilde{\phi}_{d_1 \mathrm{v}}(x)$ have definite sign:

$$\pm\,(\tilde{\mathcal{E}}_{d_1} - \tilde{\mathcal{E}}_{\mathrm{v}}) > 0 \Rightarrow \pm \mathrm{W}^{(-)}[\check{\xi}_{d_1}, \check{\xi}_{\mathrm{v}}](x) > 0 \quad (x = -1, 0, \ldots, x_{\max}). \tag{2.75}$$

Likewise the main part of the groundstate eigenvector $\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \nu](x)$ has definite sign

$$-\,\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \nu](x) > 0 \quad (x = 0, 1, \ldots, x_{\max}). \tag{2.76}$$

<u>multi virtual state vector deletion</u>

We repeat the above procedure and obtain the modified systems. The process goes almost parallel with the type I case, although some formulas appear rather different.

Let us assume that we have already deleted s virtual state vectors ($s \geq 1$), which are labeled by $\{d_1, \ldots, d_s\}$ ($d_j \in \mathcal{V}$: mutually distinct):

$$\mathcal{H}_{d_1 \ldots d_s} \stackrel{\mathrm{def}}{=} \hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1 \ldots d_s} \hat{\mathcal{A}}^{(\mathrm{ii})\,\dagger}_{d_1 \ldots d_s} + \tilde{\mathcal{E}}_{d_s}, \quad \mathcal{H}_{d_1 \ldots d_s} = (\mathcal{H}_{d_1 \ldots d_s\, x, y}) \quad (x, y = 0, 1, \ldots, x_{\max}), \tag{2.77}$$

$$\hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1 \ldots d_s} \stackrel{\mathrm{def}}{=} \sqrt{\hat{D}_{d_1 \ldots d_s}(x)} - e^{-\partial}\sqrt{\hat{B}_{d_1 \ldots d_s}(x)}, \quad \hat{\mathcal{A}}^{(\mathrm{ii})\,\dagger}_{d_1 \ldots d_s} = \sqrt{\hat{D}_{d_1 \ldots d_s}(x)} - \sqrt{\hat{B}_{d_1 \ldots d_s}(x)}\, e^{\partial}, \tag{2.78}$$

$$\hat{B}_{d_1 \ldots d_s}(x) \stackrel{\mathrm{def}}{=} \alpha B'(x) \frac{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}](x-1)}{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}](x)} \frac{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x+1)}{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)}, \tag{2.79}$$

$$\hat{D}_{d_1 \ldots d_s}(x) \stackrel{\mathrm{def}}{=} \alpha D'(x-s+1) \frac{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}](x)}{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}](x-1)} \frac{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x-1)}{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)}, \tag{2.80}$$

$$\phi_{d_1 \ldots d_s\, n}(x) \stackrel{\mathrm{def}}{=} \hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1 \ldots d_s} \phi_{d_1 \ldots d_{s-1}\, n}(x) \quad (x = 0, 1, \ldots, x_{\max}; n = 0, 1, \ldots, n_{\max}), \tag{2.81}$$

$$\tilde{\phi}_{d_1 \ldots d_s\, \mathrm{v}}(x) \stackrel{\mathrm{def}}{=} \hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1 \ldots d_s} \tilde{\phi}_{d_1 \ldots d_{s-1}\, \mathrm{v}}(x) + \delta_{x,0}\varphi_{d_1 \ldots d_s\, \mathrm{v}}, \quad (x = 0, 1, \ldots, x_{\max}; \mathrm{v} \in \mathcal{V}\backslash\{d_1, \ldots, d_s\}),$$

$$\varphi_{d_1 \ldots d_s\, \mathrm{v}} \stackrel{\mathrm{def}}{=} \phi_{d_1 \ldots d_s\, 0}(0) \frac{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](0)\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}, \check{\xi}_{\mathrm{v}}](-1)}{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s-1}}](-1)\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](0)}, \tag{2.82}$$

$$\mathcal{H}_{d_1 \ldots d_s} \phi_{d_1 \ldots d_s\, n}(x) = \mathcal{E}_n \phi_{d_1 \ldots d_s\, n}(x) \quad (x = 0, 1, \ldots, x_{\max}; n = 0, 1, \ldots, n_{\max}), \tag{2.83}$$

$$\mathcal{H}_{d_1 \ldots d_s} \tilde{\phi}_{d_1 \ldots d_s\, \mathrm{v}}(x) = \tilde{\mathcal{E}}_{\mathrm{v}} \tilde{\phi}_{d_1 \ldots d_s\, \mathrm{v}}(x) \quad (x = 1, 2, \ldots, x_{\max}; \mathrm{v} \in \mathcal{V}\backslash\{d_1, \ldots, d_s\}), \tag{2.84}$$

$$(\phi_{d_1 \ldots d_s\, n}, \phi_{d_1 \ldots d_s\, m}) \stackrel{\mathrm{def}}{=} \sum_{x=0}^{x_{\max}} \phi_{d_1 \ldots d_s\, n}(x)\phi_{d_1 \ldots d_s\, m}(x) = \prod_{j=1}^{s} (\mathcal{E}_n - \tilde{\mathcal{E}}_{d_j}) \cdot \frac{1}{d_n^2}\delta_{nm}$$
$$(n, m = 0, 1, \ldots, n_{\max}). \tag{2.85}$$

The eigenvectors and the virtual state vectors have Casoratian expressions ($x = 0, 1, \ldots, x_{\max}$):

$$\phi_{d_1 \ldots d_s\, n}(x) = \frac{(-1)^s \sqrt{\prod_{j=1}^{s} \alpha D'(x-j+1)}\, \tilde{\phi}_0(x)\, \mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu \check{P}_n](x)}{\sqrt{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)\, \mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x-1)}}, \tag{2.86}$$

$$\tilde{\phi}_{d_1 \ldots d_s\, \mathrm{v}}(x) = \frac{(-1)^s \sqrt{\prod_{j=1}^{s} \alpha D'(x-j+1)}\, \tilde{\phi}_0(x)\, \mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \check{\xi}_{\mathrm{v}}](x)}{\sqrt{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)\, \mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x-1)}}. \tag{2.87}$$

The virtual state Casoratian $\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \check{\xi}_{\mathrm{v}}](x)$ has definite sign for $x = -1, 0, 1, \ldots, x_{\max}$, and the groundstate eigenvector Casoratian $\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x)$ has definite sign for $x = 0, 1, \ldots, x_{\max}$.

The next step begins with rewriting the Hamiltonian $\mathcal{H}_{d_1 \ldots d_s}$ by choosing the next virtual state to be deleted $d_{s+1} \in \mathcal{V} \backslash \{d_1, \ldots, d_s\}$. Let us define $\hat{B}_{d_1 \ldots d_{s+1}}(x)$ and $\hat{D}_{d_1 \ldots d_{s+1}}(x)$ as in (2.79)–(2.80) by $s \to s+1$. The positivity $\hat{D}_{d_1 \ldots d_{s+1}}(x) > 0$ ($x = 0, 1, \ldots, x_{\max}$), $\hat{B}_{d_1 \ldots d_{s+1}}(x) > 0$ ($x = 0, 1, \ldots, x_{\max} - 1$) with the boundary conditions $\hat{B}_{d_1 \ldots d_{s+1}}(x_{\max}) = \hat{B}_{d_1 \ldots d_{s+1}}(-1) = 0$ are ensured. The following identities are essential

$$\begin{aligned}
&\hat{B}_{d_1 \ldots d_{s+1}}(x) \hat{D}_{d_1 \ldots d_{s+1}}(x+1) = \hat{B}_{d_1 \ldots d_s}(x) \hat{D}_{d_1 \ldots d_s}(x), \\
&\hat{B}_{d_1 \ldots d_{s+1}}(x) + \hat{D}_{d_1 \ldots d_{s+1}}(x) + \tilde{\mathcal{E}}_{d_{s+1}} = \hat{B}_{d_1 \ldots d_s}(x-1) + \hat{D}_{d_1 \ldots d_s}(x) + \tilde{\mathcal{E}}_{d_s}.
\end{aligned}$$

The Hamiltonian $\mathcal{H}_{d_1 \ldots d_s}$ is rewritten as follows:

$$\mathcal{H}_{d_1 \ldots d_s} = \hat{\mathcal{A}}^{(\mathrm{ii})\,\dagger}_{d_1 \ldots d_{s+1}} \hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1 \ldots d_{s+1}} + \tilde{\mathcal{E}}_{d_{s+1}},$$

$$\hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1 \ldots d_{s+1}} \stackrel{\mathrm{def}}{=} \sqrt{\hat{D}_{d_1 \ldots d_{s+1}}(x)} - e^{-\partial} \sqrt{\hat{B}_{d_1 \ldots d_{s+1}}(x)}, \;\; \hat{\mathcal{A}}^{(\mathrm{ii})\,\dagger}_{d_1 \ldots d_{s+1}} = \sqrt{\hat{D}_{d_1 \ldots d_{s+1}}(x)} - \sqrt{\hat{B}_{d_1 \ldots d_{s+1}}(x)}\, e^{\partial}.$$

Next let us define a new Hamiltonian $\mathcal{H}_{d_1 \ldots d_{s+1}}$ together with the eigenvectors $\phi_{d_1 \ldots d_{s+1}\, n}(x)$ and the virtual state vectors $\tilde{\phi}_{d_1 \ldots d_{s+1}\, \mathrm{v}}(x)$:

$$\begin{aligned}
&\mathcal{H}_{d_1 \ldots d_{s+1}} \stackrel{\mathrm{def}}{=} \hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1 \ldots d_{s+1}} \hat{\mathcal{A}}^{(\mathrm{ii})\,\dagger}_{d_1 \ldots d_{s+1}} + \tilde{\mathcal{E}}_{d_{s+1}}, \quad \mathcal{H}_{d_1 \ldots d_{s+1}} = (\mathcal{H}_{d_1 \ldots d_{s+1}\, x,y}) \;\; (x, y = 0, 1, \ldots, x_{\max}), \\
&\phi_{d_1 \ldots d_{s+1}\, n}(x) \stackrel{\mathrm{def}}{=} \hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1 \ldots d_{s+1}} \phi_{d_1 \ldots d_s\, n}(x) \;\; (x = 0, 1, \ldots, x_{\max}; n = 0, 1, \ldots, n_{\max}), \\
&\tilde{\phi}_{d_1 \ldots d_{s+1}\, \mathrm{v}}(x) \stackrel{\mathrm{def}}{=} \hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1 \ldots d_{s+1}} \tilde{\phi}_{d_1 \ldots d_s\, \mathrm{v}}(x) + \delta_{x,0} \varphi_{d_1 \ldots d_{s+1}\, \mathrm{v}}, \\
&\qquad\qquad (x = 0, 1, \ldots, x_{\max}; \mathrm{v} \in \mathcal{V} \backslash \{d_1, \ldots, d_{s+1}\}), \\
&\varphi_{d_1 \ldots d_{s+1}\, \mathrm{v}} \stackrel{\mathrm{def}}{=} \phi_{d_1 \ldots d_{s+1}\, 0}(0) \frac{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s+1}}](0) \mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \check{\xi}_{\mathrm{v}}](-1)}{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](-1) \mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s+1}}, \nu](0)}.
\end{aligned}$$

The orthogonality relation reads

$$(\phi_{d_1\ldots d_{s+1}\,n}, \phi_{d_1\ldots d_{s+1}\,m}) = \prod_{j=1}^{s+1}(\mathcal{E}_n - \tilde{\mathcal{E}}_{d_j}) \cdot \frac{1}{d_n^2}\delta_{nm} \quad (n, m = 0, 1, \ldots, n_{\max}).$$

The functions $\phi_{d_1\ldots d_{s+1}\,n}(x)$ and $\tilde{\phi}_{d_1\ldots d_{s+1}\,\mathrm{v}}(x)$ are expressed as Casoratians as in (2.86)–(2.87). The virtual state Casoratian $\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s+1}}, \check{\xi}_{\mathrm{v}}](x)$ has definite sign for $x = -1, 0, 1, \ldots, x_{\max}$ and the groundstate Casoratian $\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_{s+1}}, \nu](x)$ has definite sign for $x = 0, 1, \ldots, x_{\max}$. These establish the $s+1$ case.

