

# Multi-indexed Wilson and Askey-Wilson Polynomials

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## Abstract

As the third stage of the project *multi-indexed orthogonal polynomials*, we present, in the framework of ‘discrete quantum mechanics’ with pure imaginary shifts in one dimension, the multi-indexed Wilson and Askey-Wilson polynomials. They are obtained from the original Wilson and Askey-Wilson polynomials by multiple application of the discrete analogue of the Darboux transformations or the Crum-Krein-Adler deletion of ‘virtual state solutions’ of type I and II, in a similar way to the multi-indexed Laguerre, Jacobi and ( $q$ -)Racah polynomials reported earlier.

## 1 Introduction

This is a third report of the project *multi-indexed orthogonal polynomials*. Following the examples of multi-indexed Laguerre and Jacobi polynomials [1], multi-indexed ( $q$ -)Racah polynomials [2], we present multi-indexed Wilson and Askey-Wilson polynomials constructed in the framework of discrete quantum mechanics with pure imaginary shifts [3]. It is well-known that the original Wilson and Askey-Wilson polynomials are the most generic members of the Askey scheme of hypergeometric orthogonal polynomials [4, 5, 6, 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]–[29]. 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 [3, 30, 31]. 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 [32]. We strongly believe that these new orthogonal polynomials will find plenty of novel applications in various branches of science and technology in the good old tradition of orthogonal polynomials.

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 as well as pure imaginary shifts, *i.e.* the ( $q$ -)Racah polynomials and the Wilson and Askey-Wilson polynomials, etc. The main ingredients are the factorised Hamiltonians, the Crum-Krein-Adler formulas [33, 34, 35] for deletion of eigenstates, *that is* the multiple Darboux transformations [36] and the *virtual state 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 [30, 26, 3, 31, 37, 38, 39] and they were used for the exceptional Wilson and Askey-Wilson polynomials [12, 19]. In different contexts, Darboux transformations for orthogonal polynomials have been discussed by many authors [40, 41, 42].

It is important to stress that the factorised Hamiltonians in the discrete quantum mechanics, that is, those governing the ( $q$ -)Racah, Wilson, Askey-Wilson polynomials etc possess certain discrete symmetry. They lead to virtual Hamiltonians which are linearly connected with the original Hamiltonian. (See (2.14)–(2.16) of the present paper and (2.18)–(2.22), (2.59)–(2.63) of [2].) In the ordinary quantum mechanics of the radial oscillator potential ( $x^2 + \frac{g(g-1)}{x^2}$ , for the Laguerre polynomials) and the Pöschl-Teller potential ( $\frac{g(g-1)}{\sin^2 x} + \frac{h(h-1)}{\cos^2 x}$ , for the Jacobi polynomials), the discrete symmetry is well known. For the former,  $g \rightarrow 1 - g$  and/or  $x \rightarrow ix$  and for the latter  $g \rightarrow 1 - g$  and/or  $h \rightarrow 1 - h$ . To the best of our knowledge, those discrete symmetries for the ( $q$ -)Racah, Wilson and Askey-Wilson systems do not seem to be widely recognised, since they are not easily identifiable in the polynomial equations. The virtual state solutions belong to the virtual Hamiltonians. The actual contents of virtual state solutions depend on the types of the Schrödinger equations. For the ordinary Schrödinger equations with a second order differential operator, the virtual state

solutions satisfy the Schrödinger equation. But they do not belong to the Hilbert space of square integrable solutions, due to the twisted boundary condition on either one of the two boundaries, to be called the type I or II. For the multi-indexed ( $q$ -)Racah polynomials in the discrete quantum mechanics with real shifts, the virtual state ‘solutions’ fail to satisfy the Schrödinger equation at either one of the two boundary points [2]. They are called virtual state vectors of type I or II. In the present case of discrete quantum mechanics with pure imaginary shifts, the virtual state solutions satisfy the difference Schrödinger equation. But they do not belong to the Hilbert space of eigenfunctions either by the lack of square integrability or by the presence of singularities in certain rectangular domain. (See more detailed discussion in section 2.2.) In other words, the analyticity requirements supersede the boundary conditions which used to classify the virtual state solutions for the Laguerre, Jacobi and ( $q$ -)Racah cases. In section three, we will introduce two types of twistings or the discrete symmetry transformations and the corresponding virtual Hamiltonians and virtual state solutions. They are of the same structure but adopting different sets of parameters. We will call them of type I and II as in the other cases but they are not related to boundary conditions. In all these cases, the features disqualifying them to become the eigenfunctions are carried by the so called “virtual groundstate” functions  $\tilde{\phi}_0(x)$ , (3.28). The polynomial part of the virtual state solutions, to be denoted by  $\xi_v(\eta)$  (3.28), are the genuine solutions of equations determining the eigenpolynomials, but with twisted parameters. It is the virtual state polynomials  $\{\xi_v(\eta)\}$ , not the virtual groundstate  $\tilde{\phi}_0(x)$ , that play the main role in the construction of multi-indexed and exceptional [12, 19] polynomials and the set of their degrees  $\{d_1, \dots, d_M\}$  constitutes the *multi-index*. We focus on the algebraic structure of the multi-indexed orthogonal polynomials and their difference equations, which hold for any parameter range. We do not pursue the other important aspect of the problem, that is the determination of the parameter ranges in which the hermiticity of the multi-indexed Hamiltonians and the positivity of the orthogonality weight functions for the multi-indexed polynomials are ensured.

This paper is organised as follows. In section two, the basic logic of virtual states deletion in discrete quantum mechanics with pure imaginary shifts in general is outlined. Starting from the general setting of discrete quantum mechanics with pure imaginary shifts in § 2.1, the analyticity requirements in connection with the hermiticity (self-adjointness) of the Hamiltonians are briefly recapitulated in § 2.2. General procedures and formulas of multiple

virtual states deletion are reviewed in §2.3. The main logics are essentially the same as those for the multi-indexed Laguerre, Jacobi and ( $q$ -)Racah polynomials but the explicit formulas look rather different reflecting the specific properties of discrete quantum mechanics with pure imaginary shifts. After recapitulating the basic properties of the Wilson and Askey-Wilson systems in §3.1, the discrete symmetries of the the Wilson and Askey-Wilson systems are introduced in §3.2. The multi-indexed Wilson and Askey-Wilson polynomials are constructed explicitly in §3.3 for the type I and II virtual states deletions. The analyticity and hermiticity of the multi-indexed hamiltonians are discussed in some detail in section §3.4. The final section is for a summary and comments including the limits to the multi-indexed Jacobi and Laguerre polynomials. For simplicity of presentation we relegate several technical results to Appendix.

Throughout this paper we will focus on the algebraic aspects of the theory. To determine the exact ranges of validity of various formulas is another problem.

## 2 Formulation

### 2.1 Original system

Let us recapitulate the discrete quantum mechanics with pure imaginary shifts developed in [3]. The dynamical variables are the real coordinate  $x$  ( $x_1 \leq x \leq x_2$ ) and the conjugate momentum  $p = -i\partial_x$ , which are governed by the following factorised positive semi-definite Hamiltonian:

$$\mathcal{H} \stackrel{\text{def}}{=} \sqrt{V(x)} e^{\gamma p} \sqrt{V^*(x)} + \sqrt{V^*(x)} e^{-\gamma p} \sqrt{V(x)} - V(x) - V^*(x) = \mathcal{A}^\dagger \mathcal{A}, \quad (2.1)$$

$$\mathcal{A} \stackrel{\text{def}}{=} i(e^{\frac{\gamma}{2}p} \sqrt{V^*(x)} - e^{-\frac{\gamma}{2}p} \sqrt{V(x)}), \quad \mathcal{A}^\dagger \stackrel{\text{def}}{=} -i(\sqrt{V(x)} e^{\frac{\gamma}{2}p} - \sqrt{V^*(x)} e^{-\frac{\gamma}{2}p}). \quad (2.2)$$

Here the potential function  $V(x)$  is an analytic function of  $x$  and  $\gamma$  is a real constant. The  $*$ -operation on an analytic function  $f(x) = \sum_n a_n x^n$  ( $a_n \in \mathbb{C}$ ) is defined by  $f^*(x) = \sum_n a_n^* x^n$ , in which  $a_n^*$  is the complex conjugation of  $a_n$ . Obviously  $f^{**}(x) = f(x)$  and  $f(x)^* = f^*(x^*)$ . If a function satisfies  $f^* = f$ , then it takes real values on the real line. Since the momentum operator appears in exponentiated forms, the Schrödinger equation

$$\mathcal{H}\phi_n(x) = \mathcal{E}_n\phi_n(x) \quad (n = 0, 1, 2, \dots), \quad (2.3)$$

is an analytic difference equation with pure imaginary shifts instead of a differential equation. Throughout this paper we consider those systems which have a square-integrable groundstate

together with an infinite number of discrete energy levels:  $0 = \mathcal{E}_0 < \mathcal{E}_1 < \mathcal{E}_2 < \dots$ . The orthogonality relation reads

$$(\phi_n, \phi_m) \stackrel{\text{def}}{=} \int_{x_1}^{x_2} dx \phi_n^*(x) \phi_m(x) = h_n \delta_{nm} \quad (n, m = 0, 1, 2, \dots), \quad 0 < h_n < \infty. \quad (2.4)$$

The eigenfunctions  $\phi_n(x)$  can be chosen ‘real’,  $\phi_n^*(x) = \phi_n(x)$ , and the groundstate wavefunction  $\phi_0(x)$  is determined as the zero mode of the operator  $\mathcal{A}$ ,  $\mathcal{A}\phi_0(x) = 0$ , namely,

$$\sqrt{V^*(x - i\frac{\gamma}{2})} \phi_0(x - i\frac{\gamma}{2}) = \sqrt{V(x + i\frac{\gamma}{2})} \phi_0(x + i\frac{\gamma}{2}). \quad (2.5)$$

## 2.2 Analyticity requirements

The hermiticity of the Hamiltonians of discrete quantum mechanics with pure imaginary shifts is more involved than that of the ordinary quantum mechanics [3, 31]. Here we review the hermiticity of the Hamiltonian (2.1) in general, in a way applicable to those appearing in the multi-indexed Wilson and Askey-Wilson systems, *e.g.* (2.18)–(2.20), (2.26)–(2.28). Of course, the hermiticity of the original Hamiltonians of the Wilson and Askey-Wilson systems (3.4)–(3.11) is well established [3, 31].

Let us consider the functions of the form  $f(x) = \phi_0(x)\check{\mathcal{R}}(x)$ , where  $\phi_0(x)^2$  and  $\check{\mathcal{R}}(x)$  are meromorphic functions and  $\check{\mathcal{R}}^*(x) = \check{\mathcal{R}}(x)$ . For two such functions  $f_1 = \phi_0\check{\mathcal{R}}_1$  and  $f_2 = \phi_0\check{\mathcal{R}}_2$ , the condition of the hermiticity  $(f_1, \mathcal{H}f_2) = (\mathcal{H}f_1, f_2)$  becomes

$$\int_{x_1}^{x_2} dx (G(x - i\frac{\gamma}{2}) + G^*(x + i\frac{\gamma}{2})) = \int_{x_1}^{x_2} dx (G(x + i\frac{\gamma}{2}) + G^*(x - i\frac{\gamma}{2})), \quad (2.6)$$

where  $G(x)$  is defined by

$$\begin{aligned} G(x) &= V(x + i\frac{\gamma}{2})\phi_0(x + i\frac{\gamma}{2})^2\check{\mathcal{R}}_1(x + i\frac{\gamma}{2})\check{\mathcal{R}}_2(x - i\frac{\gamma}{2}), \\ (\Rightarrow G^*(x) &= V(x + i\frac{\gamma}{2})\phi_0(x + i\frac{\gamma}{2})^2\check{\mathcal{R}}_1(x - i\frac{\gamma}{2})\check{\mathcal{R}}_2(x + i\frac{\gamma}{2})). \end{aligned} \quad (2.7)$$

Although the term  $V(x) + V^*(x)$  in  $\mathcal{H}$  are canceled out in this calculation, this term  $V(x) + V^*(x)$  should be non-singular for  $x_1 \leq x \leq x_2$ , and the integral  $\int_{x_1}^{x_2} dx V(x)\phi_0(x)^2\check{\mathcal{R}}_1(x)\check{\mathcal{R}}_2(x)$  should be finite. By using the residue theorem, the condition (2.6) is rewritten as

$$\begin{aligned} & \int_{-\frac{\gamma}{2}}^{\frac{\gamma}{2}} dx (G(x_2 + ix) - G^*(x_2 - ix)) - \int_{-\frac{\gamma}{2}}^{\frac{\gamma}{2}} dx (G(x_1 + ix) - G^*(x_1 - ix)) \\ &= 2\pi \frac{\gamma}{|\gamma|} \sum_{x_0: \text{pole in } D_\gamma} \text{Res}_{x_0} (G(x) - G^*(x)), \end{aligned} \quad (2.8)$$

where the residue of the function  $G(x) - G^*(x)$  is taken at the poles in the rectangular domain  $D_\gamma$  :

$$D_\gamma \stackrel{\text{def}}{=} \{x \in \mathbb{C} \mid x_1 \leq \text{Re } x \leq x_2, |\text{Im } x| \leq \frac{1}{2}|\gamma|\}. \quad (2.9)$$

In our previous work on the exceptional Wilson and Askey-Wilson [12, 19], we required that  $G$  and  $G^*$  have no poles in the rectangular domain  $D_\gamma$ , as a sufficient condition for the hermiticity of the Hamiltonian. This was too strong a requirement. In later examples,  $\tilde{\mathcal{R}}(x) = \mathcal{R}(\eta(x))$  is a rational function of  $\eta(x)$  and  $V(x)\phi_0(x)^2$  has the form  $\sim (V\phi_0^2)_{\text{original}} \times$  (rational function of  $\eta(x)$ ). In the original Wilson and Askey Wilson theory,  $(V\phi_0^2)_{\text{original}}$  part has no poles in  $D_\gamma$ , (3.14). In the deformed theory in general, however,  $(V\phi_0^2)_{\text{original}}$  has shifted parameters and we continue to require that this part has no poles in the rectangular domain  $D_\gamma$ . We also remark that even if the (rational function of  $\eta(x)$ )-part has poles in the rectangular domain  $D_\gamma$ , there is a possibility that the sum of the residues vanish.