The standard form Hamiltonian of the type II deformed system has exactly the same form (2.54)–(2.55) as in the type I case. The explicit expressions of the potential functions $B_{d_1\ldots d_s}(x)$ and $D_{d_1\ldots d_s}(x)$ are different:

$$B_{d_1\ldots d_s}(x) \stackrel{\mathrm{def}}{=} \alpha B'(x) \frac{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x-1)}{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)} \frac{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x+1)}{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x)}, \tag{2.88}$$

$$D_{d_1\ldots d_s}(x) \stackrel{\mathrm{def}}{=} \alpha D'(x-s) \frac{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x)}{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}](x-1)} \frac{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x-1)}{\mathrm{W}^{(-)}[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_s}, \nu](x)}. \tag{2.89}$$

The positivity of $B_{d_1\ldots d_s}(x)$ and $D_{d_1\ldots d_s}(x)$ is shown above and the boundary conditions $B_{d_1\ldots d_s}(x_{\max}) = 0$ and $D_{d_1\ldots d_s}(0) = 0$ are satisfied.

2.2.3 non-coexistence of type I and type II

Here we show that the type I and II virtual state vectors cannot be used together to generate new multi-indexed orthogonal polynomials. A type I virtual state vector $\tilde{\phi}_{d_1}(x)$ (2.26) fails to satisfy the Schrödinger equation (2.23) at $x = x_{\max}$. A type II virtual state vector $\tilde{\phi}^{\mathrm{II}}_{\mathrm{w}}(x)$ (2.66) does not satisfy the equation (2.64) at $x = 0$. Like (2.37), a 'virtual state vector' obtained by combining these two in this order is given by

$$\tilde{\phi}_{d_1\mathrm{w}}(x) = \frac{-\sqrt{\alpha B'(x)}\,\tilde{\phi}_0(x)}{\sqrt{\check{\xi}_{d_1}(x)\check{\xi}_{d_1}(x+1)}}\,\mathrm{W}[\check{\xi}_{d_1}, \frac{\tilde{\phi}^{\mathrm{II}}_0}{\tilde{\phi}_0}\check{\xi}^{\mathrm{II}}_{\mathrm{w}}](x) \quad (x = 0, 1, \ldots, x_{\max}). \tag{2.90}$$

Obviously this fails to satisfy the corresponding Schrödinger equation on both boundaries, $x = 0$ and $x = x_{\max}$, and it is no longer a virtual state vector. In other words, the vector $\tilde{\phi}_{d_1\mathrm{w}}(x)$ cannot generate double-indexed orthogonal polynomials. This can be seen clearly by comparing (2.37) and (2.90). In the former $\mathrm{W}[\check{\xi}_{d_1}, \check{\xi}_{\mathrm{v}}](x)$ is well-defined for any $x \in \mathbb{C}$. On the other hand $\mathrm{W}[\check{\xi}_{d_1}, \frac{\tilde{\phi}^{\mathrm{II}}_0}{\tilde{\phi}_0}\check{\xi}^{\mathrm{II}}_{\mathrm{w}}](x)$ is not well-defined at $x = -1$ and this prevents the introduction of $\hat{\mathcal{A}}_{d_1\mathrm{w}}$ and $\hat{\mathcal{A}}^{\dagger}_{d_1\mathrm{w}}$ in the Hamiltonian $\mathcal{H}_{d_1}$:

$$\mathcal{H}_{d_1} = \hat{\mathcal{A}}^{\dagger}_{d_1\mathrm{w}}\hat{\mathcal{A}}_{d_1\mathrm{w}} + \tilde{\mathcal{E}}^{\mathrm{II}}_{\mathrm{w}},$$

$$\hat{\mathcal{A}}_{d_1\mathrm{w}} \stackrel{\mathrm{def}}{=} \sqrt{\hat{B}_{d_1\mathrm{w}}(x)} - e^{\partial}\sqrt{\hat{D}_{d_1\mathrm{w}}(x)}, \quad \hat{\mathcal{A}}^{\dagger}_{d_1\mathrm{w}} = \sqrt{\hat{B}_{d_1\mathrm{w}}(x)} - \sqrt{\hat{D}_{d_1\mathrm{w}}(x)}\, e^{-\partial},$$

$$\hat{B}_{d_1\mathrm{w}}(x) \stackrel{\mathrm{def}}{=} \alpha B'(x+1)\frac{\check{\xi}_{d_1}(x)}{\check{\xi}_{d_1}(x+1)}\frac{\mathrm{W}[\check{\xi}_{d_1}, \frac{\tilde{\phi}_0^{\mathrm{II}}}{\tilde{\phi}_0}\check{\xi}^{\mathrm{II}}_{\mathrm{w}}](x+1)}{\mathrm{W}[\check{\xi}_{d_1}, \frac{\tilde{\phi}_0^{\mathrm{II}}}{\tilde{\phi}_0}\check{\xi}^{\mathrm{II}}_{\mathrm{w}}](x)},$$

$$\hat{D}_{d_1\mathrm{w}}(x) \stackrel{\mathrm{def}}{=} \alpha D'(x)\frac{\check{\xi}_{d_1}(x+1)}{\check{\xi}_{d_1}(x)}\frac{\mathrm{W}[\check{\xi}_{d_1}, \frac{\tilde{\phi}_0^{\mathrm{II}}}{\tilde{\phi}_0}\check{\xi}^{\mathrm{II}}_{\mathrm{w}}](x-1)}{\mathrm{W}[\check{\xi}_{d_1}, \frac{\tilde{\phi}_0^{\mathrm{II}}}{\tilde{\phi}_0}\check{\xi}^{\mathrm{II}}_{\mathrm{w}}](x)}.$$

The double-indexed orthogonal polynomials cannot be constructed by using the type I and II virtual state vectors.

3 Multi-indexed (q)-Racah polynomials

In this section we apply the method of virtual state deletions to the exactly solvable systems whose eigenstates are described by the (q)-Racah polynomials. We delete M virtual state vectors labeled by

$$\mathcal{D} = \{d_1, d_2, \ldots, d_M\} \quad (d_j \in \mathcal{V} : \text{mutually distinct}), \tag{3.1}$$

and denote $\mathcal{H}_{d_1\ldots d_M}$, $\phi_{d_1\ldots d_M\, n}$, $\mathcal{A}_{d_1\ldots d_M}$, etc. by $\mathcal{H}_{\mathcal{D}}$, $\phi_{\mathcal{D}\, n}$, $\mathcal{A}_{\mathcal{D}}$, etc.

We follow the notation of [2]. Various quantities depend on a set of parameters $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \ldots)$. The eigenvectors of the models in § 5 of [2] are described by orthogonal polynomials in the sinusoidal coordinate $\eta(x;\boldsymbol{\lambda})$. The auxiliary function $\varphi(x;\boldsymbol{\lambda})$ is defined by

$$\varphi(x;\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} \frac{\eta(x+1;\boldsymbol{\lambda}) - \eta(x;\boldsymbol{\lambda})}{\eta(1;\boldsymbol{\lambda})}, \tag{3.2}$$

and it satisfies (with $\boldsymbol{\delta}$ defined in (3.6)–(3.7))

$$\frac{\varphi(x;\boldsymbol{\lambda})}{\varphi(x-1;\boldsymbol{\lambda}+2\boldsymbol{\delta})} = \varphi(1;\boldsymbol{\lambda}). \tag{3.3}$$

All the models in § 5 of [2] have shape invariance [44]. The following relations are very useful:

$$\varphi(x;\boldsymbol{\lambda}) = \sqrt{\frac{B(0;\boldsymbol{\lambda})}{B(x;\boldsymbol{\lambda})}}\,\frac{\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\phi_0(x;\boldsymbol{\lambda})}, \quad \varphi(x;\boldsymbol{\lambda}) = \sqrt{\frac{B(0;\boldsymbol{\lambda})}{D(x+1;\boldsymbol{\lambda})}}\,\frac{\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\phi_0(x+1;\boldsymbol{\lambda})}, \tag{3.4}$$

$$\frac{B(x;\boldsymbol{\lambda}+\boldsymbol{\delta})}{B(x+1;\boldsymbol{\lambda})} = \kappa^{-1}\frac{\varphi(x+1;\boldsymbol{\lambda})}{\varphi(x;\boldsymbol{\lambda})}, \quad \frac{D(x;\boldsymbol{\lambda}+\boldsymbol{\delta})}{D(x;\boldsymbol{\lambda})} = \kappa^{-1}\frac{\varphi(x-1;\boldsymbol{\lambda})}{\varphi(x;\boldsymbol{\lambda})}. \tag{3.5}$$

3.1 Original (q)-Racah system

Let us consider the Racah (R) and the q-Racah (qR) cases. Although there are four possible parameter choices indexed by $(\epsilon,\epsilon')=(\pm1,\pm1)$ in general, we restrict ourselves to the $(\epsilon,\epsilon')=(1,1)$ case for simplicity of presentation. The set of parameters $\boldsymbol{\lambda}$, which is different from the standard one $(\alpha,\beta,\gamma,\delta)$ [5], its shift $\boldsymbol{\delta}$ and κ are

$$\mathrm{R}:\ \boldsymbol{\lambda}=(a,b,c,d),\quad \boldsymbol{\delta}=(1,1,1,1),\quad \kappa=1, \tag{3.6}$$

$$q\mathrm{R}:\ q^{\boldsymbol{\lambda}}=(a,b,c,d),\quad \boldsymbol{\delta}=(1,1,1,1),\quad \kappa=q^{-1},\quad 0<q<1, \tag{3.7}$$

where $q^{\boldsymbol{\lambda}}$ stands for $q^{(\lambda_1,\lambda_2,\ldots)}=(q^{\lambda_1},q^{\lambda_2},\ldots)$. We introduce a new parameter $\tilde{d}$ defined by

$$\tilde{d}\stackrel{\mathrm{def}}{=}\begin{cases} a+b+c-d-1 & :\mathrm{R}\\ abcd^{-1}q^{-1} & :q\mathrm{R}\end{cases}. \tag{3.8}$$

Here are the fundamental data [2]:

$$B(x;\boldsymbol{\lambda})=\begin{cases} -\dfrac{(x+a)(x+b)(x+c)(x+d)}{(2x+d)(2x+1+d)} & :\mathrm{R}\\ -\dfrac{(1-aq^x)(1-bq^x)(1-cq^x)(1-dq^x)}{(1-dq^{2x})(1-dq^{2x+1})} & :q\mathrm{R}\end{cases}, \tag{3.9}$$

$$D(x;\boldsymbol{\lambda})=\begin{cases} -\dfrac{(x+d-a)(x+d-b)(x+d-c)x}{(2x-1+d)(2x+d)} & :\mathrm{R}\\ -\tilde{d}\,\dfrac{(1-a^{-1}dq^x)(1-b^{-1}dq^x)(1-c^{-1}dq^x)(1-q^x)}{(1-dq^{2x-1})(1-dq^{2x})} & :q\mathrm{R}\end{cases}, \tag{3.10}$$

$$\mathcal{E}_n(\boldsymbol{\lambda})=\begin{cases} n(n+\tilde{d}) & :\mathrm{R}\\ (q^{-n}-1)(1-\tilde{d}q^n) & :q\mathrm{R}\end{cases},\quad \eta(x;\boldsymbol{\lambda})=\begin{cases} x(x+d) & :\mathrm{R}\\ (q^{-x}-1)(1-dq^x) & :q\mathrm{R}\end{cases}, \tag{3.11}$$

$$\varphi(x;\boldsymbol{\lambda})=\begin{cases} \dfrac{2x+d+1}{d+1} & :\mathrm{R}\\ \dfrac{q^{-x}-dq^{x+1}}{1-dq} & :q\mathrm{R}\end{cases}, \tag{3.12}$$

$$\check{P}_n(x;\boldsymbol{\lambda})=P_n\big(\eta(x;\boldsymbol{\lambda});\boldsymbol{\lambda}\big)=\begin{cases} {}_4F_3\left(\begin{matrix}-n,\ n+\tilde{d},\ -x,\ x+d\\ a,\ b,\ c\end{matrix}\,\middle|\,1\right) & :\mathrm{R}\\ {}_4\phi_3\left(\begin{matrix}q^{-n},\ \tilde{d}q^n,\ q^{-x},\ dq^x\\ a,\ b,\ c\end{matrix}\,\middle|\,q\,;q\right) & :q\mathrm{R}\end{cases} \tag{3.13}$$

$$=\begin{cases} R_n\big(\eta(x;\boldsymbol{\lambda});a-1,\tilde{d}-a,c-1,d-c\big) & :\mathrm{R}\\ R_n\big(1+d+\eta(x;\boldsymbol{\lambda});aq^{-1},\tilde{d}a^{-1},cq^{-1},dc^{-1}|q\big) & :q\mathrm{R}\end{cases}, \tag{3.14}$$

$$\phi_0(x;\boldsymbol{\lambda})^2=\begin{cases} \dfrac{(a,b,c,d)_x}{(1+d-a,1+d-b,1+d-c,1)_x}\,\dfrac{2x+d}{d} & :\mathrm{R}\\ \dfrac{(a,b,c,d\,;q)_x}{(a^{-1}dq,b^{-1}dq,c^{-1}dq,q\,;q)_x\,\tilde{d}^x}\,\dfrac{1-dq^{2x}}{1-d} & :q\mathrm{R}\end{cases}, \tag{3.15}$$

$$
d_n(\boldsymbol{\lambda})^2 = \begin{cases} \dfrac{(a,b,c,\tilde{d})_n}{(1+\tilde{d}-a,1+\tilde{d}-b,1+\tilde{d}-c,1)_n}\dfrac{2n+\tilde{d}}{\tilde{d}} \\ \quad \times \dfrac{(-1)^N(1+d-a,1+d-b,1+d-c)_N}{(\tilde{d}+1)_N(d+1)_{2N}} & : \mathrm{R} \\ \dfrac{(a,b,c,\tilde{d}\,;q)_n}{(a^{-1}\tilde{d}q,b^{-1}\tilde{d}q,c^{-1}\tilde{d}q,q\,;q)_n\,d^n}\dfrac{1-\tilde{d}q^{2n}}{1-\tilde{d}} \\ \quad \times \dfrac{(-1)^N(a^{-1}dq,b^{-1}dq,c^{-1}dq\,;q)_N\,\tilde{d}^N q^{\frac{1}{2}N(N+1)}}{(\tilde{d}q\,;q)_N(dq\,;q)_{2N}} & : q\mathrm{R} \end{cases} . \tag{3.16}
$$

Here $R_n(\cdots)$ in (3.14) are the standard notation of the (q)-Racah polynomial in [5]. Here is a remark on the polynomial $\check{P}_n(x;\boldsymbol{\lambda})$, which is in fact a polynomial in the sinusoidal coordinate $\eta(x;\boldsymbol{\lambda})$ (3.11). The sinusoidal coordinate has a special dynamical meaning [2, 28, 43]. The Heisenberg operator solution for $\eta(x;\boldsymbol{\lambda})$ can be expressed in a closed form. This means that its time evolution is a sinusoidal motion. Let R be the ring of polynomials in x (the Racah case) or the ring of Laurent polynomials in q^x (the q-Racah case). Let us introduce an automorphism $\mathcal{I}$ in R by

$$
\mathcal{I}(x) = -x-d \quad : \mathrm{R}, \qquad \mathcal{I}(q^x) = q^{-x}d^{-1} \quad : q\mathrm{R}. \tag{3.17}
$$

Obviously it is an involution $\mathcal{I}^2 = \mathrm{id}$. The following remark is important.

Remark: If a (Laurent) polynomial $\check{f}$ in x (q^x) is invariant under the above involution, it is a polynomial in the sinusoidal coordinate $\eta(x;\boldsymbol{\lambda})$:

$$
\mathcal{I}\big(\check{f}(x)\big) = \check{f}(x) \;\Leftrightarrow\; \check{f}(x) = f\big(\eta(x;\boldsymbol{\lambda})\big). \tag{3.18}
$$

The system is shape invariant [44, 2],

$$
\mathcal{A}(\boldsymbol{\lambda})\mathcal{A}(\boldsymbol{\lambda})^\dagger = \kappa\mathcal{A}(\boldsymbol{\lambda}+\boldsymbol{\delta})^\dagger\mathcal{A}(\boldsymbol{\lambda}+\boldsymbol{\delta}) + \mathcal{E}_1(\boldsymbol{\lambda}), \tag{3.19}
$$

which is a sufficient condition for exact solvability and it provides the explicit formulas for the energy eigenvalues and the eigenfunctions, *i.e.* the generalised Rodrigues formula [2]. The forward and backward shift relations are

$$
\mathcal{F}(\boldsymbol{\lambda})\check{P}_n(x;\boldsymbol{\lambda}) = \mathcal{E}_n(\boldsymbol{\lambda})\check{P}_{n-1}(x;\boldsymbol{\lambda}+\boldsymbol{\delta}), \quad \mathcal{B}(\boldsymbol{\lambda})\check{P}_{n-1}(x;\boldsymbol{\lambda}+\boldsymbol{\delta}) = \check{P}_n(x;\boldsymbol{\lambda}), \tag{3.20}
$$

where the forward and backward shift operators are

$$
\mathcal{F}(\boldsymbol{\lambda}) = B(0;\boldsymbol{\lambda})\varphi(x;\boldsymbol{\lambda})^{-1}(1-e^{\partial}), \;\; \mathcal{B}(\boldsymbol{\lambda}) = B(0;\boldsymbol{\lambda})^{-1}\big(B(x;\boldsymbol{\lambda})-D(x;\boldsymbol{\lambda})e^{-\partial}\big)\varphi(x;\boldsymbol{\lambda}). \tag{3.21}
$$

We adopt the following choice of the parameter ranges:

$$\mathrm{R}: \quad a=-N, \quad 0<d<a+b, \quad 0<c<1+d, \tag{3.22}$$

$$q\mathrm{R}: \quad a=q^{-N}, \quad 0<ab<d<1, \quad qd<c<1, \tag{3.23}$$

and $x_{\max}=n_{\max}=N$. They are sufficient for the positivity of $B(x)$ and $D(x)$.

3.2 Multi-indexed (q)-Racah polynomials: type I

Let us define the twist operation $\mathfrak{t}$:

$$\mathfrak{t}(\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} (\lambda_4-\lambda_1+1, \lambda_4-\lambda_2+1, \lambda_3, \lambda_4), \quad \mathfrak{t}^2=\mathrm{id}. \tag{3.24}$$

The two functions $B'(x)$ and $D'(x)$ are defined by

$$B'(x;\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} B\bigl(x;\mathfrak{t}(\boldsymbol{\lambda})\bigr), \quad D'(x;\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} D\bigl(x;\mathfrak{t}(\boldsymbol{\lambda})\bigr), \tag{3.25}$$

namely,

$$B'(x;\boldsymbol{\lambda})=\begin{cases} -\dfrac{(x+d-a+1)(x+d-b+1)(x+c)(x+d)}{(2x+d)(2x+1+d)} & :\mathrm{R} \\ -\dfrac{(1-a^{-1}dq^{x+1})(1-b^{-1}dq^{x+1})(1-cq^x)(1-dq^x)}{(1-dq^{2x})(1-dq^{2x+1})} & :q\mathrm{R} \end{cases}, \tag{3.26}$$

$$D'(x;\boldsymbol{\lambda})=\begin{cases} -\dfrac{(x+a-1)(x+b-1)(x+d-c)x}{(2x-1+d)(2x+d)} & :\mathrm{R} \\ -\dfrac{cdq}{ab}\,\dfrac{(1-aq^{x-1})(1-bq^{x-1})(1-c^{-1}dq^x)(1-q^x)}{(1-dq^{2x-1})(1-dq^{2x})} & :q\mathrm{R} \end{cases}. \tag{3.27}$$

For M virtual states deletion, we further restrict the parameter range:

$$\mathrm{R}: \quad d+M<a+b, \qquad q\mathrm{R}: \quad ab<dq^M. \tag{3.28}$$

Then the essential properties of $B'(x)$ and $D'(x)$ (2.18)–(2.20) with $L=M$ are satisfied. The virtual Hamiltonian $\mathcal{H}'$, $\mathcal{E}'_{\mathrm{v}}$ and the virtual state vector $\tilde{\phi}_{\mathrm{v}}(x)$ are given by $\mathcal{H}(\mathfrak{t}(\boldsymbol{\lambda}))$, $\mathcal{E}_{\mathrm{v}}(\mathfrak{t}(\boldsymbol{\lambda}))$ and $\phi_{\mathrm{v}}(x;\mathfrak{t}(\boldsymbol{\lambda}))$. Namely,

$$\mathcal{H}(\boldsymbol{\lambda})=\alpha(\boldsymbol{\lambda})\mathcal{H}\bigl(\mathfrak{t}(\boldsymbol{\lambda})\bigr)+\alpha'(\boldsymbol{\lambda}), \tag{3.29}$$

$$\alpha(\boldsymbol{\lambda})=\begin{cases} 1 & :\mathrm{R} \\ abd^{-1}q^{-1} & :q\mathrm{R} \end{cases}, \quad \alpha'(\boldsymbol{\lambda})=\begin{cases} -c(a+b-d-1) & :\mathrm{R} \\ -(1-c)(1-abd^{-1}q^{-1}) & :q\mathrm{R} \end{cases}, \tag{3.30}$$

$$\tilde{\phi}_0(x;\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} \phi_0\bigl(x;\mathfrak{t}(\boldsymbol{\lambda})\bigr), \quad \tilde{\phi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} \phi_{\mathrm{v}}\bigl(x;\mathfrak{t}(\boldsymbol{\lambda})\bigr)=\tilde{\phi}_0(x;\boldsymbol{\lambda})\check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) \quad (\mathrm{v}\in\mathcal{V}), \tag{3.31}$$

$$\check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} \check{P}_{\mathrm{v}}\big(x;\mathfrak{t}(\boldsymbol{\lambda})\big), \quad \check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} \xi_{\mathrm{v}}\big(\eta(x;\boldsymbol{\lambda});\boldsymbol{\lambda}\big), \tag{3.32}$$

$$\mathcal{H}(\boldsymbol{\lambda})\tilde{\phi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) = \tilde{\mathcal{E}}_{\mathrm{v}}(\boldsymbol{\lambda})\tilde{\phi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) \quad (x=0,1,\ldots,x_{\max}-1),$$

$$\mathcal{H}(\boldsymbol{\lambda})\tilde{\phi}_{\mathrm{v}}(x_{\max};\boldsymbol{\lambda}) \neq \tilde{\mathcal{E}}_{\mathrm{v}}(\boldsymbol{\lambda})\tilde{\phi}_{\mathrm{v}}(x_{\max};\boldsymbol{\lambda}), \qquad \mathcal{E}'_{\mathrm{v}}(\boldsymbol{\lambda}) = \mathcal{E}_{\mathrm{v}}\big(\mathfrak{t}(\boldsymbol{\lambda})\big), \tag{3.33}$$

$$\tilde{\mathcal{E}}_{\mathrm{v}}(\boldsymbol{\lambda}) = \alpha(\boldsymbol{\lambda})\mathcal{E}'_{\mathrm{v}}(\boldsymbol{\lambda}) + \alpha'(\boldsymbol{\lambda}) = \begin{cases} -(c+\mathrm{v})(a+b-d-1-\mathrm{v}) & :\mathrm{R} \\ -(1-cq^{\mathrm{v}})(1-abd^{-1}q^{-1-\mathrm{v}}) & :q\mathrm{R} \end{cases}, \tag{3.34}$$

$$\nu(x;\boldsymbol{\lambda}) = \begin{cases} \dfrac{\Gamma(1-a)\Gamma(x+b)\Gamma(d-a+1)\Gamma(b-d-x)}{\Gamma(1-a-x)\Gamma(b)\Gamma(x+d-a+1)\Gamma(b-d)} & :\mathrm{R} \\ \dfrac{(a^{-1}q^{1-x},b,a^{-1}dq^{x+1},bd^{-1};q)_\infty}{(a^{-1}q,bq^x,a^{-1}dq,bd^{-1}q^{-x};q)_\infty} & :q\mathrm{R} \end{cases}. \tag{3.35}$$