### 2.3 Deletion of virtual states

In [38] we have presented the Crum-Adler scheme, *i.e.* the deletion of  $M$  eigenstates. In that case the index set of the deleted eigenstates  $\mathcal{D} \stackrel{\text{def}}{=} \{d_1, d_2, \dots, d_M\}$  ( $d_j \in \mathbb{Z}_{\geq 0}$ ) should satisfy the condition  $\prod_{j=1}^M (m - d_j) \geq 0$  ( $\forall m \in \mathbb{Z}_{\geq 0}$ ), eq. (2.8) in [38]. We now apply the Crum-Adler scheme to virtual states instead of eigenstates. The above condition eq. (2.8) in [38] is no longer necessary.

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

$$W_\gamma[f_1, \dots, f_n](x) \stackrel{\text{def}}{=} i^{\frac{1}{2}n(n-1)} \det\left(f_k(x_j^{(n)})\right)_{1 \leq j, k \leq n}, \quad x_j^{(n)} \stackrel{\text{def}}{=} x + i\left(\frac{n+1}{2} - j\right)\gamma, \quad (2.10)$$

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

$$W_\gamma[f_1, \dots, f_n]^*(x) = W_\gamma[f_1^*, \dots, f_n^*](x), \quad (2.11)$$

$$W_\gamma[gf_1, gf_2, \dots, gf_n] = \prod_{j=1}^n g(x_j^{(n)}) \cdot W_\gamma[f_1, f_2, \dots, f_n](x), \quad (2.12)$$

$$\begin{aligned} & W_\gamma[W_\gamma[f_1, f_2, \dots, f_n, g], W_\gamma[f_1, f_2, \dots, f_n, h]](x) \\ &= W_\gamma[f_1, f_2, \dots, f_n](x) W_\gamma[f_1, f_2, \dots, f_n, g, h](x) \quad (n \geq 0). \end{aligned} \quad (2.13)$$

Let us assume the existence of an analytic function  $V'(x)$  of  $x$  satisfying

$$V(x)V^*(x - i\gamma) = \alpha^2 V'(x)V'^*(x - i\gamma), \quad \alpha > 0,$$

$$V(x) + V^*(x) = \alpha(V'(x) + V'^*(x)) - \alpha', \quad \alpha' < 0, \quad (2.14)$$

where  $\alpha$  and  $\alpha'$  are constants. Then we obtain a linear relation between two Hamiltonians:

$$\mathcal{H} = \alpha\mathcal{H}' + \alpha', \quad (2.15)$$

$$\mathcal{H}' \stackrel{\text{def}}{=} \sqrt{V'(x)} e^{\gamma p} \sqrt{V'^*(x)} + \sqrt{V'^*(x)} e^{-\gamma p} \sqrt{V'(x)} - V'(x) - V'^*(x). \quad (2.16)$$

Since  $\mathcal{H}$  is positive semi-definite,  $\mathcal{H}'$  is obviously positive definite and it has no zero-mode. Let us also assume the existence of *virtual state wavefunctions*  $\tilde{\phi}_v(x)$  ( $v \in \mathcal{V}$ ), which are ‘polynomial solutions’ of degree  $v$  of the Schrödinger equation

$$\mathcal{H}\tilde{\phi}_v(x) = \tilde{\mathcal{E}}_v\tilde{\phi}_v(x) \quad \text{or} \quad \mathcal{H}'\tilde{\phi}_v(x) = \mathcal{E}'_v\tilde{\phi}_v(x), \quad \tilde{\mathcal{E}}_v \stackrel{\text{def}}{=} \alpha\mathcal{E}'_v + \alpha', \quad \tilde{\phi}_v^*(x) = \tilde{\phi}_v(x), \quad (2.17)$$

but they, including the zeromode  $\tilde{\phi}_0$ , do not belong to the Hilbert space of  $\mathcal{H}$ . Here  $\mathcal{V}$  is the index set of the virtual state wavefunctions. We require that  $\tilde{\mathcal{E}}_v < 0$  and some analytic properties of  $\tilde{\phi}_v(x)$ , which are explicitly presented in §3.

We have developed the method of virtual states deletion for ordinary quantum mechanics in [1] and for discrete quantum mechanics with real shifts in [2]. Algebraic aspects of this method are the same and can be applied to discrete quantum mechanics with pure imaginary shifts. The procedure is as follows; (i) rewrite the original Hamiltonian as  $\mathcal{H} = \hat{\mathcal{A}}_{d_1}^\dagger \hat{\mathcal{A}}_{d_1} + \tilde{\mathcal{E}}_{d_1}$  ( $d_1 \in \mathcal{V}$ ), (ii) define a new isospectral Hamiltonian  $\mathcal{H}_{d_1} \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1} \hat{\mathcal{A}}_{d_1}^\dagger + \tilde{\mathcal{E}}_{d_1}$ , whose eigenfunctions are given by  $\phi_{d_1 n}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1} \phi_n(x)$  together with virtual state wavefunctions  $\tilde{\phi}_{d_1 v}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1} \tilde{\phi}_v(x)$  ( $v \in \mathcal{V} \setminus \{d_1\}$ ),  $\mathcal{H}_{d_1} \phi_{d_1 n}(x) = \mathcal{E}_n \phi_{d_1 n}(x)$ ,  $\mathcal{H}_{d_1} \tilde{\phi}_{d_1 v}(x) = \tilde{\mathcal{E}}_v \tilde{\phi}_{d_1 v}(x)$  (iii) rewrite this as  $\mathcal{H}_{d_1} = \hat{\mathcal{A}}_{d_1 d_2}^\dagger \hat{\mathcal{A}}_{d_1 d_2} + \tilde{\mathcal{E}}_{d_2}$  ( $d_2 \in \mathcal{V} \setminus \{d_1\}$ ), (iv) define the next isospectral Hamiltonian  $\mathcal{H}_{d_1 d_2} \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1 d_2} \hat{\mathcal{A}}_{d_1 d_2}^\dagger + \tilde{\mathcal{E}}_{d_2}$ , whose eigenfunctions are given by  $\phi_{d_1 d_2 n}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1 d_2} \phi_{d_1 n}(x)$  together with virtual state wavefunctions  $\tilde{\phi}_{d_1 d_2 v}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1 d_2} \tilde{\phi}_{d_1 v}(x)$  ( $v \in \mathcal{V} \setminus \{d_1, d_2\}$ ),  $\mathcal{H}_{d_1 d_2} \phi_{d_1 d_2 n}(x) = \mathcal{E}_n \phi_{d_1 d_2 n}(x)$ ,  $\mathcal{H}_{d_1 d_2} \tilde{\phi}_{d_1 d_2 v}(x) = \tilde{\mathcal{E}}_v \tilde{\phi}_{d_1 d_2 v}(x)$ , (v) by repeating this process, we obtain  $\mathcal{H}_{d_1 \dots d_s}$  and its eigenfunctions  $\phi_{d_1 \dots d_s n}(x)$  together with virtual state wavefunctions  $\tilde{\phi}_{d_1 \dots d_s v}(x)$ , (vi)  $\mathcal{H}_{d_1 \dots d_s}$  can be written in the standard form,  $\mathcal{H}_{d_1 \dots d_s} = \mathcal{A}_{d_1 \dots d_s}^\dagger \mathcal{A}_{d_1 \dots d_s}$ . If the resulting system is well-defined, we obtain the isospectrally deformed systems just as those in refs.[1] and [2].

Here we present ‘formal’ expressions of the deformed systems, which are proved inductively. The system obtained after  $s$  virtual state deletions ( $s \geq 1$ ), which are labeled by  $\{d_1, \dots, d_s\}$  ( $d_j \in \mathcal{V}$  : mutually distinct), is

$$\mathcal{H}_{d_1 \dots d_s} \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1 \dots d_s} \hat{\mathcal{A}}_{d_1 \dots d_s}^\dagger + \tilde{\mathcal{E}}_{d_s}, \quad (2.18)$$

$$\begin{aligned}\hat{\mathcal{A}}_{d_1\dots d_s} &\stackrel{\text{def}}{=} i(e^{\frac{\gamma}{2}p}\sqrt{\hat{V}_{d_1\dots d_s}^*(x)} - e^{-\frac{\gamma}{2}p}\sqrt{\hat{V}_{d_1\dots d_s}(x)}), \\ \hat{\mathcal{A}}_{d_1\dots d_s}^\dagger &\stackrel{\text{def}}{=} -i(\sqrt{\hat{V}_{d_1\dots d_s}(x)}e^{\frac{\gamma}{2}p} - \sqrt{\hat{V}_{d_1\dots d_s}^*(x)}e^{-\frac{\gamma}{2}p}),\end{aligned}\tag{2.19}$$

$$\begin{aligned}\hat{V}_{d_1\dots d_s}(x) &\stackrel{\text{def}}{=} \sqrt{V(x - i\frac{s-1}{2}\gamma)V^*(x - i\frac{s+1}{2}\gamma)} \\ &\quad \times \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_{s-1}}](x + i\frac{\gamma}{2})}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_{s-1}}](x - i\frac{\gamma}{2})} \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x - i\gamma)}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x)},\end{aligned}\tag{2.20}$$

$$\begin{aligned}\phi_{d_1\dots d_s n}(x) &\stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1\dots d_s} \phi_{d_1\dots d_{s-1} n}(x) \quad (n = 0, 1, 2, \dots), \\ \tilde{\phi}_{d_1\dots d_s v}(x) &\stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1\dots d_s} \tilde{\phi}_{d_1\dots d_{s-1} v}(x) \quad (v \in \mathcal{V} \setminus \{d_1, \dots, d_s\}),\end{aligned}\tag{2.21}$$

$$\begin{aligned}\mathcal{H}_{d_1\dots d_s} \phi_{d_1\dots d_s n}(x) &= \mathcal{E}_n \phi_{d_1\dots d_s n}(x) \quad (n = 0, 1, 2, \dots), \\ \mathcal{H}_{d_1\dots d_s} \tilde{\phi}_{d_1\dots d_s v}(x) &= \tilde{\mathcal{E}}_v \tilde{\phi}_{d_1\dots d_s v}(x) \quad (v \in \mathcal{V} \setminus \{d_1, \dots, d_s\}),\end{aligned}\tag{2.22}$$

$$(\phi_{d_1\dots d_s n}, \phi_{d_1\dots d_s m}) = \prod_{j=1}^s (\mathcal{E}_n - \tilde{\mathcal{E}}_{d_j}) \cdot h_n \delta_{nm} \quad (n, m = 0, 1, 2, \dots).\tag{2.23}$$

Let us remark that the eigenfunctions and the virtual state solutions in all steps are ‘real’ by construction,  $\phi_{d_1\dots d_s n}^*(x) = \phi_{d_1\dots d_s n}(x)$ ,  $\tilde{\phi}_{d_1\dots d_s v}^*(x) = \tilde{\phi}_{d_1\dots d_s v}(x)$  and they have Casoratian expressions:

$$\begin{aligned}\phi_{d_1\dots d_s n}(x) &= A(x)W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \phi_n](x), \\ \tilde{\phi}_{d_1\dots d_s v}(x) &= A(x)W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \tilde{\phi}_v](x),\end{aligned}\tag{2.24}$$

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

which are shown by using (2.13).

Writing down (2.22) and dividing it by  $\phi_{d_1\dots d_s n}(x)$  or  $\tilde{\phi}_{d_1\dots d_s v}(x)$  and using (2.24), we obtain

$$\begin{aligned}&\hat{V}_{d_1\dots d_s}(x + i\frac{\gamma}{2}) + \hat{V}_{d_1\dots d_s}^*(x - i\frac{\gamma}{2}) - \tilde{\mathcal{E}}_{d_s} + \mathcal{E}_n \\ &= \sqrt{V(x - i\frac{s}{2}\gamma)V^*(x - i\frac{s+2}{2}\gamma)} \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x + i\frac{\gamma}{2})}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x - i\frac{\gamma}{2})} \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \phi_n](x - i\gamma)}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \phi_n](x)} \\ &\quad + \sqrt{V^*(x + i\frac{s}{2}\gamma)V(x + i\frac{s+2}{2}\gamma)} \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x - i\frac{\gamma}{2})}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x + i\frac{\gamma}{2})} \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \phi_n](x + i\gamma)}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \phi_n](x)},\end{aligned}\tag{2.25}$$

and a similar equation for the virtual state solution.