Note that $\alpha'(\boldsymbol{\lambda}) = \tilde{\mathcal{E}}_0(\boldsymbol{\lambda}) < 0$. The index set of the virtual state vectors is

$$\mathcal{V} = \{1,2,\ldots,\mathrm{v}_{\max}\}, \quad \mathrm{v}_{\max} = \min\big\{[\lambda_1+\lambda_2-\lambda_4-1]', [\tfrac{1}{2}(\lambda_1+\lambda_2-\lambda_3-\lambda_4)]\big\}, \tag{3.36}$$

where $[x]$ denotes the greatest integer not exceeding x and $[x]'$ denotes the greatest integer not equal or exceeding x. The negative virtual state energy conditions (2.32) is met by $\mathrm{v}_{\max} \le [\lambda_1+\lambda_2-\lambda_4-1]'$. For the positivity of $\check{\xi}_{\mathrm{v}}(x)$ (2.31), we write down $\check{\xi}(x;\boldsymbol{\lambda})$ explicitly:

$$\begin{aligned}\check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) &= \begin{cases} {}_4F_3\left(\begin{matrix}-\mathrm{v},\ \mathrm{v}-a-b+c+d+1,\ -x,\ x+d \\ d-a+1,\ d-b+1,\ c\end{matrix}\,\middle|\, 1\right) & :\mathrm{R} \\ {}_4\phi_3\left(\begin{matrix}q^{-\mathrm{v}},\ a^{-1}b^{-1}cdq^{\mathrm{v}+1},\ q^{-x},\ dq^x \\ a^{-1}dq,\ b^{-1}dq,\ c\end{matrix}\,\middle|\, q\,;q\right) & :q\mathrm{R} \end{cases} \\ &= \begin{cases} \displaystyle\sum_{k=0}^{\mathrm{v}} \frac{(-\mathrm{v},\mathrm{v}-a-b+c+d+1,-x,x+d)_k}{(d-a+1,d-b+1,c)_k}\frac{1}{k!} & :\mathrm{R} \\ \displaystyle\sum_{k=0}^{\mathrm{v}} \frac{(q^{-\mathrm{v}},a^{-1}b^{-1}cdq^{\mathrm{v}+1},q^{-x},dq^x;q)_k}{(a^{-1}dq,b^{-1}dq,c;q)_k}\frac{q^k}{(q;q)_k} & :q\mathrm{R} \end{cases}.\end{aligned} \tag{3.37}$$

Each k-th term in the sum is non-negative for $2\mathrm{v}_{\max} \le \lambda_1+\lambda_2-\lambda_3-\lambda_4$.

Let us denote the eigenvector $\phi_{\mathcal{D}\,n}(x;\boldsymbol{\lambda})$ in (2.52) after M-deletions ($s=M$) by $\phi^{\mathrm{gen}}_{\mathcal{D}\,n}(x;\boldsymbol{\lambda})$. We define two polynomials $\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})$ and $\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})$, to be called the denominator polynomial and the multi-indexed orthogonal polynomial, respectively, from the Casoratians as follows:

$$\mathrm{W}[\check{\xi}_{d_1},\ldots,\check{\xi}_{d_M}](x;\boldsymbol{\lambda}) = \mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda})\varphi_M(x;\boldsymbol{\lambda})\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}), \tag{3.38}$$

$$\mathrm{W}[\check{\xi}_{d_1},\ldots,\check{\xi}_{d_M},\nu\check{P}_n](x;\boldsymbol{\lambda}) = \mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})\varphi_{M+1}(x;\boldsymbol{\lambda})\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})\nu(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}}), \tag{3.39}$$

$$\tilde{\boldsymbol{\delta}} \stackrel{\mathrm{def}}{=} (0,0,1,1), \qquad \mathfrak{t}(\boldsymbol{\lambda})+\beta\boldsymbol{\delta} = \mathfrak{t}(\boldsymbol{\lambda}+\beta\tilde{\boldsymbol{\delta}}) \quad (\forall\beta\in\mathbb{R}). \tag{3.40}$$

The constants $\mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda})$ and $\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})$ are specified later. The auxiliary function $\varphi_M(x;\boldsymbol{\lambda})$ is defined by [42]:

$$\varphi_M(x;\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} \prod_{1\le j<k\le M} \frac{\eta(x+k-1;\boldsymbol{\lambda})-\eta(x+j-1;\boldsymbol{\lambda})}{\eta(k-j;\boldsymbol{\lambda})}$$

$$= \prod_{1\le j<k\le M} \varphi\big(x+j-1;\boldsymbol{\lambda}+(k-j-1)\boldsymbol{\delta}\big), \tag{3.41}$$

and $\varphi_0(x;\boldsymbol{\lambda})=\varphi_1(x;\boldsymbol{\lambda})=1$. The eigenvector (2.52) is rewritten as

$$\phi^{\mathrm{gen}}_{\mathcal{D}\,n}(x;\boldsymbol{\lambda}) = (-1)^M \kappa^{\frac{1}{4}M(M-1)} \frac{\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})}{\mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda})} \sqrt{\prod_{j=1}^{M} \alpha(\boldsymbol{\lambda}) B'\big(0;\boldsymbol{\lambda}+(j-1)\tilde{\boldsymbol{\delta}}\big)}$$
$$\times \frac{\phi_0(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})}{\sqrt{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}} \check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}). \tag{3.42}$$

The multi-indexed orthogonal polynomial $\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})$ (3.39) has an expression

$$\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}) = \mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})^{-1}\varphi_{M+1}(x;\boldsymbol{\lambda})^{-1}$$
$$\times \begin{vmatrix} \check{\xi}_{d_1}(x_1) & \cdots & \check{\xi}_{d_M}(x_1) & r_1(x_1)\check{P}_n(x_1) \\ \check{\xi}_{d_1}(x_2) & \cdots & \check{\xi}_{d_M}(x_2) & r_2(x_2)\check{P}_n(x_2) \\ \vdots & \cdots & \vdots & \vdots \\ \check{\xi}_{d_1}(x_{M+1}) & \cdots & \check{\xi}_{d_M}(x_{M+1}) & r_{M+1}(x_{M+1})\check{P}_n(x_{M+1}) \end{vmatrix}, \tag{3.43}$$

where $x_j \overset{\mathrm{def}}{=} x+j-1$ and $r_j(x)=r_j(x;\boldsymbol{\lambda},M)$ $(1\le j\le M+1)$ are given by

$$r_j\big(x+j-1;\boldsymbol{\lambda},M\big) \overset{\mathrm{def}}{=} \begin{cases} \dfrac{(x+a,x+b)_{j-1}(x+d-a+j,x+d-b+j)_{M+1-j}}{(d-a+1,d-b+1)_M} & :\mathrm{R} \\[2ex] \dfrac{(aq^x,bq^x;q)_{j-1}(a^{-1}dq^{x+j},b^{-1}dq^{x+j};q)_{M+1-j}}{(abd^{-1}q^{-1})^{j-1}q^{Mx}(a^{-1}dq,b^{-1}dq;q)_M} & :q\mathrm{R} \end{cases}. \tag{3.44}$$

Reflecting the involution properties (3.18) of the basic polynomials $\check{P}_n(x)$ and $\check{\xi}_{d_j}(x)$, $\check{\Xi}_{\mathcal{D}}$ (3.38) and $\check{P}_{\mathcal{D},n}$ (3.43) are also polynomials in η:

$$\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}) \overset{\mathrm{def}}{=} \Xi_{\mathcal{D}}\big(\eta(x;\boldsymbol{\lambda}+(M-1)\tilde{\boldsymbol{\delta}});\boldsymbol{\lambda}\big), \quad \check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}) \overset{\mathrm{def}}{=} P_{\mathcal{D},n}\big(\eta(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}});\boldsymbol{\lambda}\big), \tag{3.45}$$

and their degrees are generically ℓ and $\ell+n$, respectively. Here ℓ is

$$\ell \overset{\mathrm{def}}{=} \sum_{j=1}^{M} d_j - \tfrac{1}{2}M(M-1). \tag{3.46}$$

We adopt the standard normalisation for $\check{\Xi}_{\mathcal{D}}$ and $\check{P}_{\mathcal{D},n}$: $\check{\Xi}_{\mathcal{D}}(0;\boldsymbol{\lambda})=1$, $\check{P}_{\mathcal{D},n}(0;\boldsymbol{\lambda})=1$, which determine the constants $\mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda})$ and $\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})$,

$$\mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda}) \overset{\mathrm{def}}{=} \frac{1}{\varphi_M(0;\boldsymbol{\lambda})} \prod_{1\le j<k\le M} \frac{\tilde{\mathcal{E}}_{d_j}(\boldsymbol{\lambda})-\tilde{\mathcal{E}}_{d_k}(\boldsymbol{\lambda})}{\alpha(\boldsymbol{\lambda})B'(j-1;\boldsymbol{\lambda})}, \tag{3.47}$$

$$\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda}) \stackrel{\text{def}}{=} (-1)^M \mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda}) \tilde{d}_{\mathcal{D},n}(\boldsymbol{\lambda})^2, \quad \tilde{d}_{\mathcal{D},n}(\boldsymbol{\lambda})^2 \stackrel{\text{def}}{=} \frac{\varphi_M(0;\boldsymbol{\lambda})}{\varphi_{M+1}(0;\boldsymbol{\lambda})} \prod_{j=1}^{M} \frac{\mathcal{E}_n(\boldsymbol{\lambda}) - \tilde{\mathcal{E}}_{d_j}(\boldsymbol{\lambda})}{\alpha(\boldsymbol{\lambda}) B'(j-1;\boldsymbol{\lambda})}. \tag{3.48}$$

The use of *dual polynomials* $Q_x(\mathcal{E}(n)) \stackrel{\text{def}}{=} P_n(\eta(x))$ [2] is essential for the derivation of these results. The three term recurrence relations of $\{Q_x(\mathcal{E})\}$ are specified by $B(x)$ and $D(x)$. The denominator polynomial $\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})$ is positive for $x = 0, 1, \ldots, x_{\max} + 1$. The lowest degree multi-indexed orthogonal polynomial $\check{P}_{\mathcal{D},0}(x;\boldsymbol{\lambda})$ is related to $\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})$ by the parameter shift $\boldsymbol{\lambda} \to \boldsymbol{\lambda} + \boldsymbol{\delta}$:

$$\check{P}_{\mathcal{D},0}(x;\boldsymbol{\lambda}) = \check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda} + \boldsymbol{\delta}). \tag{3.49}$$

The potential functions $B_{\mathcal{D}}$ and $D_{\mathcal{D}}$ (2.57)–(2.58) after M-deletion ($s = M$) can be expressed neatly in terms of the denominator polynomial:

$$B_{\mathcal{D}}(x;\boldsymbol{\lambda}) = B(x;\boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}) \frac{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})} \frac{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})}, \tag{3.50}$$

$$D_{\mathcal{D}}(x;\boldsymbol{\lambda}) = D(x;\boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}) \frac{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})} \frac{\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})}. \tag{3.51}$$