The deformed Hamiltonian  $\mathcal{H}_{d_1\dots d_s}$  can be rewritten in the standard form:

$$\mathcal{H}_{d_1\dots d_s} = \mathcal{A}_{d_1\dots d_s}^\dagger \mathcal{A}_{d_1\dots d_s},\tag{2.26}$$



$$\begin{aligned}\mathcal{A}_{d_1\dots d_s} &\stackrel{\text{def}}{=} i\left(e^{\frac{\gamma}{2}p}\sqrt{V_{d_1\dots d_s}^*(x)} - e^{-\frac{\gamma}{2}p}\sqrt{V_{d_1\dots d_s}(x)}\right), \\ \mathcal{A}_{d_1\dots d_s}^\dagger &\stackrel{\text{def}}{=} -i\left(\sqrt{V_{d_1\dots d_s}(x)}e^{\frac{\gamma}{2}p} - \sqrt{V_{d_1\dots d_s}^*(x)}e^{-\frac{\gamma}{2}p}\right),\end{aligned}\tag{2.27}$$

$$\begin{aligned}V_{d_1\dots d_s}(x) &\stackrel{\text{def}}{=} \sqrt{V(x - i\frac{s}{2}\gamma)V^*(x - i\frac{s+2}{2}\gamma)} \\ &\quad \times \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x + i\frac{\gamma}{2})}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}](x - i\frac{\gamma}{2})} \frac{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \phi_0](x - i\gamma)}{W_\gamma[\tilde{\phi}_{d_1}, \dots, \tilde{\phi}_{d_s}, \phi_0](x)},\end{aligned}\tag{2.28}$$

in which the  $\mathcal{A}$  operator annihilates the groundstate,

$$\mathcal{A}_{d_1\dots d_s}\phi_{d_1\dots d_s 0}(x) = 0.\tag{2.29}$$

The conditions for the equality of (2.26) and (2.18) are

$$\begin{aligned}V_{d_1\dots d_s}(x)V_{d_1\dots d_s}^*(x - i\gamma) &= \hat{V}_{d_1\dots d_s}(x - i\frac{\gamma}{2})\hat{V}_{d_1\dots d_s}^*(x - i\frac{\gamma}{2}), \\ V_{d_1\dots d_s}(x) + V_{d_1\dots d_s}^*(x) &= \hat{V}_{d_1\dots d_s}(x + i\frac{\gamma}{2}) + \hat{V}_{d_1\dots d_s}^*(x - i\frac{\gamma}{2}) - \tilde{\mathcal{E}}_{d_s}.\end{aligned}\tag{2.30}$$

The first equation is trivially satisfied and the second equation is a consequence of (2.25) with  $n = 0$ .

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

In order that this deformed system is well-defined *i.e.* Hamiltonian  $\mathcal{H}_{d_1\dots d_s}$  is hermitian, we have to study the singularities of  $V_{d_1\dots d_s}(x)$  and  $\phi_{d_1\dots d_s n}(x)$ . We will do this for explicit examples in section §3.4.

### 3 Multi-indexed Wilson and Askey-Wilson Polynomials

In this section we apply the method of virtual states deletion to the exactly solvable systems whose eigenstates are described by the Wilson (W) and Askey-Wilson (AW) polynomials. We delete  $M$  virtual states labeled by

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

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

We follow the notation of [3]. Various quantities depend on a set of parameters  $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \dots)$ .

### 3.1 Original Wilson and Askey-Wilson systems

Let us consider the Wilson and Askey-Wilson cases. Various parameters are

$$\begin{aligned} W : x_1 = 0, x_2 = \infty, \gamma = 1, \quad \boldsymbol{\lambda} &= (a_1, a_2, a_3, a_4), \quad \boldsymbol{\delta} = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right), \quad \kappa = 1, \\ AW : x_1 = 0, x_2 = \pi, \gamma = \log q, \quad q^\lambda &= (a_1, a_2, a_3, a_4), \quad \boldsymbol{\delta} = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right), \quad \kappa = q^{-1}, \end{aligned} \quad (3.2)$$

where  $q^\lambda$  stands for  $q^{(\lambda_1, \lambda_2, \dots)} = (q^{\lambda_1}, q^{\lambda_2}, \dots)$  and  $0 < q < 1$ . The parameters are restricted by

$$\{a_1^*, a_2^*, a_3^*, a_4^*\} = \{a_1, a_2, a_3, a_4\} \quad (\text{as a set}); \quad W : \operatorname{Re} a_i > 0, \quad AW : |a_i| < 1. \quad (3.3)$$

Here are the fundamental data [3]:

$$V(x; \boldsymbol{\lambda}) = \begin{cases} (2ix(2ix+1))^{-1} \prod_{j=1}^4 (a_j + ix) & : W \\ ((1 - e^{2ix})(1 - qe^{2ix}))^{-1} \prod_{j=1}^4 (1 - a_j e^{ix}) & : AW \end{cases}, \quad (3.4)$$

$$\eta(x) = \begin{cases} x^2 & : W \\ \cos x & : AW \end{cases}, \quad \varphi(x) = \begin{cases} 2x & : W \\ 2 \sin x & : AW \end{cases}, \quad (3.5)$$

$$\mathcal{E}_n(\boldsymbol{\lambda}) = \begin{cases} n(n+b_1-1) & : W \\ (q^{-n}-1)(1-b_4q^{n-1}) & : AW \end{cases}, \quad \begin{aligned} b_1 &\stackrel{\text{def}}{=} a_1 + a_2 + a_3 + a_4, \\ b_4 &\stackrel{\text{def}}{=} a_1 a_2 a_3 a_4, \end{aligned} \quad (3.6)$$

$$\phi_n(x; \boldsymbol{\lambda}) = \phi_0(x; \boldsymbol{\lambda}) \check{P}_n(x; \boldsymbol{\lambda}), \quad (3.7)$$

$$\begin{aligned} \check{P}_n(x; \boldsymbol{\lambda}) = P_n(\eta(x); \boldsymbol{\lambda}) &= \begin{cases} W_n(\eta(x); a_1, a_2, a_3, a_4) & : W \\ p_n(\eta(x); a_1, a_2, a_3, a_4 | q) & : AW \end{cases} \\ &= \begin{cases} \begin{aligned} &(a_1 + a_2)_n (a_1 + a_3)_n (a_1 + a_4)_n \\ &\times {}_4F_3 \left( \begin{matrix} -n, n + b_1 - 1, a_1 + ix, a_1 - ix \\ a_1 + a_2, a_1 + a_3, a_1 + a_4 \end{matrix} \middle| 1 \right) \end{aligned} & : W \\ \begin{aligned} &a_1^{-n} (a_1 a_2, a_1 a_3, a_1 a_4; q)_n \\ &\times {}_4\phi_3 \left( \begin{matrix} q^{-n}, b_4 q^{n-1}, a_1 e^{ix}, a_1 e^{-ix} \\ a_1 a_2, a_1 a_3, a_1 a_4 \end{matrix} \middle| q; q \right) \end{aligned} & : AW \end{cases} \\ &= c_n(\boldsymbol{\lambda}) \eta(x)^n + (\text{lower order terms}), \end{aligned} \quad (3.8)$$

$$c_n(\boldsymbol{\lambda}) = \begin{cases} (-1)^n (n + b_1 - 1)_n & : W \\ 2^n (b_4 q^{n-1}; q)_n & : AW \end{cases}, \quad (3.9)$$

$$\phi_0(x; \boldsymbol{\lambda}) = \begin{cases} \sqrt{(\Gamma(2ix)\Gamma(-2ix))^{-1} \prod_{j=1}^4 \Gamma(a_j + ix)\Gamma(a_j - ix)} & : W \\ \sqrt{(e^{2ix}; q)_\infty (e^{-2ix}; q)_\infty \prod_{j=1}^4 (a_j e^{ix}; q)_\infty^{-1} (a_j e^{-ix}; q)_\infty^{-1}} & : AW \end{cases}, \quad (3.10)$$

$$h_n(\boldsymbol{\lambda}) = \begin{cases} 2\pi n! (n + b_1 - 1)_n \prod_{1 \leq i < j \leq 4} \Gamma(n + a_i + a_j) \cdot \Gamma(2n + b_1)^{-1} & : W \\ 2\pi (b_4 q^{n-1}; q)_n (b_4 q^{2n}; q)_\infty (q^{n+1}; q)_\infty^{-1} \prod_{1 \leq i < j \leq 4} (a_i a_j q^n; q)_\infty^{-1} & : AW \end{cases}. \quad (3.11)$$

Here  $W_n$  and  $p_n$  in (3.8) are the Wilson and the Askey-Wilson polynomials [6] and the symbols  $(a)_n$  and  $(a; q)_n$  are  $(q)$ -shifted factorials. We have  $\phi_0^*(x; \boldsymbol{\lambda}) = \phi_0(x; \boldsymbol{\lambda})$  and  $\check{P}_n^*(x; \boldsymbol{\lambda}) =$

$\check{P}_n(x; \boldsymbol{\lambda})$ . Note that

$$\phi_0(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = \varphi(x) \sqrt{V(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})} \phi_0(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}), \quad (3.12)$$

$$V(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = \kappa^{-1} \frac{\varphi(x - i\gamma)}{\varphi(x)} V(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}). \quad (3.13)$$

The sinusoidal coordinate  $\eta(x)$  has a special dynamical meaning [30, 3, 43]. The Heisenberg operator solution for  $\eta(x)$  can be expressed in a closed form and its time evolution is a sinusoidal motion. The hermiticity of the Hamiltonian is satisfied because the function  $V\phi_0^2$  has the property

$$(3.3) \Leftrightarrow V(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) \phi_0(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})^2 \text{ has no poles in the rectangular domain } D_\gamma, \quad (3.14)$$

and the function  $G$  (2.7) ( $\check{\mathcal{R}}(x) = \check{P}_n(x; \boldsymbol{\lambda})$ ) satisfies  $G(x_1 + ix) = G^*(x_1 - ix)$ ,  $G(x_2 + ix) = 0 = G^*(x_2 - ix)$  for W and  $G(x_1 + ix) = G^*(x_1 - ix)$ ,  $G(x_2 + ix) = G^*(x_2 - ix)$  for AW. Note that eq.(3.12) implies

$$V(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) \phi_0(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})^2 = \frac{\phi_0(x; \boldsymbol{\lambda} + \boldsymbol{\delta})^2}{\varphi(x)^2}. \quad (3.15)$$

The system is shape invariant [44, 3],

$$\mathcal{A}(\boldsymbol{\lambda}) \mathcal{A}(\boldsymbol{\lambda})^\dagger = \kappa \mathcal{A}(\boldsymbol{\lambda} + \boldsymbol{\delta})^\dagger \mathcal{A}(\boldsymbol{\lambda} + \boldsymbol{\delta}) + \mathcal{E}_1(\boldsymbol{\lambda}), \quad (3.16)$$

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 formulas [3]. The action of the operators  $\mathcal{A}(\boldsymbol{\lambda})$  and  $\mathcal{A}(\boldsymbol{\lambda})^\dagger$  on the eigenfunctions is

$$\mathcal{A}(\boldsymbol{\lambda}) \phi_n(x; \boldsymbol{\lambda}) = f_n(\boldsymbol{\lambda}) \phi_{n-1}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}), \quad \mathcal{A}(\boldsymbol{\lambda})^\dagger \phi_{n-1}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = b_{n-1}(\boldsymbol{\lambda}) \phi_n(x; \boldsymbol{\lambda}). \quad (3.17)$$

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

$$f_n(\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \begin{cases} -n(n + b_1 - 1) & : \text{W} \\ q^{\frac{n}{2}}(q^{-n} - 1)(1 - b_4 q^{n-1}) & : \text{AW} \end{cases}, \quad b_{n-1}(\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \begin{cases} -1 & : \text{W} \\ q^{-\frac{n}{2}} & : \text{AW} \end{cases}. \quad (3.18)$$

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

$$\mathcal{F}(\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \phi_0(x; \boldsymbol{\lambda} + \boldsymbol{\delta})^{-1} \circ \mathcal{A}(\boldsymbol{\lambda}) \circ \phi_0(x; \boldsymbol{\lambda}) = i\varphi(x)^{-1}(e^{\frac{\gamma}{2}p} - e^{-\frac{\gamma}{2}p}), \quad (3.19)$$

$$\mathcal{B}(\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \phi_0(x; \boldsymbol{\lambda})^{-1} \circ \mathcal{A}(\boldsymbol{\lambda})^\dagger \circ \phi_0(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = -i(V(x; \boldsymbol{\lambda})e^{\frac{\gamma}{2}p} - V^*(x; \boldsymbol{\lambda})e^{-\frac{\gamma}{2}p})\varphi(x), \quad (3.20)$$

and their action on the polynomials is

$$\mathcal{F}(\boldsymbol{\lambda})\check{P}_n(x; \boldsymbol{\lambda}) = f_n(\boldsymbol{\lambda})\check{P}_{n-1}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}), \quad \mathcal{B}(\boldsymbol{\lambda})\check{P}_{n-1}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = b_{n-1}(\boldsymbol{\lambda})\check{P}_n(x; \boldsymbol{\lambda}). \quad (3.21)$$

The second order difference operator  $\tilde{\mathcal{H}}(\boldsymbol{\lambda})$  acting on the polynomial eigenfunctions is square root free. It is defined by

$$\begin{aligned} \tilde{\mathcal{H}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \phi_0(x; \boldsymbol{\lambda})^{-1} \circ \mathcal{H}(\boldsymbol{\lambda}) \circ \phi_0(x; \boldsymbol{\lambda}) = \mathcal{B}(\boldsymbol{\lambda})\mathcal{F}(\boldsymbol{\lambda}) \\ &= V(x; \boldsymbol{\lambda})(e^{\gamma p} - 1) + V^*(x; \boldsymbol{\lambda})(e^{-\gamma p} - 1), \end{aligned} \quad (3.22)$$

$$\tilde{\mathcal{H}}(\boldsymbol{\lambda})\check{P}_n(x; \boldsymbol{\lambda}) = \mathcal{E}_n(\boldsymbol{\lambda})\check{P}_n(x; \boldsymbol{\lambda}). \quad (3.23)$$

### 3.2 Discrete symmetries of the Wilson and Askey-Wilson systems

Since the potential function  $V(x; \boldsymbol{\lambda})$  (3.4) is invariant under the permutation of  $(a_1, a_2, a_3, a_4)$ , the system is symmetric in  $(a_1, a_2, a_3, a_4)$ . So are the groundstate wavefunction  $\phi_0(x; \boldsymbol{\lambda})$  (3.10) and the eigenpolynomial  $\check{P}_n(x; \boldsymbol{\lambda})$  (3.8).

In the following we restrict the parameters as follows:

$$a_1, a_2 \in \mathbb{R} \quad \text{or} \quad a_2^* = a_1; \quad a_3, a_4 \in \mathbb{R} \quad \text{or} \quad a_4^* = a_3. \quad (3.24)$$

Let us introduce twist operations  $\mathfrak{t}^{\text{I}}$ ,  $\mathfrak{t}^{\text{II}}$  and constants  $\tilde{\boldsymbol{\delta}}^{\text{I}}$ ,  $\tilde{\boldsymbol{\delta}}^{\text{II}}$ ,

$$\begin{aligned} \mathfrak{t}^{\text{I}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} (1 - \lambda_1, 1 - \lambda_2, \lambda_3, \lambda_4), & \tilde{\boldsymbol{\delta}}^{\text{I}} &\stackrel{\text{def}}{=} \left(-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right), \\ \mathfrak{t}^{\text{II}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} (\lambda_1, \lambda_2, 1 - \lambda_3, 1 - \lambda_4), & \tilde{\boldsymbol{\delta}}^{\text{II}} &\stackrel{\text{def}}{=} \left(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right). \end{aligned} \quad (3.25)$$

By using these twist operations, we define deformed potential functions  $V'$  by

$$V'^{\text{I}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} V(x; \mathfrak{t}^{\text{I}}(\boldsymbol{\lambda})), \quad V'^{\text{II}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} V(x; \mathfrak{t}^{\text{II}}(\boldsymbol{\lambda})). \quad (3.26)$$

These  $V'$ s satisfy (2.14) with

$$\begin{aligned} \alpha^{\text{I}}(\boldsymbol{\lambda}) &= \begin{cases} 1 & : \text{W} \\ a_1 a_2 q^{-1} & : \text{AW} \end{cases}, & \alpha'^{\text{I}}(\boldsymbol{\lambda}) &= \begin{cases} -(a_1 + a_2 - 1)(a_3 + a_4) & : \text{W} \\ -(1 - a_1 a_2 q^{-1})(1 - a_3 a_4) & : \text{AW} \end{cases}, \\ \alpha^{\text{II}}(\boldsymbol{\lambda}) &= \begin{cases} 1 & : \text{W} \\ a_3 a_4 q^{-1} & : \text{AW} \end{cases}, & \alpha'^{\text{II}}(\boldsymbol{\lambda}) &= \begin{cases} -(a_3 + a_4 - 1)(a_1 + a_2) & : \text{W} \\ -(1 - a_3 a_4 q^{-1})(1 - a_1 a_2) & : \text{AW} \end{cases}. \end{aligned} \quad (3.27)$$

(For  $\alpha > 0$ , we have  $a_1 a_2 > 0$  and  $a_3 a_4 > 0$  for AW case. For  $\alpha' < 0$ , we will restrict the parameters further as in (3.36).) We obtain a linear relation between the two Hamiltonians (2.15). The virtual state wavefunctions satisfying (2.17) are given by

$$\tilde{\phi}_0^{\text{I}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \phi_0(x; \mathfrak{t}^{\text{I}}(\boldsymbol{\lambda})), \quad \tilde{\phi}_v^{\text{I}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \phi_v(x; \mathfrak{t}^{\text{I}}(\boldsymbol{\lambda})) = \tilde{\phi}_0^{\text{I}}(x; \boldsymbol{\lambda}) \tilde{\xi}_v^{\text{I}}(x; \boldsymbol{\lambda}) \quad (v \in \mathcal{V}^{\text{I}}),$$

$$\begin{aligned}
\check{\xi}_v^{\text{I}}(x; \boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \xi_v^{\text{I}}(\eta(x); \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \check{P}_v(x; \mathbf{t}^{\text{I}}(\boldsymbol{\lambda})) = P_v(\eta(x); \mathbf{t}^{\text{I}}(\boldsymbol{\lambda})), \\
\check{\phi}_0^{\text{II}}(x; \boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \phi_0(x; \mathbf{t}^{\text{II}}(\boldsymbol{\lambda})), \quad \check{\phi}_v^{\text{II}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \phi_v(x; \mathbf{t}^{\text{II}}(\boldsymbol{\lambda})) = \check{\phi}_0^{\text{II}}(x; \boldsymbol{\lambda}) \check{\xi}_v^{\text{II}}(x; \boldsymbol{\lambda}) \quad (v \in \mathcal{V}^{\text{II}}), \\
\check{\xi}_v^{\text{II}}(x; \boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \xi_v^{\text{II}}(\eta(x); \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \check{P}_v(x; \mathbf{t}^{\text{II}}(\boldsymbol{\lambda})) = P_v(\eta(x); \mathbf{t}^{\text{II}}(\boldsymbol{\lambda})).
\end{aligned} \tag{3.28}$$

The virtual state polynomials  $\xi_v(\eta; \boldsymbol{\lambda})$  are polynomials of degree  $v$  in  $\eta$ . They are chosen ‘real,’  $\check{\phi}_0^*(x; \boldsymbol{\lambda}) = \check{\phi}_0(x; \boldsymbol{\lambda})$ ,  $\check{\xi}_v^*(x; \boldsymbol{\lambda}) = \check{\xi}_v(x; \boldsymbol{\lambda})$  and the virtual energies are  $\mathcal{E}'_v(\boldsymbol{\lambda}) = \mathcal{E}_v(\mathbf{t}(\boldsymbol{\lambda}))$ :

$$\begin{aligned}
\check{\mathcal{E}}_v^{\text{I}}(\boldsymbol{\lambda}) &= \begin{cases} -(a_1 + a_2 - v - 1)(a_3 + a_4 + v) & : \text{W} \\ -(1 - a_1 a_2 q^{-v-1})(1 - a_3 a_4 q^v) & : \text{AW} \end{cases}, \\
\check{\mathcal{E}}_v^{\text{II}}(\boldsymbol{\lambda}) &= \begin{cases} -(a_3 + a_4 - v - 1)(a_1 + a_2 + v) & : \text{W} \\ -(1 - a_3 a_4 q^{-v-1})(1 - a_1 a_2 q^v) & : \text{AW} \end{cases}.
\end{aligned} \tag{3.29}$$

Note that  $\alpha'(\boldsymbol{\lambda}) = \check{\mathcal{E}}_0(\boldsymbol{\lambda}) < 0$  and

$$\begin{aligned}
\text{W} : \quad \check{\mathcal{E}}_v^{\text{I}}(\boldsymbol{\lambda}) < 0 &\Leftrightarrow a_1 + a_2 > v + 1, \quad \check{\mathcal{E}}_v^{\text{II}}(\boldsymbol{\lambda}) < 0 \Leftrightarrow a_3 + a_4 > v + 1, \\
\text{AW} : \quad \check{\mathcal{E}}_v^{\text{I}}(\boldsymbol{\lambda}) < 0 &\Leftrightarrow 0 < a_1 a_2 < q^{v+1}, \quad \check{\mathcal{E}}_v^{\text{II}}(\boldsymbol{\lambda}) < 0 \Leftrightarrow 0 < a_3 a_4 < q^{v+1},
\end{aligned} \tag{3.30}$$

for  $v \geq 0$ . We choose  $\mathcal{V}^{\text{I}}$  and  $\mathcal{V}^{\text{II}}$  as

$$\mathcal{V}^{\text{I}} = \{1, 2, \dots, [\lambda_1 + \lambda_2 - 1]'\}, \quad \mathcal{V}^{\text{II}} = \{1, 2, \dots, [\lambda_3 + \lambda_4 - 1]'\}, \tag{3.31}$$

where  $[x]'$  denotes the greatest integer not equal or exceeding  $x$ . We will not use the label 0 states for deletion, see (3.58)–(3.59).

For later use, we define the following functions (recall  $x_j^{(n)}$  in (2.10)):

$$\begin{aligned}
\nu^{\text{I}}(x; \boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \frac{\phi_0(x; \boldsymbol{\lambda})}{\check{\phi}_0^{\text{I}}(x; \boldsymbol{\lambda})}, \quad r_j^{\text{I}}(x_j^{(M)}; \boldsymbol{\lambda}, M) \stackrel{\text{def}}{=} \frac{\nu^{\text{I}}(x_j^{(M)}; \boldsymbol{\lambda})}{\nu^{\text{I}}(x; \boldsymbol{\lambda} + (M-1)\check{\boldsymbol{\delta}}^{\text{I}})} \quad (1 \leq j \leq M), \\
\nu^{\text{II}}(x; \boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \frac{\phi_0(x; \boldsymbol{\lambda})}{\check{\phi}_0^{\text{II}}(x; \boldsymbol{\lambda})}, \quad r_j^{\text{II}}(x_j^{(M)}; \boldsymbol{\lambda}, M) \stackrel{\text{def}}{=} \frac{\nu^{\text{II}}(x_j^{(M)}; \boldsymbol{\lambda})}{\nu^{\text{II}}(x; \boldsymbol{\lambda} + (M-1)\check{\boldsymbol{\delta}}^{\text{II}})} \quad (1 \leq j \leq M).
\end{aligned} \tag{3.32}$$

Their explicit forms are

$$r_j^{\text{I}}(x_j^{(M)}; \boldsymbol{\lambda}, M) = \alpha^{\text{I}}(\boldsymbol{\lambda} + (M-1)\check{\boldsymbol{\delta}}^{\text{I}})^{-\frac{1}{2}(M-1)} \kappa^{\frac{1}{2}(M-1)^2 - (j-1)(M-j)} \tag{3.33}$$

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

$$r_j^{\text{II}}(x_j^{(M)}; \boldsymbol{\lambda}, M) = \alpha^{\text{II}}(\boldsymbol{\lambda} + (M-1)\check{\boldsymbol{\delta}}^{\text{II}})^{-\frac{1}{2}(M-1)} \kappa^{\frac{1}{2}(M-1)^2 - (j-1)(M-j)} \tag{3.34}$$

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

The auxiliary function  $\varphi_M(x)$  [38] is defined by:

$$\begin{aligned} \varphi_M(x) &\stackrel{\text{def}}{=} \varphi(x)^{\lfloor \frac{M}{2} \rfloor} \prod_{k=1}^{M-2} (\varphi(x - i\frac{k}{2}\gamma) \varphi(x + i\frac{k}{2}\gamma))^{\lfloor \frac{M-k}{2} \rfloor} \\ &= \prod_{1 \leq j < k \leq M} \frac{\eta(x_j^{(M)}) - \eta(x_k^{(M)})}{\varphi(i\frac{j}{2}\gamma)} \times \begin{cases} 1 & : \text{W} \\ (-2)^{\frac{1}{2}M(M-1)} & : \text{AW} \end{cases}, \end{aligned} \quad (3.35)$$

and  $\varphi_0(x) = \varphi_1(x) = 1$ . Here  $[x]$  denotes the greatest integer not exceeding  $x$ .

### 3.3 Explicit Forms of Multi-indexed Wilson and Askey-Wilson polynomials

We delete  $M = M_I + M_{II}$  virtual states  $\mathcal{D} = \{d_1^I, \dots, d_{M_I}^I, d_1^{II}, \dots, d_{M_{II}}^{II}\}$ , where  $d_j^I$  and  $d_j^{II}$  are labels of the type I and II virtual states, respectively. We restrict the parameter range further as follows:

$$\begin{aligned} \text{W} : \quad & \text{Re } a_i > \frac{1}{2}(\max_j \{d_j^I\} + 1) \quad (i = 1, 2), \quad \text{Re } a_i > \frac{1}{2}(\max_j \{d_j^{II}\} + 1) \quad (i = 3, 4), \quad (3.36) \\ \text{AW} : \quad & |a_i| < q^{\frac{1}{2}(\max_j \{d_j^I\} + 1)} \quad (i = 1, 2), \quad |a_i| < q^{\frac{1}{2}(\max_j \{d_j^{II}\} + 1)} \quad (i = 3, 4), \quad a_1 a_2, a_3 a_4 > 0. \end{aligned}$$

Then the condition  $\tilde{\mathcal{E}}_v(\boldsymbol{\lambda}) < 0$  ( $v \in \mathcal{D}$ ) is satisfied, see (3.30). We assume that the parameters are so chosen that  $\tilde{\xi}_v(x; \boldsymbol{\lambda}) \neq 0$  for  $x_1 \leq x \leq x_2$ . For example, if we take the parameters as

- $a_i \in \mathbb{R}, \quad -1 < \lambda_j - \lambda_k < 1 \quad (j = 1, 2; k = 3, 4),$
- $a_1, a_2 \in \mathbb{R}, \quad a_4^* = a_3, \quad \lambda_1 + \lambda_2 + 2v < \lambda_3 + \lambda_4,$
- $a_3, a_4 \in \mathbb{R}, \quad a_2^* = a_1, \quad \lambda_3 + \lambda_4 + 2v < \lambda_1 + \lambda_2,$

then  $\tilde{\xi}_v(x; \boldsymbol{\lambda})$  and  $\tilde{\xi}_v(x; \boldsymbol{\lambda} + \boldsymbol{\delta})$  have a definite sign for real  $x$ .