These formulas look similar to those in the exceptional polynomials [23]. The groundstate eigenvector $\phi_{\mathcal{D}\,0}$ is expressed by $\phi_0(x)$ (2.8) and $\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})$:

$$\begin{aligned}\phi_{\mathcal{D}\,0}(x;\boldsymbol{\lambda}) &= \sqrt{\prod_{y=0}^{x-1} \frac{B_{\mathcal{D}}(y)}{D_{\mathcal{D}}(y+1)}} = \phi_0(x;\boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}) \sqrt{\frac{\check{\Xi}_{\mathcal{D}}(1;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}}\, \check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta}) \\ &= \psi_{\mathcal{D}}(x;\boldsymbol{\lambda}) \check{P}_{\mathcal{D},0}(x;\boldsymbol{\lambda}) \propto \phi^{\text{gen}}_{\mathcal{D}\,0}(x;\boldsymbol{\lambda}),\end{aligned} \tag{3.52}$$

$$\psi_{\mathcal{D}}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \sqrt{\check{\Xi}_{\mathcal{D}}(1;\boldsymbol{\lambda})}\, \frac{\phi_0(x;\boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}})}{\sqrt{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})\, \check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}}, \quad \psi_{\mathcal{D}}(0;\boldsymbol{\lambda}) = 1. \tag{3.53}$$

We arrive at the normalised eigenvector $\phi_{\mathcal{D}\,n}(x;\boldsymbol{\lambda})$ with the orthogonality relation,

$$\phi_{\mathcal{D}\,n}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x;\boldsymbol{\lambda}) \check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}) \propto \phi^{\text{gen}}_{\mathcal{D}\,n}(x;\boldsymbol{\lambda}), \quad \phi_{\mathcal{D}\,n}(0;\boldsymbol{\lambda}) = 1, \tag{3.54}$$

$$\sum_{x=0}^{x_{\max}} \frac{\psi_{\mathcal{D}}(x;\boldsymbol{\lambda})^2}{\check{\Xi}_{\mathcal{D}}(1;\boldsymbol{\lambda})} \check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}) \check{P}_{\mathcal{D},m}(x;\boldsymbol{\lambda}) = \frac{\delta_{nm}}{d_n(\boldsymbol{\lambda})^2 \tilde{d}_{\mathcal{D},n}(\boldsymbol{\lambda})^2} \quad (n, m = 0, 1, \ldots, n_{\max}). \tag{3.55}$$

It is worthwhile to emphasise that the above orthogonality relation is a rational equation of $\boldsymbol{\lambda}$ or $q^{\boldsymbol{\lambda}}$, and it is valid for any value of $\boldsymbol{\lambda}$ (except for the zeros of denominators) but the weight function may not be positive definite.

The shape invariance of the original system is inherited by the deformed systems. The matrix $\hat{\mathcal{A}}_{d_1 \ldots d_{s+1}}(\boldsymbol{\lambda})$ intertwines the two Hamiltonians $\mathcal{H}_{d_1 \ldots d_s}(\boldsymbol{\lambda})$ and $\mathcal{H}_{d_1 \ldots d_{s+1}}(\boldsymbol{\lambda})$,

$$\hat{\mathcal{A}}_{d_1 \ldots d_{s+1}}(\boldsymbol{\lambda})^\dagger \hat{\mathcal{A}}_{d_1 \ldots d_{s+1}}(\boldsymbol{\lambda}) = \mathcal{H}_{d_1 \ldots d_s}(\boldsymbol{\lambda}) - \tilde{\mathcal{E}}_{d_{s+1}}(\boldsymbol{\lambda}),$$

$$\hat{\mathcal{A}}_{d_1\dots d_{s+1}}(\boldsymbol{\lambda})\hat{\mathcal{A}}_{d_1\dots d_{s+1}}(\boldsymbol{\lambda})^\dagger = \mathcal{H}_{d_1\dots d_{s+1}}(\boldsymbol{\lambda}) - \tilde{\mathcal{E}}_{d_{s+1}}(\boldsymbol{\lambda}),$$

and it has the inverse. By the same argument given in § 4 of [19], the shape invariance of $\mathcal{H}(\boldsymbol{\lambda})$ is inherited by $\mathcal{H}_{d_1}(\boldsymbol{\lambda})$, $\mathcal{H}_{d_1 d_2}(\boldsymbol{\lambda})$, $\cdots$. Therefore the Hamiltonian $\mathcal{H}_{\mathcal{D}}(\boldsymbol{\lambda})$ is shape invariant:

$$\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})^\dagger = \kappa\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda}+\boldsymbol{\delta})^\dagger\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda}+\boldsymbol{\delta}) + \mathcal{E}_1(\boldsymbol{\lambda}). \tag{3.56}$$

As a consequence of the shape invariance and the normalisation, the actions of $\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})$ and $\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})^\dagger$ on the eigenvectors $\phi_{\mathcal{D}\,n}(x;\boldsymbol{\lambda})$ are

$$\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})\phi_{\mathcal{D}\,n}(x;\boldsymbol{\lambda}) = \frac{\mathcal{E}_n(\boldsymbol{\lambda})}{\sqrt{B_{\mathcal{D}}(0;\boldsymbol{\lambda})}}\,\phi_{\mathcal{D}\,n-1}(x;\boldsymbol{\lambda}+\boldsymbol{\delta}) \quad (x=0,1,\dots,x_{\max}-1), \tag{3.57}$$

$$\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})^\dagger\phi_{\mathcal{D}\,n-1}(x;\boldsymbol{\lambda}+\boldsymbol{\delta}) = \sqrt{B_{\mathcal{D}}(0;\boldsymbol{\lambda})}\,\phi_{\mathcal{D}\,n}(x;\boldsymbol{\lambda}) \quad (x=0,1,\dots,x_{\max}). \tag{3.58}$$

The forward and backward shift operators are defined by

$$\begin{aligned}\mathcal{F}_{\mathcal{D}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \sqrt{B_{\mathcal{D}}(0;\boldsymbol{\lambda})}\,\psi_{\mathcal{D}}\,(x;\boldsymbol{\lambda}+\boldsymbol{\delta})^{-1}\circ\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})\circ\psi_{\mathcal{D}}\,(x;\boldsymbol{\lambda})\\ &= \frac{B(0;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})}{\varphi(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}\Big(\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda}+\boldsymbol{\delta}) - \check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})e^{\partial}\Big),\end{aligned} \tag{3.59}$$

$$\begin{aligned}\mathcal{B}_{\mathcal{D}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \frac{1}{\sqrt{B_{\mathcal{D}}(0;\boldsymbol{\lambda})}}\,\psi_{\mathcal{D}}\,(x;\boldsymbol{\lambda})^{-1}\circ\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})^\dagger\circ\psi_{\mathcal{D}}\,(x;\boldsymbol{\lambda}+\boldsymbol{\delta})\\ &= \frac{1}{B(0;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})}\\ &\quad\times\Big(B(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}) - D(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})e^{-\partial}\Big)\varphi(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}}),\end{aligned} \tag{3.60}$$

and their actions on $\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})$ are

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

As in the original (q)-Racah theory (3.20), these formulas are useful for the explicit calculation of the multi-indexed polynomials. The similarity transformed Hamiltonian is

$$\begin{aligned}\widetilde{\mathcal{H}}_{\mathcal{D}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x;\boldsymbol{\lambda})^{-1}\circ\mathcal{H}_{\mathcal{D}}(\boldsymbol{\lambda})\circ\psi_{\mathcal{D}}(x;\boldsymbol{\lambda}) = \mathcal{B}_{\mathcal{D}}(\boldsymbol{\lambda})\mathcal{F}_{\mathcal{D}}(\boldsymbol{\lambda})\\ &= B(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\,\frac{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}\left(\frac{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})} - e^{\partial}\right)\\ &\quad + D(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\,\frac{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})}\left(\frac{\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})} - e^{-\partial}\right),\end{aligned} \tag{3.61}$$

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

$$\widetilde{\mathcal{H}}_{\mathcal{D}}(\boldsymbol{\lambda})\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}) = \mathcal{E}_n(\boldsymbol{\lambda})\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}). \tag{3.62}$$

Other intertwining relations are

$$\kappa^{\frac{1}{2}}\hat{\mathcal{A}}_{d_1\dots d_{s+1}}(\boldsymbol{\lambda}+\boldsymbol{\delta})\mathcal{A}_{d_1\dots d_s}(\boldsymbol{\lambda})=\mathcal{A}_{d_1\dots d_{s+1}}(\boldsymbol{\lambda})\hat{\mathcal{A}}_{d_1\dots d_{s+1}}(\boldsymbol{\lambda}),$$
$$\kappa^{-\frac{1}{2}}\hat{\mathcal{A}}_{d_1\dots d_{s+1}}(\boldsymbol{\lambda})\mathcal{A}_{d_1\dots d_s}(\boldsymbol{\lambda})^{\dagger}=\mathcal{A}_{d_1\dots d_{s+1}}(\boldsymbol{\lambda})^{\dagger}\hat{\mathcal{A}}_{d_1\dots d_{s+1}}(\boldsymbol{\lambda}+\boldsymbol{\delta}),$$

with the potential functions given in (2.45)–(2.46) (with $s\to s+1$).

Including the level 0 deletion corresponds to $M-1$ virtual states deletion.

$$\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})\Big|_{d_M=0}=\check{P}_{\mathcal{D}',n}(x;\boldsymbol{\lambda}+\tilde{\boldsymbol{\delta}}),\quad \mathcal{D}'=\{d_1-1,\dots,d_{M-1}-1\}. \tag{3.63}$$

This formula is similar to those in the multi-indexed Jacobi theory, eqs.(48)–(49) in [1]. The denominator polynomial $\Xi_{\mathcal{D}}$ behaves similarly. This is why we have restricted $d_j\geq 1$.

The exceptional X_ℓ (q)-Racah orthogonal polynomials presented in [23] correspond to the simplest case $M=1$, $\mathcal{D}=\{\ell\}$, $\ell\geq 1$:

$$\check{\xi}_\ell(x;\boldsymbol{\lambda})=\check{\Xi}_{\{\ell\}}(x;\boldsymbol{\lambda}+\ell\boldsymbol{\delta}-\tilde{\boldsymbol{\delta}}),\quad \check{P}_{\ell,n}(x;\boldsymbol{\lambda})=\check{P}_{\{\ell\},n}(x;\boldsymbol{\lambda}+\ell\boldsymbol{\delta}-\tilde{\boldsymbol{\delta}}). \tag{3.64}$$