Let us write down  $\phi_{\mathcal{D}n}$  (2.24) concretely. The Casoratians in (2.24) are reduced to the following determinants, by which we define two polynomials  $\tilde{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})$  and  $\tilde{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda})$ , to be called the denominator polynomial and the multi-indexed orthogonal polynomial, respectively:

$$i^{\frac{1}{2}M(M-1)} \begin{vmatrix} \bar{X}_{d_1^I}^{(M)} & \cdots & \bar{X}_{d_{M_I}^I}^{(M)} & \bar{Y}_{d_1^{II}}^{(M)} & \cdots & \bar{Y}_{d_{M_{II}}^{II}}^{(M)} \end{vmatrix} = \varphi_M(x) \tilde{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda}) \times A,$$

$$A = \begin{cases} \prod_{k=3,4} \prod_{j=1}^{M_I-1} (a_k - \frac{M-1}{2} + ix, a_k - \frac{M-1}{2} - ix)_j \\ \quad \times \prod_{k=1,2} \prod_{j=1}^{M_{II}-1} (a_k - \frac{M-1}{2} + ix, a_k - \frac{M-1}{2} - ix)_j & : W \\ \prod_{k=3,4} \prod_{j=1}^{M_I-1} a_k^{-j} q^{\frac{1}{4}j(j+1)} (a_k q^{-\frac{M-1}{2}} e^{ix}, a_k q^{-\frac{M-1}{2}} e^{-ix}; q)_j \\ \quad \times \prod_{k=1,2} \prod_{j=1}^{M_{II}-1} a_k^{-j} q^{\frac{1}{4}j(j+1)} (a_k q^{-\frac{M-1}{2}} e^{ix}, a_k q^{-\frac{M-1}{2}} e^{-ix}; q)_j & : AW \end{cases}, \quad (3.37)$$

$$i^{\frac{1}{2}M(M+1)} \left| \begin{array}{cccccc} \vec{X}_{d_I^I}^{(M+1)} & \dots & \vec{X}_{d_{M_I}^I}^{(M+1)} & \vec{Y}_{d_I^{II}}^{(M+1)} & \dots & \vec{Y}_{d_{M_{II}}^{II}}^{(M+1)} & \vec{Z}_n^{(M+1)} \end{array} \right|$$

$$= \varphi_{M+1}(x) \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) \times B,$$

$$B = \begin{cases} \prod_{k=3,4} \prod_{j=1}^{M_I} (a_k - \frac{M}{2} + ix, a_k - \frac{M}{2} - ix)_j \\ \quad \times \prod_{k=1,2} \prod_{j=1}^{M_{II}} (a_k - \frac{M}{2} + ix, a_k - \frac{M}{2} - ix)_j & : W \\ \prod_{k=3,4} \prod_{j=1}^{M_I} a_k^{-j} q^{\frac{1}{4}j(j+1)} (a_k q^{-\frac{M}{2}} e^{ix}, a_k q^{-\frac{M}{2}} e^{-ix}; q)_j \\ \quad \times \prod_{k=1,2} \prod_{j=1}^{M_{II}} a_k^{-j} q^{\frac{1}{4}j(j+1)} (a_k q^{-\frac{M}{2}} e^{ix}, a_k q^{-\frac{M}{2}} e^{-ix}; q)_j & : AW \end{cases}, \quad (3.38)$$

where

$$\begin{aligned} (\vec{X}_v^{(M)})_j &= r_j^{II}(x_j^{(M)}; \boldsymbol{\lambda}, M) \check{\xi}_v^I(x_j^{(M)}; \boldsymbol{\lambda}), \quad (1 \leq j \leq M), \\ (\vec{Y}_v^{(M)})_j &= r_j^I(x_j^{(M)}; \boldsymbol{\lambda}, M) \check{\xi}_v^{II}(x_j^{(M)}; \boldsymbol{\lambda}), \\ (\vec{Z}_n^{(M)})_j &= r_j^{II}(x_j^{(M)}; \boldsymbol{\lambda}, M) r_j^I(x_j^{(M)}; \boldsymbol{\lambda}, M) \check{P}_n(x_j^{(M)}; \boldsymbol{\lambda}). \end{aligned} \quad (3.39)$$

They are ‘real’,  $\check{\Xi}_{\mathcal{D}}^*(x; \boldsymbol{\lambda}) = \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})$  and  $\check{P}_{\mathcal{D},n}^*(x; \boldsymbol{\lambda}) = \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda})$ . After some calculation, the eigenfunction (2.24) is rewritten as

$$\begin{aligned} \phi_{\mathcal{D}n}(x; \boldsymbol{\lambda}) &= \alpha^I (\boldsymbol{\lambda}^{[M_I, M_{II}]})^{\frac{1}{2}M_I} \alpha^{II} (\boldsymbol{\lambda}^{[M_I, M_{II}]})^{\frac{1}{2}M_{II}} \kappa^{-\frac{1}{4}M_I(M_I+1) - \frac{1}{4}M_{II}(M_{II}+1) + \frac{5}{2}M_I M_{II}} \\ &\quad \times \psi_{\mathcal{D}}(x; \boldsymbol{\lambda}) \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}), \end{aligned} \quad (3.40)$$

$$\psi_{\mathcal{D}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{\phi_0(x; \boldsymbol{\lambda}^{[M_I, M_{II}]})}{\sqrt{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}}, \quad \boldsymbol{\lambda}^{[M_I, M_{II}]} \stackrel{\text{def}}{=} \boldsymbol{\lambda} + M_I \tilde{\boldsymbol{\delta}}^I + M_{II} \tilde{\boldsymbol{\delta}}^{II}. \quad (3.41)$$

The ground state  $\phi_{\mathcal{D}0}$  is annihilated by  $\mathcal{A}_{\mathcal{D}}$ ,  $\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})\phi_{\mathcal{D}0}(x; \boldsymbol{\lambda}) = 0$ . By construction  $\psi_{\mathcal{D}}(x; \boldsymbol{\lambda})$  is positive definite in  $x_1 \leq x \leq x_2$ . By using the properties of  $\eta(x)$ ,  $r_j(x; \boldsymbol{\lambda}, M)$ ,  $\varphi_M(x)$  and the determinants, we can show that these  $\check{\Xi}_{\mathcal{D}}(x)$  (3.37) and  $\check{P}_{\mathcal{D},n}(x)$  (3.38) are polynomials in the sinusoidal coordinate  $\eta(x)$ :

$$\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \Xi_{\mathcal{D}}(\eta(x); \boldsymbol{\lambda}), \quad \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} P_{\mathcal{D},n}(\eta(x); \boldsymbol{\lambda}), \quad (3.42)$$

and their degrees are generically  $\ell$  and  $\ell + n$ , respectively (See (A.6)–(A.7)). Here  $\ell$  is

$$\ell \stackrel{\text{def}}{=} \sum_{j=1}^{M_I} d_j^I + \sum_{j=1}^{M_{II}} d_j^{II} - \frac{1}{2}M_I(M_I - 1) - \frac{1}{2}M_{II}(M_{II} - 1) + M_I M_{II}. \quad (3.43)$$

We assume that the parameters are so chosen that  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda}) \neq 0$  for  $x_1 \leq x \leq x_2$ . We have also  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) \neq 0$  ( $x_1 \leq x \leq x_2$ ). By using these and (A.16)–(A.19), we can show that  $\check{\Xi}_{\mathcal{D}}(x \mp i\frac{\gamma}{2}; \boldsymbol{\lambda}) \neq 0$  ( $x_1 \leq x \leq x_2$ ). 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  $\boldsymbol{\lambda} \rightarrow \boldsymbol{\lambda} + \boldsymbol{\delta}$ :

$$\check{P}_{\mathcal{D},0}(x; \boldsymbol{\lambda}) = A \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}), \quad (3.44)$$

where the proportionality constant  $A$  is given in (A.1). This can be shown by using (A.9)–(A.12) etc. The potential function  $V_{\mathcal{D}}$  (2.28) after  $M$  deletions ( $s = M$ ) can be expressed neatly in terms of the denominator polynomial:

$$V_{\mathcal{D}}(x; \boldsymbol{\lambda}) = V(x; \boldsymbol{\lambda}^{[M_{\text{I}}, M_{\text{II}}]}) \frac{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}}(x - i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})}. \quad (3.45)$$

The orthogonality relation (2.23) is

$$\begin{aligned} \int_{x_1}^{x_2} dx \psi_{\mathcal{D}}(x; \boldsymbol{\lambda})^2 \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) \check{P}_{\mathcal{D},m}(x; \boldsymbol{\lambda}) &= h_{\mathcal{D},n}(\boldsymbol{\lambda}) \delta_{nm} \quad (n, m = 0, 1, 2, \dots), \\ h_{\mathcal{D},n}(\boldsymbol{\lambda}) &= h_n(\boldsymbol{\lambda}) \kappa^{\frac{1}{2}M_{\text{I}}(M_{\text{I}}+1) + \frac{1}{2}M_{\text{II}}(M_{\text{II}}+1) - 5M_{\text{I}}M_{\text{II}}} \alpha^{\text{I}}(\boldsymbol{\lambda}^{[M_{\text{I}}, M_{\text{II}}]})^{-M_{\text{I}}} \alpha^{\text{II}}(\boldsymbol{\lambda}^{[M_{\text{I}}, M_{\text{II}}]})^{-M_{\text{II}}} \\ &\quad \times \prod_{j=1}^{M_{\text{I}}} (\mathcal{E}_n(\boldsymbol{\lambda}) - \tilde{\mathcal{E}}_{d_j^{\text{I}}}(\boldsymbol{\lambda})) \cdot \prod_{j=1}^{M_{\text{II}}} (\mathcal{E}_n(\boldsymbol{\lambda}) - \tilde{\mathcal{E}}_{d_j^{\text{II}}}(\boldsymbol{\lambda})). \end{aligned} \quad (3.46)$$

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

$$\begin{aligned} \hat{\mathcal{A}}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda})^\dagger \hat{\mathcal{A}}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda}) &= \mathcal{H}_{d_1 \dots d_s}(\boldsymbol{\lambda}) - \tilde{\mathcal{E}}_{d_{s+1}}(\boldsymbol{\lambda}), \\ \hat{\mathcal{A}}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda}) \hat{\mathcal{A}}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda})^\dagger &= \mathcal{H}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda}) - \tilde{\mathcal{E}}_{d_{s+1}}(\boldsymbol{\lambda}). \end{aligned} \quad (3.47)$$

It is important that they have no zero mode, so that the eigenstates of the two Hamiltonians are mapped one to one. In other words, the two Hamiltonians  $\mathcal{H}_{d_1 \dots d_s}(\boldsymbol{\lambda})$  and  $\mathcal{H}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda})$  are exactly isospectral. By the same argument given in §4 of [19], the shape invariance of  $\mathcal{H}(\boldsymbol{\lambda})$  is inherited by  $\mathcal{H}_{d_1}(\boldsymbol{\lambda})$ ,  $\mathcal{H}_{d_1 d_2}(\boldsymbol{\lambda})$ ,  $\dots$ . Therefore the Hamiltonian  $\mathcal{H}_{\mathcal{D}}(\boldsymbol{\lambda})$  is shape invariant:

$$\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda}) \mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})^\dagger = \kappa \mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda} + \boldsymbol{\delta})^\dagger \mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda} + \boldsymbol{\delta}) + \mathcal{E}_1(\boldsymbol{\lambda}). \quad (3.48)$$

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

$$\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda}) \phi_{\mathcal{D}n}(x; \boldsymbol{\lambda}) = \kappa^{\frac{M}{2}} f_n(\boldsymbol{\lambda}) \phi_{\mathcal{D}n-1}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}),$$



$$\mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})^\dagger \phi_{\mathcal{D}n-1}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = \kappa^{-\frac{M}{2}} b_{n-1}(\boldsymbol{\lambda}) \phi_{\mathcal{D}n}(x; \boldsymbol{\lambda}). \quad (3.49)$$

The forward and backward shift operators are defined by

$$\begin{aligned} \mathcal{F}_{\mathcal{D}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})^{-1} \circ \mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda}) \circ \psi_{\mathcal{D}}(x; \boldsymbol{\lambda}) \\ &= \frac{i}{\varphi(x) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})} \left( \check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda} + \boldsymbol{\delta}) e^{\frac{\gamma}{2}p} - \check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda} + \boldsymbol{\delta}) e^{-\frac{\gamma}{2}p} \right), \end{aligned} \quad (3.50)$$

$$\begin{aligned} \mathcal{B}_{\mathcal{D}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x; \boldsymbol{\lambda})^{-1} \circ \mathcal{A}_{\mathcal{D}}(\boldsymbol{\lambda})^\dagger \circ \psi_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) \\ &= \frac{-i}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \left( V(x; \boldsymbol{\lambda}^{[M_I, M_{II}]}) \check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) e^{\frac{\gamma}{2}p} \right. \\ &\quad \left. - V^*(x; \boldsymbol{\lambda}^{[M_I, M_{II}]}) \check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) e^{-\frac{\gamma}{2}p} \right) \varphi(x), \end{aligned} \quad (3.51)$$

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

$$\mathcal{F}_{\mathcal{D}}(\boldsymbol{\lambda}) \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) = f_n(\boldsymbol{\lambda}) \check{P}_{\mathcal{D},n-1}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}), \quad \mathcal{B}_{\mathcal{D}}(\boldsymbol{\lambda}) \check{P}_{\mathcal{D},n-1}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = b_{n-1}(\boldsymbol{\lambda}) \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}). \quad (3.52)$$

The similarity transformed Hamiltonian is square root free:

$$\begin{aligned} \tilde{\mathcal{H}}_{\mathcal{D}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x; \boldsymbol{\lambda})^{-1} \circ \mathcal{H}_{\mathcal{D}}(\boldsymbol{\lambda}) \circ \psi_{\mathcal{D}}(x; \boldsymbol{\lambda}) = \mathcal{B}_{\mathcal{D}}(\boldsymbol{\lambda}) \mathcal{F}_{\mathcal{D}}(\boldsymbol{\lambda}) \\ &= V(x; \boldsymbol{\lambda}^{[M_I, M_{II}]}) \frac{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})} \left( e^{\gamma p} - \frac{\check{\Xi}_{\mathcal{D}}(x - i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \right) \\ &\quad + V^*(x; \boldsymbol{\lambda}^{[M_I, M_{II}]}) \frac{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})} \left( e^{-\gamma p} - \frac{\check{\Xi}_{\mathcal{D}}(x + i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \right), \end{aligned} \quad (3.53)$$