3.3 Multi-indexed (q)-Racah polynomials: type II

For the type II, the virtual Hamiltonian $\mathcal{H}'$ (3.72) is defined by twisting parameters combined with the coordinate reflection $x\to N-x$. Since N is a part of the parameters, the twist operator $\mathfrak{t}$

$$\mathfrak{t}(\boldsymbol{\lambda})\stackrel{\text{def}}{=}(\lambda_1-\lambda_4+1,\lambda_1+\lambda_2-\lambda_4,\lambda_1-\lambda_3+1,2\lambda_1-\lambda_4),\quad \mathfrak{t}^2\neq\mathrm{id}, \tag{3.65}$$

is not an involution. The two functions $B'(x)$ and $D'(x)$ are defined by

$$B'(x;\boldsymbol{\lambda})\stackrel{\text{def}}{=}D\big(N-x;\mathfrak{t}(\boldsymbol{\lambda})\big),\quad D'(x;\boldsymbol{\lambda})\stackrel{\text{def}}{=}B\big(N-x;\mathfrak{t}(\boldsymbol{\lambda})\big), \tag{3.66}$$

namely,

$$B'(x;\boldsymbol{\lambda})=\begin{cases}-\dfrac{(x+a)(x+b)(x+d-c+1)(x+1)}{(2x+d)(2x+1+d)} & :\mathrm{R}\\[2ex] -\dfrac{(1-aq^x)(1-bq^x)(1-c^{-1}dq^{x+1})(1-q^{x+1})}{(1-dq^{2x})(1-dq^{2x+1})} & :q\mathrm{R}\end{cases}, \tag{3.67}$$

$$D'(x;\boldsymbol{\lambda})=\begin{cases}-\dfrac{(x+d-a)(x+d-b)(x+c-1)(x+d-1)}{(2x-1+d)(2x+d)} & :\mathrm{R}\\[2ex] -\dfrac{abq}{cd}\,\dfrac{(1-a^{-1}dq^x)(1-b^{-1}dq^x)(1-cq^{x-1})(1-dq^{x-1})}{(1-dq^{2x-1})(1-dq^{2x})} & :q\mathrm{R}\end{cases}, \tag{3.68}$$

and we recall $\lambda_1 = -N$. Note that $\varphi\big(N-x;\mathfrak{t}(\boldsymbol{\lambda})\big) = \varphi(x-1;\boldsymbol{\lambda})/\varphi(N-1;\boldsymbol{\lambda})$ and (3.5) implies

$$\frac{D'(x;\boldsymbol{\lambda}+\tilde{\boldsymbol{\delta}})}{D'(x-1;\boldsymbol{\lambda})} = \kappa^{-1}\frac{\varphi(x-2;\boldsymbol{\lambda})}{\varphi(x-1;\boldsymbol{\lambda})}, \quad \frac{B'(x;\boldsymbol{\lambda}+\tilde{\boldsymbol{\delta}})}{B'(x;\boldsymbol{\lambda})} = \kappa^{-1}\frac{\varphi(x;\boldsymbol{\lambda})}{\varphi(x-1;\boldsymbol{\lambda})}, \tag{3.69}$$

$$\tilde{\boldsymbol{\delta}} \stackrel{\text{def}}{=} (0,0,-1,-1), \quad \mathfrak{t}(\boldsymbol{\lambda}) + \beta\boldsymbol{\delta} = \mathfrak{t}(\boldsymbol{\lambda}+\beta\tilde{\boldsymbol{\delta}}) \ \ (\forall\beta\in\mathbb{R}). \tag{3.70}$$

For M virtual states deletion, we restrict the parameter range:

$$\mathrm{R}: \quad M<c, \quad 2M<1+d, \qquad q\mathrm{R}: \quad c<q^M, \quad qd<q^{2M}, \tag{3.71}$$

so that the essential properties of B' and D' (2.59)–(2.61) with $L=M$ are satisfied. The virtual Hamiltonian $\mathcal{H}'$, $\mathcal{E}'_{\mathrm{v}}$ and the virtual state vectors $\tilde{\phi}_{\mathrm{v}}(x)$ are $\mathcal{H}(\mathfrak{t}(\boldsymbol{\lambda}))|_{x\to N-x}$, $\mathcal{E}_{\mathrm{v}}(\mathfrak{t}(\boldsymbol{\lambda}))$ and $\phi_{\mathrm{v}}(N-x;\mathfrak{t}(\boldsymbol{\lambda}))$, namely,

$$\mathcal{H}(\boldsymbol{\lambda}) = \alpha(\boldsymbol{\lambda})\mathcal{H}\big(\mathfrak{t}(\boldsymbol{\lambda})\big)|_{x\to N-x} + \alpha'(\boldsymbol{\lambda}), \tag{3.72}$$

$$\alpha(\boldsymbol{\lambda}) = \begin{cases} 1 & :\mathrm{R} \\ cq^{-1} & :q\mathrm{R} \end{cases}, \quad \alpha'(\boldsymbol{\lambda}) = \begin{cases} -(c-1)(a+b-d) & :\mathrm{R} \\ -(1-cq^{-1})(1-abd^{-1}) & :q\mathrm{R} \end{cases}, \tag{3.73}$$

$$\tilde{\phi}_0(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \phi_0\big(N-x;\mathfrak{t}(\boldsymbol{\lambda})\big)\phi_0\big(N;\mathfrak{t}(\boldsymbol{\lambda})\big)^{-1}, \quad \tilde{\phi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \tilde{\phi}_0(x;\boldsymbol{\lambda})\check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) \quad (\mathrm{v}\in\mathcal{V}), \tag{3.74}$$

$$\check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \check{P}_{\mathrm{v}}\big(N-x;\mathfrak{t}(\boldsymbol{\lambda})\big), \quad \check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \xi_{\mathrm{v}}\big(\eta(x;\boldsymbol{\lambda});\boldsymbol{\lambda}\big), \tag{3.75}$$

$$\mathcal{H}(\boldsymbol{\lambda})\tilde{\phi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) = \tilde{\mathcal{E}}_{\mathrm{v}}(\boldsymbol{\lambda})\tilde{\phi}_{\mathrm{v}}(x;\boldsymbol{\lambda}) \ \ (x=1,\dots,x_{\max}),$$

$$\mathcal{H}(\boldsymbol{\lambda})\tilde{\phi}_{\mathrm{v}}(0;\boldsymbol{\lambda}) \neq \tilde{\mathcal{E}}_{\mathrm{v}}(\boldsymbol{\lambda})\tilde{\phi}_{\mathrm{v}}(0;\boldsymbol{\lambda}), \qquad \mathcal{E}'_{\mathrm{v}}(\boldsymbol{\lambda}) = \mathcal{E}_{\mathrm{v}}\big(\mathfrak{t}(\boldsymbol{\lambda})\big), \tag{3.76}$$

$$\tilde{\mathcal{E}}_{\mathrm{v}}(\boldsymbol{\lambda}) = \alpha(\boldsymbol{\lambda})\mathcal{E}'_{\mathrm{v}}(\boldsymbol{\lambda}) + \alpha'(\boldsymbol{\lambda}) = \begin{cases} -(c-\mathrm{v}-1)(a+b-d+\mathrm{v}) & :\mathrm{R} \\ -(1-cq^{-\mathrm{v}-1})(1-abd^{-1}q^{\mathrm{v}}) & :q\mathrm{R} \end{cases}, \tag{3.77}$$

$$\nu(x;\boldsymbol{\lambda}) = \begin{cases} \dfrac{\Gamma(x+c)\Gamma(x+d)}{\Gamma(c)\Gamma(d)}\dfrac{\Gamma(d-c+1)}{\Gamma(x+d-c+1)\Gamma(x+1)} & :\mathrm{R} \\ (c^{-1}q)^x\dfrac{(c,d;q)_\infty}{(cq^x,dq^x;q)_\infty}\dfrac{(c^{-1}dq^{x+1},q^{x+1};q)_\infty}{(c^{-1}dq,q;q)_\infty} & :q\mathrm{R} \end{cases}. \tag{3.78}$$

Note that $\check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda})$ is normalised to be unity at $x=N$, instead of $x=0$ in the type I case. Here $\alpha'(\boldsymbol{\lambda}) = \tilde{\mathcal{E}}_0(\boldsymbol{\lambda}) < 0$ holds by definition. The first equation in (3.4) implies

$$\frac{\varphi(x-1;\boldsymbol{\lambda})}{\varphi(N-1;\boldsymbol{\lambda})} = \sqrt{\frac{D'(N;\boldsymbol{\lambda})}{D'(x;\boldsymbol{\lambda})}}\,\frac{\tilde{\phi}_0(x;\boldsymbol{\lambda}+\tilde{\boldsymbol{\delta}})}{\tilde{\phi}_0(x;\boldsymbol{\lambda})}\,\frac{\phi_0\big(N;\mathfrak{t}(\boldsymbol{\lambda}+\tilde{\boldsymbol{\delta}})\big)}{\phi_0\big(N;\mathfrak{t}(\boldsymbol{\lambda})\big)}. \tag{3.79}$$

Due the invariance under the involution (3.17) $\check{\xi}_{\mathrm{v}}(-x-\lambda_4;\boldsymbol{\lambda}) = \check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda})$, $\check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda})$ is a polynomial in $\eta(x;\boldsymbol{\lambda})$ by Remark (3.18). The index set of the virtual state vectors is

$$\mathcal{V} = \{1,2,\dots,\mathrm{v}_{\max}\}, \quad \mathrm{v}_{\max} \stackrel{\text{def}}{=} \min\big\{[\lambda_3-1]', [\tfrac{1}{2}(-\lambda_1-\lambda_2+\lambda_3+\lambda_4)]\big\}. \tag{3.80}$$

The negative energy condition (2.67) is satisfied by $\mathrm{v}_{\max} \leq [\lambda_3 - 1]'$. The other limit is determined by the positivity of the virtual state vectors as in the type I case (3.37).

Let us denote $\phi_{\mathcal{D}\,n}(x;\boldsymbol{\lambda})$ in (2.86) with $s = M$ by $\phi^{\mathrm{gen}}_{\mathcal{D}\,n}(x;\boldsymbol{\lambda})$ and evaluate it explicitly. The polynomials $\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})$, $\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})$ are defined in terms of the Casoratians as follows:

$$\mathrm{W}^{(-)}[\check{\xi}_{d_1},\ldots,\check{\xi}_{d_M}](x;\boldsymbol{\lambda}) = \mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda})\varphi^{(-)}_M(x;\boldsymbol{\lambda})\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}), \tag{3.81}$$

$$\mathrm{W}^{(-)}[\check{\xi}_{d_1},\ldots,\check{\xi}_{d_M},\nu\check{P}_n](x;\boldsymbol{\lambda}) = \mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})\varphi^{(-)}_{M+1}(x;\boldsymbol{\lambda})\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})\nu(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}}), \tag{3.82}$$

where $\mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda})$ and $\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})$ are specified later. The auxiliary function $\varphi^{(-)}_M(x;\boldsymbol{\lambda})$ is defined by

$$\begin{aligned}\varphi^{(-)}_M(x;\boldsymbol{\lambda}) &\stackrel{\mathrm{def}}{=} \prod_{1\leq j<k\leq M}\frac{\eta(x-j+1;\boldsymbol{\lambda})-\eta(x-k+1;\boldsymbol{\lambda})}{\eta(k-j;\boldsymbol{\lambda})} = \varphi_M(x-M+1;\boldsymbol{\lambda})\\ &= \prod_{1\leq j<k\leq M}\varphi\big(x-k+1;\boldsymbol{\lambda}+(k-j-1)\boldsymbol{\delta}\big),\end{aligned} \tag{3.83}$$

and $\varphi^{(-)}_0(x;\boldsymbol{\lambda}) = \varphi^{(-)}_1(x;\boldsymbol{\lambda}) = 1$. The eigenvector (2.86) is rewritten as

$$\begin{aligned}\phi^{\mathrm{gen}}_{\mathcal{D}\,n}(x;\boldsymbol{\lambda}) = (-1)^M\kappa^{\frac{1}{4}M(M-1)}\frac{\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})}{\mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda})}&\sqrt{\prod_{j=1}^M\alpha(\boldsymbol{\lambda})D'\big(N;\boldsymbol{\lambda}+(j-1)\tilde{\boldsymbol{\delta}}\big)}\\ &\times\frac{\phi_0\big(N;\mathfrak{t}(\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\big)}{\phi_0\big(N;\mathfrak{t}(\boldsymbol{\lambda})\big)}\prod_{j=1}^M\frac{\varphi\big(N-1;\boldsymbol{\lambda}-(j-1)\boldsymbol{\delta}\big)}{\prod_{k=0}^{j-2}\varphi\big(1;\boldsymbol{\lambda}+(2k-j+1)\boldsymbol{\delta}\big)}\\ &\times\frac{\phi_0(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})}{\sqrt{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda})}}\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}).\end{aligned} \tag{3.84}$$

The multi-indexed orthogonal polynomial $\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})$ (3.82) has the same Casoratian expression (3.43) as in the type I case with $\varphi_{M+1}(x)$ replaced by $\varphi^{(-)}_{M+1}(x)$ and $x_j \stackrel{\mathrm{def}}{=} x-j+1$, $r_j(x) = r_j(x;\boldsymbol{\lambda},M)$ $(1\leq j\leq M+1)$ are given by

$$r_j\big(x-j+1;\boldsymbol{\lambda},M\big) \stackrel{\mathrm{def}}{=} \begin{cases}\dfrac{(x-c+d-j+2,x-j+2)_{j-1}(x+c-M,x+d-M)_{M+1-j}}{(c-M,d-M)_M} & :\mathrm{R}\\[2ex] \dfrac{(c^{-1}dq^{x-j+2},q^{x-j+2};q)_{j-1}(cq^{x-M},dq^{x-M};q)_{M+1-j}}{(c^{-1}q)^{j-1}q^{Mx}(cq^{-M},dq^{-M};q)_M} & :q\mathrm{R}\end{cases}. \tag{3.85}$$

As in the type I case, $\check{\Xi}_{\mathcal{D}}$ (3.81) and $\check{P}_{\mathcal{D},n}$ (3.82) are degree ℓ and $\ell+n$ polynomials in η, with the same form of the sinusoidal coordinate dependence (3.45), but the actual values of $\tilde{\boldsymbol{\delta}}$ are different in the type I (3.40) and type II (3.70). The degree formula is also the same as that in the type I, (3.46). The normalisation of $\check{\Xi}_{\mathcal{D}}$ and $\check{P}_{\mathcal{D},n}$ are chosen to be, $\check{\Xi}_{\mathcal{D}}(N;\boldsymbol{\lambda}) = 1$,

$\check{P}_{\mathcal{D},n}(N;\boldsymbol{\lambda})=1$, which determine the constants $\mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda})$ and $\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})$,

$$\mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{1}{\varphi_M^{(-)}(N;\boldsymbol{\lambda})} \prod_{1\le j<k\le M} \frac{\tilde{\mathcal{E}}_{d_j}(\boldsymbol{\lambda})-\tilde{\mathcal{E}}_{d_k}(\boldsymbol{\lambda})}{\alpha(\boldsymbol{\lambda})D'(N-j+1;\boldsymbol{\lambda})}, \tag{3.86}$$

$$\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda})\tilde{d}_{\mathcal{D},n}(\boldsymbol{\lambda})^2 \frac{\kappa^{-\frac{1}{2}M(M-1)}}{\check{P}_n(N;\boldsymbol{\lambda})} \prod_{j=1}^{M} \frac{\tilde{\mathcal{E}}_{j-1}(\boldsymbol{\lambda})\varphi\big(j;\boldsymbol{\lambda}-(j+1)\boldsymbol{\delta}\big)}{\alpha(\boldsymbol{\lambda})D'\big(0;\boldsymbol{\lambda}+(j-1)\tilde{\boldsymbol{\delta}}\big)},$$

$$\tilde{d}_{\mathcal{D},n}(\boldsymbol{\lambda})^2 \stackrel{\text{def}}{=} \kappa^{\frac{1}{2}M(M-1)}\check{P}_n(N;\boldsymbol{\lambda})^2 \prod_{j=1}^{M} \frac{\mathcal{E}_n(\boldsymbol{\lambda})-\tilde{\mathcal{E}}_{d_j}(\boldsymbol{\lambda})}{\tilde{\mathcal{E}}_{j-1}(\boldsymbol{\lambda})} \cdot \prod_{j=1}^{M} \frac{\alpha(\boldsymbol{\lambda})D'\big(0;\boldsymbol{\lambda}+(j-1)\tilde{\boldsymbol{\delta}}\big)}{\tilde{\mathcal{E}}_{j-1}(\boldsymbol{\lambda})}. \tag{3.87}$$

The denominator polynomial $\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})$ is positive for $x=-1,0,1,\ldots,x_{\max}$. The lowest degree polynomial $\check{P}_{\mathcal{D},0}(x;\boldsymbol{\lambda})$ is related to $\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})$ by the parameter shift $\boldsymbol{\lambda}\to\boldsymbol{\lambda}+\boldsymbol{\delta}$ and the coordinate shift $x\to x-1$:

$$\check{P}_{\mathcal{D},0}(x;\boldsymbol{\lambda}) = \check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda}+\boldsymbol{\delta}). \tag{3.88}$$

The normalisation $\Xi_{\mathcal{D}}\big(N;(-N,\lambda_2,\ \lambda_3,\lambda_4)\big)=1$, means $\Xi_{\mathcal{D}}\big(N-1;(-N+1,\lambda_2+1,\lambda_3+1,\lambda_4+1)\big)=1$. Based on this relation, the potential functions $B_{\mathcal{D}}$ and $D_{\mathcal{D}}$ (2.88)–(2.89) with $s=M$ are expressed in terms of the denominator polynomials

$$B_{\mathcal{D}}(x;\boldsymbol{\lambda}) = B(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\,\frac{\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})}\frac{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda}+\boldsymbol{\delta})}, \tag{3.89}$$

$$D_{\mathcal{D}}(x;\boldsymbol{\lambda}) = D(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\,\frac{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda})}\frac{\check{\Xi}_{\mathcal{D}}(x-2;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda}+\boldsymbol{\delta})}. \tag{3.90}$$

With a different normalisation $\phi_{\mathcal{D}\,0}(N;\boldsymbol{\lambda})=1$, the ground state $\phi_{\mathcal{D}\,0}$ is calculated to be

$$\begin{aligned}
\phi_{\mathcal{D}\,0}(x;\boldsymbol{\lambda}) &= \Big(\prod_{y=0}^{x-1}\frac{B_{\mathcal{D}}(y)}{D_{\mathcal{D}}(y+1)}\Big)^{\frac{1}{2}} \times \Big(\prod_{y=0}^{N-1}\frac{B_{\mathcal{D}}(y)}{D_{\mathcal{D}}(y+1)}\Big)^{-\frac{1}{2}} = \sqrt{\prod_{y=x}^{N-1}\frac{D_{\mathcal{D}}(y+1)}{B_{\mathcal{D}}(y)}} \\
&= \frac{\phi_0(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})}{\phi_0(N;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})}\sqrt{\frac{\check{\Xi}_{\mathcal{D}}(N-1;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda})}}\,\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda}+\boldsymbol{\delta}) \\
&= \psi_{\mathcal{D}}(x;\boldsymbol{\lambda})\check{P}_{\mathcal{D},0}(x;\boldsymbol{\lambda}) \propto \phi^{\text{gen}}_{\mathcal{D}\,0}(x;\boldsymbol{\lambda}),
\end{aligned} \tag{3.91}$$

$$\psi_{\mathcal{D}}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{\sqrt{\check{\Xi}_{\mathcal{D}}(N-1;\boldsymbol{\lambda})}}{\phi_0(N;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})}\,\frac{\phi_0(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})}{\sqrt{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})\,\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda})}}, \quad \psi_{\mathcal{D}}(N;\boldsymbol{\lambda})=1. \tag{3.92}$$

By changing the overall normalisation we define the eigenvector $\phi_{\mathcal{D}\,n}(x;\boldsymbol{\lambda})$,

$$\phi_{\mathcal{D}\,n}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x;\boldsymbol{\lambda})\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}) \propto \phi^{\text{gen}}_{\mathcal{D}\,n}(x;\boldsymbol{\lambda}), \quad \phi_{\mathcal{D}\,n}(N;\boldsymbol{\lambda})=1. \tag{3.93}$$

The orthogonality relation (2.85) reads ($n, m = 0, 1, \ldots, n_{\max}$)

$$\sum_{x=0}^{x_{\max}} \frac{\phi_0(N; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}})^2 \psi_{\mathcal{D}}(x; \boldsymbol{\lambda})^2}{\check{\Xi}_{\mathcal{D}}(N-1; \boldsymbol{\lambda})} \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) \check{P}_{\mathcal{D},m}(x; \boldsymbol{\lambda}) = \frac{\delta_{nm}}{d_n(\boldsymbol{\lambda})^2 \tilde{d}_{\mathcal{D},n}(\boldsymbol{\lambda})^2}. \tag{3.94}$$

The shape invariance of $\mathcal{H}(\boldsymbol{\lambda})$ is inherited by $\mathcal{H}_{d_1}(\boldsymbol{\lambda})$, $\mathcal{H}_{d_1 d_2}(\boldsymbol{\lambda})$, $\cdots$. The Hamiltonian $\mathcal{H}_{\mathcal{D}}(\boldsymbol{\lambda})$ is shape invariant. As a consequence of the shape invariance and the normalisation, the actions of $\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})$ and $\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})^\dagger$ on the eigenvectors $\phi_{\mathcal{D}\,n}(x; \boldsymbol{\lambda})$ are

$$\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda}) \phi_{\mathcal{D}\,n}(x; \boldsymbol{\lambda}) = -\frac{\mathcal{E}_n(\boldsymbol{\lambda})}{\sqrt{D_{\mathcal{D}}(N; \boldsymbol{\lambda})}} \phi_{\mathcal{D}\,n-1}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) \quad (x = 0, 1, \ldots, x_{\max} - 1), \tag{3.95}$$

$$\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})^\dagger \phi_{\mathcal{D}\,n-1}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = -\sqrt{D_{\mathcal{D}}(N; \boldsymbol{\lambda})}\, \phi_{\mathcal{D}\,n}(x; \boldsymbol{\lambda}) \quad (x = 0, 1, \ldots, x_{\max}). \tag{3.96}$$

The forward and backward shift operators are defined by

$$\begin{aligned}
\mathcal{F}_{\mathcal{D}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} -\sqrt{D_{\mathcal{D}}(N; \boldsymbol{\lambda})}\, \psi_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})^{-1} \circ \mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda}) \circ \psi_{\mathcal{D}}(x; \boldsymbol{\lambda}) \\
&= \frac{-D(N; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}) \varphi(N-1; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}})}{\varphi(x; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})} \Big(\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) - \check{\Xi}_{\mathcal{D}}(x-1; \boldsymbol{\lambda} + \boldsymbol{\delta}) e^{\partial} \Big),
\end{aligned} \tag{3.97}$$

$$\begin{aligned}
\mathcal{B}_{\mathcal{D}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} -\frac{1}{\sqrt{D_{\mathcal{D}}(N; \boldsymbol{\lambda})}}\, \psi_{\mathcal{D}}(x; \boldsymbol{\lambda})^{-1} \circ \mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})^\dagger \circ \psi_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) \\
&= -\frac{1}{D(N; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}) \varphi(N-1; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}})} \frac{1}{\check{\Xi}_{\mathcal{D}}(x-1; \boldsymbol{\lambda} + \boldsymbol{\delta})} \\
&\quad \times \Big(B(x; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}) \check{\Xi}_{\mathcal{D}}(x-1; \boldsymbol{\lambda}) - D(x; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda}) e^{-\partial} \Big) \varphi(x; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}),
\end{aligned} \tag{3.98}$$

and their actions on $\check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda})$ are

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

The similarity transformed Hamiltonian is

$$\begin{aligned}
\widetilde{\mathcal{H}}_{\mathcal{D}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x; \boldsymbol{\lambda})^{-1} \circ \mathcal{H}_{\mathcal{D}}(\boldsymbol{\lambda}) \circ \psi_{\mathcal{D}}(x; \boldsymbol{\lambda}) = \mathcal{B}_{\mathcal{D}}(\boldsymbol{\lambda}) \mathcal{F}_{\mathcal{D}}(\boldsymbol{\lambda}) \\
&= B(x; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}) \frac{\check{\Xi}_{\mathcal{D}}(x-1; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})} \left(\frac{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x-1; \boldsymbol{\lambda} + \boldsymbol{\delta})} - e^{\partial} \right) \\
&\quad + D(x; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}) \frac{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x-1; \boldsymbol{\lambda})} \left(\frac{\check{\Xi}_{\mathcal{D}}(x-2; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x-1; \boldsymbol{\lambda} + \boldsymbol{\delta})} - e^{-\partial} \right),
\end{aligned} \tag{3.99}$$

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

$$\widetilde{\mathcal{H}}_{\mathcal{D}}(\boldsymbol{\lambda}) \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) = \mathcal{E}_n(\boldsymbol{\lambda}) \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}). \tag{3.100}$$

Here are other intertwining relations

$$\kappa^{\frac{1}{2}}\hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1\ldots d_{s+1}}(\boldsymbol{\lambda}+\boldsymbol{\delta})\mathcal{A}_{d_1\ldots d_s}(\boldsymbol{\lambda}) = \mathcal{A}_{d_1\ldots d_{s+1}}(\boldsymbol{\lambda})\hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1\ldots d_{s+1}}(\boldsymbol{\lambda}),$$
$$\kappa^{-\frac{1}{2}}\hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1\ldots d_{s+1}}(\boldsymbol{\lambda})\mathcal{A}_{d_1\ldots d_s}(\boldsymbol{\lambda})^{\dagger} = \mathcal{A}_{d_1\ldots d_{s+1}}(\boldsymbol{\lambda})^{\dagger}\hat{\mathcal{A}}^{(\mathrm{ii})}_{d_1\ldots d_{s+1}}(\boldsymbol{\lambda}+\boldsymbol{\delta}),$$

with the potential functions given in (2.79)–(2.80) (with $s \to s+1$). The effects of the level 0 deletion are the same as in the type I case (3.63).