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

$$\tilde{\mathcal{H}}_{\mathcal{D}}(\boldsymbol{\lambda}) \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) = \mathcal{E}_n(\boldsymbol{\lambda}) \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}). \quad (3.54)$$

Other intertwining relations are (see (A.16)–(A.19))

$$\kappa^{\frac{1}{2}} \hat{\mathcal{A}}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda} + \boldsymbol{\delta}) \mathcal{A}_{d_1 \dots d_s}(\boldsymbol{\lambda}) = \mathcal{A}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda}) \hat{\mathcal{A}}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda}), \quad (3.55)$$

$$\kappa^{-\frac{1}{2}} \hat{\mathcal{A}}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda}) \mathcal{A}_{d_1 \dots d_s}(\boldsymbol{\lambda})^\dagger = \mathcal{A}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda})^\dagger \hat{\mathcal{A}}_{d_1 \dots d_{s+1}}(\boldsymbol{\lambda} + \boldsymbol{\delta}), \quad (3.56)$$

with the potential function  $\hat{V}_{d_1 \dots d_{s+1}}$  given in (2.20) (with  $s \rightarrow s+1$ )

$$\begin{aligned} \hat{V}_{d_1 \dots d_{s+1}}(x; \boldsymbol{\lambda}) &= \frac{\Xi_{d_1 \dots d_s}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) \Xi_{d_1 \dots d_{s+1}}(x - i\gamma; \boldsymbol{\lambda})}{\Xi_{d_1 \dots d_s}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) \Xi_{d_1 \dots d_{s+1}}(x; \boldsymbol{\lambda})} \\ &\quad \times \begin{cases} \alpha^{\text{I}}(\boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) V'^{\text{I}}(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) & : d_{s+1} \text{ is of type I} \\ \alpha^{\text{II}}(\boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) V'^{\text{II}}(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) & : d_{s+1} \text{ is of type II} \end{cases}, \end{aligned} \quad (3.57)$$

where  $s_I$  and  $s_{II}$  are the numbers of the type I and II states in  $\{d_1, \dots, d_s\}$ , respectively.

Although we have restricted  $d_j \geq 1$ , there is no obstruction for deletion of  $d_j = 0$ . Including the level 0 deletion corresponds to  $M - 1$  virtual states deletion:

$$\begin{aligned} \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) \Big|_{d_{M_I}^I=0} &= A \check{P}_{\mathcal{D}',n}(x; \boldsymbol{\lambda} + \tilde{\boldsymbol{\delta}}^I), \\ \mathcal{D}' &= \{d_1^I - 1, \dots, d_{M_I-1}^I - 1, d_1^{II} + 1, \dots, d_{M_{II}}^{II} + 1\}, \end{aligned} \quad (3.58)$$

$$\begin{aligned} \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) \Big|_{d_{M_{II}}^{II}=0} &= B \check{P}_{\mathcal{D}',n}(x; \boldsymbol{\lambda} + \tilde{\boldsymbol{\delta}}^{II}), \\ \mathcal{D}' &= \{d_1^I + 1, \dots, d_{M_I}^I + 1, d_1^{II} - 1, \dots, d_{M_{II}-1}^{II} - 1\}, \end{aligned} \quad (3.59)$$

where the proportionality constants  $A$  and  $B$  are given in (A.2)–(A.3). These can be shown by using (3.21), (A.9), (A.11) etc. The denominator polynomial  $\Xi_{\mathcal{D}}$  behaves similarly due to (3.44). This is why we have restricted  $d_j \geq 1$ .

The exceptional  $X_\ell$  Wilson and Askey-Wilson orthogonal polynomials presented in [12, 19] correspond to the simplest case  $M = 1$ ,  $\mathcal{D} = \{\ell\}$  of type I,  $\ell \geq 1$ :

$$\begin{aligned} \check{\xi}_\ell(x; \boldsymbol{\lambda}) &= \check{\Xi}_{\{\ell^I\}}(x; \boldsymbol{\lambda} + \ell \boldsymbol{\delta} - \tilde{\boldsymbol{\delta}}^I), \\ \check{P}_{\ell,n}(x; \boldsymbol{\lambda}) &= \check{P}_{\{\ell^I\},n}(x; \boldsymbol{\lambda} + \ell \boldsymbol{\delta} - \tilde{\boldsymbol{\delta}}^I) \times \begin{cases} -(a_1 + a_2 + n)^{-1} & : W \\ (a_1 a_2 q^n)^{\frac{1}{2}} (1 - a_1 a_2 q^n)^{-1} & : AW \end{cases}. \end{aligned} \quad (3.60)$$

As observed in some multi-indexed Laguerre and Jacobi polynomials [1], it can happen that two systems with different sets  $\mathcal{D}$  turn out to be equivalent. Namely the denominator polynomials with different sets  $\mathcal{D}$  may be proportional to each other. For example, the denominator polynomial of  $k$  deletions of type I virtual states,  $\mathcal{D}_1 = \{m^I, (m+1)^I, \dots, (m+k-1)^I\}$ , and that of  $m$  deletions of type II virtual states,  $\mathcal{D}_2 = \{k^{II}, (k+1)^{II}, \dots, (k+m-1)^{II}\}$ , are related,

$$\check{\Xi}_{\mathcal{D}_1}(x; \boldsymbol{\lambda} + m \tilde{\boldsymbol{\delta}}^{II}) = A \check{\Xi}_{\mathcal{D}_2}(x; \boldsymbol{\lambda} + k \tilde{\boldsymbol{\delta}}^I) \quad (k, m \geq 1), \quad (3.61)$$

where the proportionality constant  $A$  is given in (A.4). From this and (3.45), we have

$$V_{\mathcal{D}_1}(x; \boldsymbol{\lambda} + m \tilde{\boldsymbol{\delta}}^{II}) = V_{\mathcal{D}_2}(x; \boldsymbol{\lambda} + k \tilde{\boldsymbol{\delta}}^I). \quad (3.62)$$

Therefore these two systems are equivalent under the shift of parameters. Classification of the equivalent classes leading to the same polynomials is a challenging future problem.

For the cases of type I only ( $M_I = M$ ,  $M_{II} = 0$ ,  $\mathcal{D} = \{d_1, \dots, d_M\}$ ), the expressions (3.37) and (3.38) are slightly simplified,

$$W_\gamma[\check{\xi}_{d_1}^I, \dots, \check{\xi}_{d_M}^I](x; \boldsymbol{\lambda}) = \varphi_M(x) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda}), \quad (3.63)$$

$$\begin{aligned}
& \nu^I(x; \boldsymbol{\lambda} + M\tilde{\boldsymbol{\delta}}^I)^{-1} W_\gamma[\check{\xi}_{d_1}^I, \dots, \check{\xi}_{d_M}^I, \nu^I \check{P}_n](x; \boldsymbol{\lambda}) = \varphi_{M+1}(x) \check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda}) \\
& = i^{\frac{1}{2}M(M+1)} \left| \begin{array}{cccc} \check{\xi}_{d_1}^I(x_1^{(M+1)}; \boldsymbol{\lambda}) & \cdots & \check{\xi}_{d_M}^I(x_1^{(M+1)}; \boldsymbol{\lambda}) & r_1^I(x_1^{(M+1)}) \check{P}_n(x_1^{(M+1)}; \boldsymbol{\lambda}) \\ \check{\xi}_{d_1}^I(x_2^{(M+1)}; \boldsymbol{\lambda}) & \cdots & \check{\xi}_{d_M}^I(x_2^{(M+1)}; \boldsymbol{\lambda}) & r_2^I(x_2^{(M+1)}) \check{P}_n(x_2^{(M+1)}; \boldsymbol{\lambda}) \\ \vdots & \cdots & \vdots & \vdots \\ \check{\xi}_{d_1}^I(x_{M+1}^{(M+1)}; \boldsymbol{\lambda}) & \cdots & \check{\xi}_{d_M}^I(x_{M+1}^{(M+1)}; \boldsymbol{\lambda}) & r_{M+1}^I(x_{M+1}^{(M+1)}) \check{P}_n(x_{M+1}^{(M+1)}; \boldsymbol{\lambda}) \end{array} \right|, \quad (3.64)
\end{aligned}$$

where  $r_j^I(x) = r_j^I(x; \boldsymbol{\lambda}, M+1)$ . The cases of type II only ( $M_I = 0$ ,  $M_{II} = M$ ) are similar.

### 3.4 Analyticity and Hermiticity

At the end of this section we comment on the hermiticity of the Hamiltonian  $\mathcal{H}_{\mathcal{D}}$ . The functions  $V(x)$ ,  $\phi_0(x)$  and  $\check{\mathcal{R}}(x)$  in § 2.2 correspond to  $V_{\mathcal{D}}(x; \boldsymbol{\lambda})$ ,  $\phi_{\mathcal{D}0}(x; \boldsymbol{\lambda}) \propto \psi_{\mathcal{D}}(x; \boldsymbol{\lambda}) \check{P}_{\mathcal{D},0}(x; \boldsymbol{\lambda})$  and  $\check{P}_{\mathcal{D},n}(x; \boldsymbol{\lambda})/\check{P}_{\mathcal{D},0}(x; \boldsymbol{\lambda})$ , respectively. So the function  $G(x)$  (2.7) becomes (up to an overall constant)

$$G(x) = \frac{V(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}^{[M_I, M_{II}]}) \phi_0(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}^{[M_I, M_{II}]})^2}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})^2} \check{P}_{\mathcal{D},n}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{P}_{\mathcal{D},m}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}), \quad (3.65)$$

and we have

$$\begin{aligned}
G(x) - G^*(x) &= V(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}^{[M_I, M_{II}]}) \phi_0(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}^{[M_I, M_{II}]})^2 \times \frac{\mathcal{P}(x)}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})} \times \frac{1}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})}, \\
\mathcal{P}(x) &= \check{P}_{\mathcal{D},n}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{P}_{\mathcal{D},m}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) - \check{P}_{\mathcal{D},n}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{P}_{\mathcal{D},m}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}). \quad (3.66)
\end{aligned}$$

From (3.14) and (3.36), this  $V\phi_0^2$  part  $V(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}^{[M_I, M_{II}]}) \phi_0(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}^{[M_I, M_{II}]})^2$  has no poles in the rectangular domain  $D_\gamma$ . The function  $\mathcal{P}(x)$  can be divided by  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})$ ;  $\mathcal{P}(x)/\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda}) = i\varphi(x) \times (\text{polynomial in } \eta(x))$ . Thus the potential singularities of  $G - G^*$  originate from the zeros of  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})$ . The left hand side of the condition (2.8) vanishes because of  $G(x_1 + ix) = G^*(x_1 - ix)$ ,  $G(x_2 + ix) = 0 = G^*(x_2 - ix)$  for W and  $G(x_1 + ix) = G^*(x_1 - ix)$ ,  $G(x_2 + ix) = G^*(x_2 - ix)$  for AW, on the assumption that there is no singularity on the integration paths. If  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})$  has no zeros in  $D_\gamma$ , the function  $G - G^*$  has no poles in  $D_\gamma$  and the condition (2.8) is satisfied. If  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})$  has zeros in  $D_\gamma$ , they appear as complex conjugate pairs,  $\alpha \pm i\beta$  ( $x_1 \leq \alpha \leq x_2$ ,  $0 < \beta \leq \frac{1}{2}|\gamma|$ ), because of  $\check{\Xi}_{\mathcal{D}}^* = \check{\Xi}_{\mathcal{D}}$  and  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda}) \neq 0$  ( $x_1 \leq x \leq x_2$ ). In order to satisfy the condition (2.8), the sum of the residues of  $G - G^*$  should vanish.

The term  $V_{\mathcal{D}} + V_{\mathcal{D}}^*$  in  $\mathcal{H}_{\mathcal{D}}$  is

$$V_{\mathcal{D}}(x; \boldsymbol{\lambda}) + V_{\mathcal{D}}^*(x; \boldsymbol{\lambda}) = V(x; \boldsymbol{\lambda}^{[M_I, M_{II}]}) \frac{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}}(x - i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})}$$

$$+ V^*(x; \boldsymbol{\lambda}^{[M_I, M_{II}]}) \frac{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}}(x + i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})}.$$

This does not cause any obstruction for the hermiticity. The potential singularities in the interval  $x_1 \leq x \leq x_2$  are (i)  $V(x; \boldsymbol{\lambda}^{[M_I, M_{II}]})$  and  $V^*(x; \boldsymbol{\lambda}^{[M_I, M_{II}]})$  at  $x = x_1, x_2$ , (ii) zeros of  $\check{\Xi}_{\mathcal{D}}(x \mp i\frac{\gamma}{2}; \boldsymbol{\lambda})$  in the denominators, (iii) zeros of  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})$  in the denominators. For case (i), the singularities cancel out as in the original case  $V(x; \boldsymbol{\lambda}) + V^*(x; \boldsymbol{\lambda})$ . For case (ii), we can show  $\check{\Xi}_{\mathcal{D}}(x \mp i\frac{\gamma}{2}; \boldsymbol{\lambda}) \neq 0$  ( $x_1 \leq x \leq x_2$ ) by using  $\check{\Xi}_{d_1 \dots d_s}(x; \boldsymbol{\lambda}) \neq 0$ ,  $\check{\Xi}_{d_1 \dots d_s}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) \neq 0$  ( $x_1 \leq x \leq x_2$ ) and (A.16)–(A.19). For case (iii), (2.30) and (3.57) imply that the denominator factor  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})$  disappears, namely  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})$  does not give singularities.

Thus the Hamiltonian  $\mathcal{H}_{\mathcal{D}}$  is well-defined and hermitian, if  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})$  has no zeros in  $D_{\gamma}$  or the residues coming from the zeros of  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})$  cancel. At present we have no general proof of the cancellation nor generic procedures to restrict the parameters so that there will be no zeros of  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})$  in the rectangular domain  $D_{\gamma}$ . Existence of such parameter ranges that  $\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})$  has no zeros in  $D_{\gamma}$  can be verified by numerical calculation for small  $M$ .

## 4 Summary and Comments

By following the examples of the multi-indexed Laguerre, Jacobi [1] and ( $q$ -)Racah [2] polynomials, the multi-indexed Wilson (W) and Askey-Wilson (AW) polynomials are constructed within the framework of discrete quantum mechanics with pure imaginary shifts [3, 26]. The method is, as in the previous cases, multiple Darboux-Crum transformations [33, 34, 36] by using the virtual state solutions. The virtual state solutions are derived through certain discrete symmetries of the original Wilson and Askey-Wilson Hamiltonians and by definition they are not eigenfunctions of the discrete Schrödinger equation. The type I and II virtual state solutions are introduced (3.28) but they are not related with specific boundary conditions, in contradistinction with the multi-indexed Laguerre, Jacobi or ( $q$ -)Racah cases. Main emphasis is on the algebraic structure and the difference equations for the multi-indexed W and AW polynomials, (3.52), (3.54) etc., which hold for any parameter range. So far we do not have a comprehensive method to determine the parameter ranges which ensure the hermiticity of the deformed Hamiltonians and thus the orthogonality of the multi-indexed W and AW polynomials. The one-indexed, *i.e.*  $\mathcal{D} = \{\ell\}$ ,  $\ell \geq 1$ , of type I are identical with the exceptional W or AW polynomials reported earlier [12, 19].

Like the other exceptional polynomials, the multi-indexed W and AW polynomials do not satisfy the three term recurrence relations. As in the ordinary Sturm-Liouville problems, the multi-indexed orthogonal polynomial  $P_{\mathcal{D},n}(y; \boldsymbol{\lambda})$  has  $n$  zeros in the orthogonality range,  $0 < y < \infty$  (W) or  $-1 < y < 1$  (AW) (the oscillation theorem). It is well known that various hypergeometric orthogonal polynomials in the Askey scheme are obtained from the Wilson and Askey-Wilson polynomials in certain limits. Similarly, from the multi-indexed W and AW polynomials presented in the previous section, we can obtain the multi-indexed version of various orthogonal polynomials, such as the continuous (dual) Hahn, etc. In that sense, the multi-indexed Wilson polynomials are also obtained from the multi-indexed Askey-Wilson polynomials. Here we briefly discuss the limits to the multi-indexed Jacobi and Laguerre cases. In an appropriate limit the discrete quantum mechanics with pure imaginary shifts reduces to the ordinary quantum mechanics [45]. Explicitly the W and the AW systems reduce to the Laguerre (L) and the Jacobi (J) systems, respectively in the following way [45]:

$$\begin{aligned} \text{W} : \boldsymbol{\lambda} &= \left( \frac{c^2}{\omega_1}, \frac{c^2}{\omega_2}, g_1, g_2 \right), \quad 1 = \omega_1 + \omega_2, \quad g = g_1 + g_2 - \frac{1}{2}, \\ \frac{4}{a_1 a_2} \mathcal{H}^{\text{W}} \times c^2 &\xrightarrow{c \rightarrow \infty} \mathcal{H}^{\text{L}} = p^2 + x^2 + \frac{g(g-1)}{x^2} - 1 - 2g, \end{aligned} \quad (4.1)$$

$$\begin{aligned} \text{AW} : q^\lambda &= (-q^{h_1}, -q^{h_2}, q^{g_1}, q^{g_2}), \quad g = g_1 + g_2 - \frac{1}{2}, \quad h = h_1 + h_2 - \frac{1}{2}, \quad q = e^{-\frac{1}{c}}, \quad x = 2x^J, \\ (a_1 a_2 a_3 a_4 q^{-1})^{-\frac{1}{2}} \mathcal{H}^{\text{AW}} \times c^2 &\xrightarrow{c \rightarrow \infty} \frac{1}{4} \mathcal{H}^{\text{J}}, \quad \mathcal{H}^{\text{J}} = (p^J)^2 + \frac{g(g-1)}{\sin^2 x^J} + \frac{h(h-1)}{\cos^2 x^J} - (g+h)^2. \end{aligned} \quad (4.2)$$

The ground state wavefunction  $\phi_0(x)$  (3.10) and the eigenpolynomial  $P_n(x)$  (3.8) also reduce to those of L and J cases after an appropriate overall rescaling. For the deformed systems we have the same correspondence under the same limit. For the AW case, the type I and II twists (3.25) reduce to those of the J cases given in [1],  $(g, h) \rightarrow (g, 1-h)$  and  $(g, h) \rightarrow (1-g, h)$ . For the W case, the type II twist (3.25) reduces to that of the L case given in [1],  $g \rightarrow 1-g$ . For the type I of W case, there is subtlety because of negative components of  $\mathbf{t}^{\text{I}}(\boldsymbol{\lambda}) = (1 - \frac{c^2}{\omega_1}, 1 - \frac{c^2}{\omega_2}, g_1, g_2)$ . For example, in order to obtain the limit of the ground state wavefunction, we need certain regularization. The limit of type I becomes unchanging  $g$  and effectively changing  $x$  to  $ix$ . This corresponds to the type I of L given in [1]. Therefore the deformed W and AW systems reduce to the deformed L and J systems in [1]. The multi-indexed Wilson and Askey-Wilson polynomials (3.38) reduce to the multi-indexed Laguerre and Jacobi polynomials given in [1] after an appropriate overall rescaling.

When all the parameters  $a_i$ 's are real, we have four other twists,

$$\begin{aligned} \mathfrak{t}^{(13)}(\boldsymbol{\lambda}) &= (1 - \lambda_1, \lambda_2, 1 - \lambda_3, \lambda_4), & \mathfrak{t}^{(14)}(\boldsymbol{\lambda}) &= (1 - \lambda_1, \lambda_2, \lambda_3, 1 - \lambda_4), \\ \mathfrak{t}^{(23)}(\boldsymbol{\lambda}) &= (\lambda_1, 1 - \lambda_2, 1 - \lambda_3, \lambda_4), & \mathfrak{t}^{(24)}(\boldsymbol{\lambda}) &= (\lambda_1, 1 - \lambda_2, \lambda_3, 1 - \lambda_4), \end{aligned}$$

because of the permutation symmetry of the  $a_i$ 's. Algebraically, any one of the six twists defines a deformed Hamiltonian. According to the parameter configuration, *e.g.*  $a_1 < a_2 < a_3 < a_4$ , etc, the compatibility of any two or more twists and the hermiticity of the resulting multi-indexed Hamiltonians would be determined. The detailed analysis of these allowed parameter ranges is beyond the scope of the present paper.

With the present paper, the project of generic construction of multi-indexed orthogonal polynomials of a single variable is now complete. It is a real challenge to pursue the possibility of constructing multi-indexed orthogonal polynomials of several variables.

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## A Several Formulas

In Appendix we provide several formulas which are not included in the main text for smooth presentation.

First we give various proportionality constants:

$$A \text{ in (3.44)} = \begin{cases} \prod_{j=1}^{M_I} (-a_1 - a_2 + d_j^I + 1) \cdot \prod_{j=1}^{M_{II}} (-a_3 - a_4 + d_j^{II} + 1) & : W \\ q^{2M_I M_{II}} \prod_{j=1}^{M_I} (a_1 a_2 q^{-d_j^I - 1})^{-\frac{1}{2}} (1 - a_1 a_2 q^{-d_j^I - 1}) \\ \quad \times \prod_{j=1}^{M_{II}} (a_3 a_4 q^{-d_j^{II} - 1})^{-\frac{1}{2}} (1 - a_3 a_4 q^{-d_j^{II} - 1}) & : AW \end{cases}, \quad (\text{A.1})$$

$$A \text{ in (3.58)} = \begin{cases} (-1)^{M_{II}+1} (a_1 + a_2 + n - 1) \prod_{j=1}^{M_I-1} d_j^I (-a_1 - a_2 + a_3 + a_4 + d_j^I + 1) & : W \\ (-1)^{M_I-1} (a_1 a_2 q^{n-1})^{-\frac{1}{2}} (1 - a_1 a_2 q^{n-1}) \\ \quad \times \prod_{j=1}^{M_I-1} q^{-\frac{1}{2} d_j^I} (1 - q^{d_j^I}) (1 - a_1^{-1} a_2^{-1} a_3 a_4 q^{d_j^I + 1}) \\ \quad \times (a_1^{-1} a_2^{-1} a_3 a_4)^{\frac{1}{2} M_{II}} \prod_{j=1}^{M_{II}} q^{M_I + j - \frac{1}{2} d_j^{II}} & : AW \end{cases}, \quad (\text{A.2})$$

$$B \text{ in (3.59)} = \begin{cases} -(a_3 + a_4 + n - 1) \prod_{j=1}^{M_{\text{II}}-1} d_j^{\text{II}} (-a_3 - a_4 + a_1 + a_2 + d_j^{\text{II}} + 1) & : \text{W} \\ (-1)^{M_{\text{I}}+M_{\text{II}}-1} (a_3 a_4 q^{n-1})^{-\frac{1}{2}} (1 - a_3 a_4 q^{n-1}) \\ \quad \times \prod_{j=1}^{M_{\text{II}}-1} q^{-\frac{1}{2}d_j^{\text{II}}} (1 - q^{d_j^{\text{II}}}) (1 - a_3^{-1} a_4^{-1} a_1 a_2 q^{d_j^{\text{II}}+1}) \\ \quad \times (a_1 a_2 a_3^{-1} a_4^{-1})^{\frac{1}{2}M_{\text{I}}} \prod_{j=1}^{M_{\text{I}}} q^{M_{\text{II}}+j-\frac{1}{2}d_j^{\text{I}}} & : \text{AW} \end{cases}, \quad (\text{A.3})$$

$$A \text{ in (3.61)} = \begin{cases} (-1)^{km} \frac{\prod_{j=1}^k (-j)^{k-j} \prod_{j=1}^{\lfloor \frac{1}{2}k \rfloor} (a_3 + a_4 - a_1 - a_2 + 2j)_{2k-4j+1}}{\prod_{j=1}^m (-j)^{m-j} \prod_{j=1}^{\lfloor \frac{1}{2}m \rfloor} (a_1 + a_2 - a_3 - a_4 + 2j)_{2m-4j+1}} & : \text{W} \\ (-a_1^{-1} a_2^{-1} a_3 a_4)^{km} q^{\frac{1}{2}(k-m)(3km-(k-m-1)(k-m+1))} \\ \quad \times \frac{\prod_{j=1}^k (1 - q^j)^{k-j} \prod_{j=1}^{\lfloor \frac{1}{2}k \rfloor} (a_1^{-1} a_2^{-1} a_3 a_4 q^{2j}; q)_{2k-4j+1}}{\prod_{j=1}^m (1 - q^j)^{m-j} \prod_{j=1}^{\lfloor \frac{1}{2}m \rfloor} (a_1 a_2 a_3^{-1} a_4^{-1} q^{2j}; q)_{2m-4j+1}} & : \text{AW} \end{cases}. \quad (\text{A.4})$$

Next we give the coefficients of the highest degree term of the polynomials  $\Xi_{\mathcal{D}}$  and  $P_{\mathcal{D},n}$ ,

$$\begin{aligned} \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda}) &= c_{\mathcal{D}}^{\Xi}(\boldsymbol{\lambda}) \eta(x)^{\ell} + (\text{lower order terms}), \\ \check{P}_{\mathcal{D}}(x; \boldsymbol{\lambda}) &= c_{\mathcal{D},n}^P(\boldsymbol{\lambda}) \eta(x)^{\ell+n} + (\text{lower order terms}). \end{aligned} \quad (\text{A.5})$$