3.4 Relations between type I and II

We discuss the discrete symmetries of the original (q)-Racah Hamiltonian (3.9)–(3.10) and their twisting together with the type I & II virtual state vectors. It is obvious that $B(x;\boldsymbol{\lambda})$ and $D(x;\boldsymbol{\lambda})$ (3.9)–(3.10) are symmetric under the permutation

$$\lambda_1 \leftrightarrow \lambda_2, \quad \lambda_1 \leftrightarrow \lambda_3, \quad \lambda_2 \leftrightarrow \lambda_3. \tag{3.101}$$

On top of the type I twisting (3.24), to be denoted by $\mathfrak{t}^{\mathrm{I}}$ in this subsection, one wonders if another twisting $\mathfrak{t}'$ obtained from $\mathfrak{t}^{\mathrm{I}}$ by $\lambda_2 \leftrightarrow \lambda_3$

$$\mathfrak{t}'(\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} (\lambda_4-\lambda_1+1, \lambda_2, \lambda_4-\lambda_3+1, \lambda_4), \quad \mathfrak{t}'^2 = \mathrm{id},$$

might work. Of course, it does not, since the above symmetry (3.101) is spontaneously broken by the actual choice of the parameter ranges (3.22)–(3.23). The positivity of $B'(x)$ and $D'(x)$ is lost when twisted by $\mathfrak{t}'$.

Another ingredient is the reflection $\mathcal{R}$ with respect to the mid-point of the grid, which is obviously an involution:

$$\mathcal{R}(x) \stackrel{\mathrm{def}}{=} N-x, \quad \mathcal{R}^2 = \mathrm{id}.$$

The reflection is also realised by an involution $\mathfrak{t}^{(\mathrm{r})}$ of the parameter changes together with $B \leftrightarrow D$:

$$\mathfrak{t}^{(\mathrm{r})}(\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} (\lambda_1, \lambda_1+\lambda_2-\lambda_4, \lambda_1+\lambda_3-\lambda_4, 2\lambda_1-\lambda_4), \quad (\mathfrak{t}^{(\mathrm{r})})^2 = \mathrm{id},$$
$$B(N-x;\boldsymbol{\lambda}) = D\big(x;\mathfrak{t}^{(\mathrm{r})}(\boldsymbol{\lambda})\big), \quad D(N-x;\boldsymbol{\lambda}) = B\big(x;\mathfrak{t}^{(\mathrm{r})}(\boldsymbol{\lambda})\big) \quad (N=-\lambda_1).$$

The type II twisting (3.65), to be denoted by $\mathfrak{t}^{\mathrm{II}}$ in this subsection, is obtained by applying $\mathfrak{t}'$ after $\mathfrak{t}^{(\mathrm{r})}$:

$$\mathfrak{t}^{\mathrm{II}} = \mathfrak{t}' \circ \mathfrak{t}^{(\mathrm{r})}, \quad \mathfrak{t}' \circ \mathfrak{t}^{(\mathrm{r})} \neq \mathfrak{t}^{(\mathrm{r})} \circ \mathfrak{t}' \ \Big(\Rightarrow (\mathfrak{t}^{\mathrm{II}})^2 \neq \mathrm{id}\Big).$$

This is a justification for the type II twisting.

Various quantities for the type I and II twistings are related by another involution $\mathfrak{t}^{(\mathrm{ex})}$:

$$
\begin{aligned}
&\mathfrak{t}^{(\mathrm{ex})}(\boldsymbol{\lambda}) \stackrel{\mathrm{def}}{=} (\lambda_1, \lambda_1-\lambda_2+1, \lambda_1-\lambda_3+1, 2\lambda_1-\lambda_4) \stackrel{\mathrm{def}}{=} \boldsymbol{\lambda}^{(\mathrm{ex})}, \quad (\mathfrak{t}^{(\mathrm{ex})})^2 = \mathrm{id},\\
&\mathfrak{t}^{\mathrm{II}} = \mathfrak{t}^{\mathrm{I}} \circ \mathfrak{t}^{(\mathrm{ex})}, \quad \mathfrak{t}^{\mathrm{I}} = \mathfrak{t}^{\mathrm{II}} \circ \mathfrak{t}^{(\mathrm{ex})}, \quad \mathfrak{t}^{\mathrm{I}} \circ \mathfrak{t}^{(\mathrm{ex})} \neq \mathfrak{t}^{(\mathrm{ex})} \circ \mathfrak{t}^{\mathrm{I}},\\
&B'^{\mathrm{II}}(x;\boldsymbol{\lambda}) = D'^{\mathrm{I}}(N-x;\boldsymbol{\lambda}^{(\mathrm{ex})}), \quad D'^{\mathrm{II}}(x;\boldsymbol{\lambda}) = B'^{\mathrm{I}}(N-x;\boldsymbol{\lambda}^{(\mathrm{ex})}), \quad \mathcal{E}'^{\mathrm{II}}_{\mathrm{v}}(\boldsymbol{\lambda}) = \mathcal{E}'^{\mathrm{I}}_{\mathrm{v}}(\boldsymbol{\lambda}^{(\mathrm{ex})}),\\
&\tilde{\phi}^{\mathrm{II}}_0(x;\boldsymbol{\lambda}) = \tilde{\phi}^{\mathrm{I}}_0(N-x;\boldsymbol{\lambda}^{(\mathrm{ex})})\phi_0(N;\mathfrak{t}^{\mathrm{II}}(\boldsymbol{\lambda}))^{-1}, \quad \check{\xi}^{\mathrm{II}}_{\mathrm{v}}(x;\boldsymbol{\lambda}) = \check{\xi}^{\mathrm{I}}_{\mathrm{v}}(N-x;\boldsymbol{\lambda}^{(\mathrm{ex})}),\\
&\check{\Xi}^{\mathrm{II}}_{\mathcal{D}}(x;\boldsymbol{\lambda}) = \check{\Xi}^{\mathrm{I}}_{\mathcal{D}}(N-x;\boldsymbol{\lambda}^{(\mathrm{ex})}),
\end{aligned}
$$

where $N = -\lambda_1$. However, the Hamiltonians (potential functions $B_{\mathcal{D}}$ and $D_{\mathcal{D}}$) and the multi-indexed orthogonal polynomials are different,

$$
\begin{aligned}
&B^{\mathrm{II}}_{\mathcal{D}}(x;\boldsymbol{\lambda}) \neq (\mathrm{const}) \times D^{\mathrm{I}}_{\mathcal{D}}(N-x;\boldsymbol{\lambda}^{(\mathrm{ex})}), \quad D^{\mathrm{II}}_{\mathcal{D}}(x;\boldsymbol{\lambda}) \neq (\mathrm{const}) \times B^{\mathrm{I}}_{\mathcal{D}}(N-x;\boldsymbol{\lambda}^{(\mathrm{ex})}),\\
&\check{P}^{\mathrm{II}}_{\mathcal{D},n}(x;\boldsymbol{\lambda}) \neq (\mathrm{const}) \times \check{P}^{\mathrm{I}}_{\mathcal{D},n}(N-x;\boldsymbol{\lambda}^{(\mathrm{ex})}).
\end{aligned}
$$

4 Summary and Comments

Following the examples of multi-indexed Laguerre and Jacobi polynomials [1], multi-indexed (q)-Racah polynomials, the discrete quantum mechanics counterparts, are constructed. These new polynomials could be considered further generalisation of Bannai-Ito polynomials [45]. The next stage will be the construction of multi-indexed Askey-Wilson and Wilson polynomials. The basic logic is the same for the ordinary quantum mechanics as well as for the discrete quantum mechanics with real [2] or pure imaginary shifts [28]. Starting from the factorised Hamiltonians of exactly solvable quantum mechanical systems, a series of new 'deformed' exactly solvable quantum systems are generated by applying Crum-Krein-Adler formulas [36, 37] or multiple Darboux transformations [39] through deletion of various virtual states instead of eigenstates. The virtual state vectors are polynomial 'solutions' of a virtual Hamiltonian which is obtained by twisting the discrete symmetry of the original Hamiltonian. They fail to satisfy the Schrödinger equation of the virtual Hamiltonian at one of the boundaries, at $x = x_{\max}$ for the type I and $x = 0$ for the type II. When there is only one extra index $\mathcal{D} = \{\ell\}$ ($\ell \geq 1$), the multi-indexed (q)-Racah polynomials reduce to the exceptional polynomials [23, 26]. But the type II exceptional (q)-Racah polynomials are new. Like the exceptional polynomials, the multi-indexed (q)-Racah polynomials do not

satisfy the three term recurrence relations. On the other hand, their dual polynomials satisfy the three term recurrence relations because of the tri-diagonal form of the Hamiltonian. As for the parameter ranges in which (2.20), (2.31)–(2.32), (2.61) and (2.67) are satisfied, we have taken conservative ones, (3.22)–(3.23), (3.28), (3.36), (3.71) and (3.80). It is quite possible that the valid parameter ranges could be enlarged. The difference equations for the multi-indexed (q)-Racah polynomials, (3.62) and (3.100) etc., are purely algebraic and they hold for any parameter ranges.

Various orthogonal polynomials are obtained from the (q)-Racah polynomials in certain limits. Similarly, from the multi-indexed (q)-Racah polynomials presented in the previous section, we can obtain the multi-indexed version of various orthogonal polynomials, such as the (q)-Hahn, dual (q)-Hahn, alternative q-Hahn, etc. The infinite dimensional cases, the little q-Jacobi, (q)-Meixner, etc will be reported in a separate publication. In these cases, the treatment of the type II twisting becomes delicate.

As in the ordinary Sturm-Liouville case (the oscillation theorem) the multi-indexed orthogonal polynomial $P_{\mathcal{D},n}(y;\boldsymbol{\lambda})$ has n zeros in the orthogonality range, $0 < y < \eta(x_{\max};\boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}})$. This is a general property of the eigenvectors of a Jacobi matrix.

In §2.2.3 it is shown that the type I and II virtual states cannot be used together to construct new eigenvectors. If we relax the conditions of positive definite orthogonality weight functions, multi-indexed polynomials based on the type I and II together could be allowed.

Let us emphasise that the discrete symmetries of the original (q)-Racah systems and their twisting, which are essential for the construction of virtual Hamiltonians and virtual state vectors, are easily recognised in the present parametrisation (3.9)–(3.10) [2], but rather unclear in the original parametrisation [3, 4, 5]. This is a good reason to promote the (q)-Racah systems in our parametrisation.

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