For  $\mathcal{D} = \{d_1^{\text{I}}, \dots, d_{M_{\text{I}}}^{\text{I}}, d_1^{\text{II}}, \dots, d_{M_{\text{II}}}^{\text{II}}\}$ , they are

$$\begin{aligned} c_{\mathcal{D}}^{\Xi}(\boldsymbol{\lambda}) &= \prod_{j=1}^{M_{\text{I}}} c_{d_j^{\text{I}}}(\mathbf{t}^{\text{I}}(\boldsymbol{\lambda})) \cdot \prod_{j=1}^{M_{\text{II}}} c_{d_j^{\text{II}}}(\mathbf{t}^{\text{II}}(\boldsymbol{\lambda})) \\ &\times \begin{cases} \prod_{1 \leq j < k \leq M_{\text{I}}} (d_k^{\text{I}} - d_j^{\text{I}}) \cdot \prod_{1 \leq j < k \leq M_{\text{II}}} (d_k^{\text{II}} - d_j^{\text{II}}) \\ \quad \times \prod_{j=1}^{M_{\text{I}}} \prod_{k=1}^{M_{\text{II}}} (-a_3 - a_4 - d_j^{\text{I}} + a_1 + a_2 + d_k^{\text{II}}) & : \text{W} \\ \prod_{1 \leq j < k \leq M_{\text{I}}} \frac{1}{2} q^{\frac{1}{2}(d_j^{\text{I}} - d_k^{\text{I}})} (1 - q^{d_k^{\text{I}} - d_j^{\text{I}}}) \cdot \prod_{1 \leq j < k \leq M_{\text{II}}} \frac{1}{2} q^{\frac{1}{2}(d_j^{\text{II}} - d_k^{\text{II}})} (1 - q^{d_k^{\text{II}} - d_j^{\text{II}}}) \\ \quad \times \prod_{j=1}^{M_{\text{I}}} \prod_{k=1}^{M_{\text{II}}} \frac{2}{\sqrt{a_1 a_2 a_3 a_4}} q^{j+k-2-\frac{1}{2}(d_j^{\text{I}}+d_k^{\text{II}})} (a_3 a_4 q^{d_j^{\text{I}}} - a_1 a_2 q^{d_k^{\text{II}}}) & : \text{AW} \end{cases}, \end{aligned} \quad (\text{A.6})$$

$$\begin{aligned} c_{\mathcal{D},n}^P(\boldsymbol{\lambda}) &= c_{\mathcal{D}}^{\Xi}(\boldsymbol{\lambda}) c_n(\boldsymbol{\lambda}) \\ &\times \begin{cases} \prod_{j=1}^{M_{\text{I}}} (-a_1 - a_2 - n + d_j^{\text{I}} + 1) \cdot \prod_{j=1}^{M_{\text{II}}} (-a_3 - a_4 - n + d_j^{\text{II}} + 1) & : \text{W} \\ q^{2M_{\text{I}}M_{\text{II}}} \prod_{j=1}^{M_{\text{I}}} (a_1 a_2)^{-\frac{1}{2}} q^{\frac{1}{2}(d_j^{\text{I}}+1-n)} (1 - a_1 a_2 q^{n-d_j^{\text{I}}-1}) \\ \quad \times \prod_{j=1}^{M_{\text{II}}} (a_3 a_4)^{-\frac{1}{2}} q^{\frac{1}{2}(d_j^{\text{II}}+1-n)} (1 - a_3 a_4 q^{n-d_j^{\text{II}}-1}) & : \text{AW} \end{cases}. \end{aligned} \quad (\text{A.7})$$

The virtual state wavefunction  $\tilde{\phi}_{\mathcal{D}\text{v}}$  (2.24) for  $\mathcal{D} = \{d_1^{\text{I}}, \dots, d_{M_{\text{I}}}^{\text{I}}, d_1^{\text{II}}, \dots, d_{M_{\text{II}}}^{\text{II}}\}$  is given by

$$\tilde{\phi}_{\mathcal{D}\text{v}}(x; \boldsymbol{\lambda}) = \frac{\check{\Xi}_{\mathcal{D}\text{v}}(x; \boldsymbol{\lambda})}{\sqrt{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}}$$

$$\begin{aligned}
& \times (a_1 a_2)^{\frac{1}{2}M_I} (a_3 a_4)^{\frac{1}{2}M_{II}} \kappa^{\frac{3}{4}M(M+1) - \frac{1}{2}M_I(M_I+1) - \frac{1}{2}M_{II}(M_{II}+1)} \\
& \times \begin{cases} \kappa^{\frac{1}{2}M_{II}(M_{II}-1) - M_I M_{II}} \tilde{\phi}_0^I(x; \boldsymbol{\lambda}^{[M_I, M_{II}]}) & : v \text{ is of type I} \\ \kappa^{\frac{1}{2}M_I(M_I-1) - M_I M_{II}} \tilde{\phi}_0^{II}(x; \boldsymbol{\lambda}^{[M_I, M_{II}]}) & : v \text{ is of type II} \end{cases} . \quad (\text{A.8})
\end{aligned}$$

The polynomial  $\xi_v$  with parameters  $\boldsymbol{\lambda}$  and  $\boldsymbol{\lambda} + \boldsymbol{\delta}$  are related in the following way [19]:

$$\frac{i}{\varphi(x)} \left( v_1^*(x; \boldsymbol{\lambda} + \tilde{\boldsymbol{\delta}}^I) e^{\frac{\gamma}{2}p} - v_1(x; \boldsymbol{\lambda} + \tilde{\boldsymbol{\delta}}^I) e^{-\frac{\gamma}{2}p} \right) \check{\xi}_v^I(x; \boldsymbol{\lambda}) = \hat{f}_{0,v}^I(\boldsymbol{\lambda}) \check{\xi}_v^I(x; \boldsymbol{\lambda} + \boldsymbol{\delta}), \quad (\text{A.9})$$

$$\frac{-i}{\varphi(x)} \left( v_2(x; \boldsymbol{\lambda}) e^{\frac{\gamma}{2}p} - v_2^*(x; \boldsymbol{\lambda}) e^{-\frac{\gamma}{2}p} \right) \check{\xi}_v^I(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = \hat{b}_{0,v}^I(\boldsymbol{\lambda}) \check{\xi}_v^I(x; \boldsymbol{\lambda}), \quad (\text{A.10})$$

$$\frac{i}{\varphi(x)} \left( v_2^*(x; \boldsymbol{\lambda} + \tilde{\boldsymbol{\delta}}^{II}) e^{\frac{\gamma}{2}p} - v_2(x; \boldsymbol{\lambda} + \tilde{\boldsymbol{\delta}}^{II}) e^{-\frac{\gamma}{2}p} \right) \check{\xi}_v^{II}(x; \boldsymbol{\lambda}) = \hat{f}_{0,v}^{II}(\boldsymbol{\lambda}) \check{\xi}_v^{II}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}), \quad (\text{A.11})$$

$$\frac{-i}{\varphi(x)} \left( v_1(x; \boldsymbol{\lambda}) e^{\frac{\gamma}{2}p} - v_1^*(x; \boldsymbol{\lambda}) e^{-\frac{\gamma}{2}p} \right) \check{\xi}_v^{II}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) = \hat{b}_{0,v}^{II}(\boldsymbol{\lambda}) \check{\xi}_v^{II}(x; \boldsymbol{\lambda}), \quad (\text{A.12})$$

where the functions  $v_1$  and  $v_2$  are

$$v_1(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \begin{cases} \prod_{j=1}^2 (a_j + ix) & : W \\ e^{-ix} \prod_{j=1}^2 (1 - a_j e^{ix}) & : AW \end{cases}, \quad v_2(x; \boldsymbol{\lambda}) \stackrel{\text{def}}{=} \begin{cases} \prod_{j=3}^4 (a_j + ix) & : W \\ e^{-ix} \prod_{j=3}^4 (1 - a_j e^{ix}) & : AW \end{cases}, \quad (\text{A.13})$$

and the constants  $\hat{f}_{s,v}$  and  $\hat{b}_{s,v}$  are

$$\hat{f}_{s,v}^I(\boldsymbol{\lambda}) = \begin{cases} a_1 + a_2 - v - 1 & : W \\ -q^{\frac{1}{2}(v-s)} (1 - a_1 a_2 q^{-v-1}) & : AW \end{cases}, \quad \hat{b}_{s,v}^I(\boldsymbol{\lambda}) = \begin{cases} a_3 + a_4 + v & : W \\ -q^{-\frac{1}{2}(v-s)} (1 - a_3 a_4 q^v) & : AW \end{cases}, \quad (\text{A.14})$$

$$\hat{f}_{s,v}^{II}(\boldsymbol{\lambda}) = \begin{cases} a_3 + a_4 - v - 1 & : W \\ -q^{\frac{1}{2}(v-s)} (1 - a_3 a_4 q^{-v-1}) & : AW \end{cases}, \quad \hat{b}_{s,v}^{II}(\boldsymbol{\lambda}) = \begin{cases} a_1 + a_2 + v & : W \\ -q^{-\frac{1}{2}(v-s)} (1 - a_1 a_2 q^v) & : AW \end{cases}. \quad (\text{A.15})$$

These relations are generalized to the denominator polynomials  $\Xi_{d_1 \dots d_s v}$ . In the rest of Appendix we consider the set  $\mathcal{D} = \{d_1, \dots, d_s\}$ , in which the number of type I virtual states is  $s_I$  and that of type II is  $s_{II}$ ,  $s = s_I + s_{II}$ . When  $v$  is of type I, the denominator polynomials  $\Xi_{\mathcal{D}v}$  with  $\boldsymbol{\lambda}$  and  $\boldsymbol{\lambda} + \boldsymbol{\delta}$  are related as

$$\begin{aligned}
& \frac{i}{\varphi(x) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})} \left( v_1^*(x; \boldsymbol{\lambda}^{[s_I, s_{II}]} + \tilde{\boldsymbol{\delta}}^I) \check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda} + \boldsymbol{\delta}) e^{\frac{\gamma}{2}p} \right. \\
& \quad \left. - v_1(x; \boldsymbol{\lambda}^{[s_I, s_{II}]} + \tilde{\boldsymbol{\delta}}^I) \check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda} + \boldsymbol{\delta}) e^{-\frac{\gamma}{2}p} \right) \check{\Xi}_{\mathcal{D}v}(x; \boldsymbol{\lambda}) \\
& \quad = \kappa^{-s_{II}} \hat{f}_{s,v}^I(\boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}v}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}), \quad (\text{A.16}) \\
& \frac{-i}{\varphi(x) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \left( v_2(x; \boldsymbol{\lambda}^{[s_I, s_{II}]} + \tilde{\boldsymbol{\delta}}^I) \check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) e^{\frac{\gamma}{2}p} \right. \\
& \quad \left. - v_2^*(x; \boldsymbol{\lambda}^{[s_I, s_{II}]} + \tilde{\boldsymbol{\delta}}^I) \check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) e^{-\frac{\gamma}{2}p} \right) \check{\Xi}_{\mathcal{D}v}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})
\end{aligned}$$



$$= \kappa^{s_{\text{II}}} \hat{b}_{s, \text{v}}^{\text{I}}(\boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}_{\text{v}}}(x; \boldsymbol{\lambda}). \quad (\text{A.17})$$

When  $\text{v}$  is of type II, they are

$$\begin{aligned} & \frac{i}{\varphi(x) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda})} \left( v_2^*(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]} + \tilde{\boldsymbol{\delta}}^{\text{II}}) \check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda} + \boldsymbol{\delta}) e^{\frac{\gamma}{2}p} \right. \\ & \quad \left. - v_2(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]} + \tilde{\boldsymbol{\delta}}^{\text{II}}) \check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda} + \boldsymbol{\delta}) e^{-\frac{\gamma}{2}p} \right) \check{\Xi}_{\mathcal{D}_{\text{v}}}(x; \boldsymbol{\lambda}) \\ & = \kappa^{-s_{\text{I}}} \hat{f}_{s, \text{v}}^{\text{II}}(\boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}_{\text{v}}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}), \end{aligned} \quad (\text{A.18})$$

$$\begin{aligned} & \frac{-i}{\varphi(x) \check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \left( v_1(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) \check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda}) e^{\frac{\gamma}{2}p} \right. \\ & \quad \left. - v_1^*(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) \check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda}) e^{-\frac{\gamma}{2}p} \right) \check{\Xi}_{\mathcal{D}_{\text{v}}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta}) \\ & = \kappa^{s_{\text{I}}} \hat{b}_{s, \text{v}}^{\text{II}}(\boldsymbol{\lambda}) \check{\Xi}_{\mathcal{D}_{\text{v}}}(x; \boldsymbol{\lambda}). \end{aligned} \quad (\text{A.19})$$

These relations are used to show (3.55)–(3.56), and imply the difference equations of  $\check{\Xi}_{\mathcal{D}_{\text{v}}}$ ; when  $\text{v}$  is of type I, they are

$$\begin{aligned} & \left( \alpha^{\text{I}}(\boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) V'^{\text{I}}(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) \frac{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})} e^{\gamma p} \right. \\ & \quad + \alpha^{\text{I}}(\boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) V'^{\text{I}*}(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) \frac{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})} e^{-\gamma p} \\ & \quad - V(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) \frac{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})} \frac{\check{\Xi}_{\mathcal{D}}(x - i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \\ & \quad \left. - V^*(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) \frac{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})} \frac{\check{\Xi}_{\mathcal{D}}(x + i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \right) \Xi_{\mathcal{D}_{\text{v}}}(x; \boldsymbol{\lambda}) \\ & = \tilde{\mathcal{E}}_{\text{v}}^{\text{I}}(\boldsymbol{\lambda}) \Xi_{\mathcal{D}_{\text{v}}}(x; \boldsymbol{\lambda}), \end{aligned} \quad (\text{A.20})$$

and when  $\text{v}$  is of type II, they are

$$\begin{aligned} & \left( \alpha^{\text{II}}(\boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) V'^{\text{II}}(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) \frac{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})} e^{\gamma p} \right. \\ & \quad + \alpha^{\text{II}}(\boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) V'^{\text{II}*}(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) \frac{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})} e^{-\gamma p} \\ & \quad - V(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) \frac{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})} \frac{\check{\Xi}_{\mathcal{D}}(x - i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \\ & \quad \left. - V^*(x; \boldsymbol{\lambda}^{[s_{\text{I}}, s_{\text{II}}]}) \frac{\check{\Xi}_{\mathcal{D}}(x - i\frac{\gamma}{2}; \boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x + i\frac{\gamma}{2}; \boldsymbol{\lambda})} \frac{\check{\Xi}_{\mathcal{D}}(x + i\gamma; \boldsymbol{\lambda} + \boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x; \boldsymbol{\lambda} + \boldsymbol{\delta})} \right) \Xi_{\mathcal{D}_{\text{v}}}(x; \boldsymbol{\lambda}) \\ & = \tilde{\mathcal{E}}_{\text{v}}^{\text{II}}(\boldsymbol{\lambda}) \Xi_{\mathcal{D}_{\text{v}}}(x; \boldsymbol{\lambda}). \end{aligned} \quad (\text{A.21})$$

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