Lecture Note
NCTU Yau Center, Mini Course
Exactly solvable (discrete) quantum mechanics and new orthogonal polynomials

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Abstract

A comprehensive introduction to exactly solvable quantum mechanics in one dimension and its *difference equation versions* is presented. This provides a unified theory of *classical* orthogonal polynomials. An important recent progress of *integrable deformations* of these exactly solvable quantum mechanical systems is also covered. New types of *infinitely many* orthogonal polynomials are discovered as the main parts of the eigenfunctions of the deformed integrable systems. These new polynomials are called the *exceptional* and/or *multi-indexed* and *Krein-Adler* orthogonal polynomials. These new polynomials are rational deformations of the classical orthogonal polynomials generated by multiple Darboux transformations. The discrete symmetries of the original solvable quantum mechanical systems provide the seed polynomials from the original eigenpolynomials.

Contents

1 Introduction

It is well known that the Hermite, Laguerre and Jacobi polynomials constitute the main parts of the eigenfunctions of the exactly solvable Quantum Mechanics (QM) in one dimension [1, 2]. The eigenvalue problem of self-adjoint operators is the natural setting of the orthogonality of these polynomials and their orthogonality weight are simply the square of the *ground state eigenfunctions*. This has led to quantum mechanical reformulation of all the classical orthogonal polynomials in the Askey scheme [3, 4, 5] for which the Schrödinger equations are second order difference equations [6, 7, 8, 9].

The reformulation has turned out quite fruitful, providing universal expressions for various formulas, *e.g.* the Rodrigues formulas as well as the Heisenberg operator solutions, the creation/annihilation operators and coherent states, etc. Many new properties and formulas have been uncovered for the orthogonal polynomials of a *discrete variable* [10], *e.g.* the (dual) (q-)Hahn, (q-)Racah polynomials etc. [6, 9]. For this group, the corresponding quantum mechanical setting is simply the eigenvalue problem of *tri-diagonal real symmetric* (Jacobi) matrices of finite or infinite dimensions [6, 9]. The *duality* [11, 12, 13] is recognised as a universal property of the polynomials of this group and the *dual polynomial* [14] is identified for each polynomial [6, 9] except for those having the Jackson integral measures. All the polynomials belonging to this group are shown to provide *exactly solvable Birth and Death processes* [15], which are well-known stochastic (Markov) processes [16, 4]. An even more interesting finding is that the Jackson integral measures arise naturally through the *self-adjoint extension processes* of certain infinite matrix formulations, including the big q-Jacobi (Laguerre), Al-Salam-Carlitz I, discrete q-Hermite polynomials, [6, 9].

The quantum mechanical formulation of orthogonal polynomials has provided not only the *unified theory classical orthogonal polynomials* but also opened new dimensions for *non-classical orthogonal polynomials*. They satisfy second order differential or difference equations but not three term recurrence relations. This means that there are '*holes*' in their degrees but they still form complete sets in proper Hilbert spaces. They are obtained from the eigenfunctions (vectors) of the original systems through Darboux-Crum transformations [17]–[20] by using certain seed solutions. Depending on the nature of the seed solutions, there are two types of non-classical orthogonal polynomials. When a part of the eigenfunctions (vectors) is used, the obtained polynomials are called *Krein-Adler polynomials* [21],[22]. By applying certain discrete transformations of the original systems to the eigen functions (vectors), seed solutions called *virtual state solutions (vectors)* are obtained. The non-classical orthogonal polynomials obtained by using virtual state solutions are called *exceptional* and/or *multi-indexed orthogonal polynomials* [23]–[27]. Of course, using both eigenfunctions and virtual state solutions as seed solutions for multiple Darboux-Crum transformations is possible and it leads to mixed type non-classical orthogonal polynomials.

We emphasise the strategy and main results and omit details. The contents of this chapter are as follows. In section 2, the new orthogonal polynomials satisfying second order differential equations are surveyed. Starting from QM formulation of the Hermite, Laguerre and Jacobi polynomials, their discrete symmetries and the virtual state solutions are explicitly presented. Based on the Darboux-Crum transformations, the multi-indexed Laguerre and Jacobi polynomials are derived. The general forms of the Krein-Adler polynomials for the Hermite, Laguerre and Jacobi are presented. Explicit examples of the multi-indexed Laguerre and Jacobi polynomials are displayed. In the second part of the note, the non-classical orthogonal polynomials satisfying second order difference equations with *real shifts* are presented. The overview of the Simplest QM is presented in section 3. It is the eigenvalue problems of certain tri-diagonal real symmetric matrices and the the Hamiltonians, eigenvectors, etc. for various explicit examples are explained. In section 4 the duality and dual polynomials are explained. The fundamental structure of the solution spaces of the Simplest QM is explored in 5. The shape invariance, a sufficient condition for exact solvability is introduced in section 6. These exactly solvable QM are also solvable in the Heisenberg picture, which is explained in 7. The construction of the non-classical orthogonal polynomials is explained by deforming the Racah and q-Racah systems. The hamiltonians, their discrete symmetry transformations and the corresponding virtual state vectors are presented. The discrete QM analogue of the Darboux transformation is introduced by using a virtual state vector as one seed 'solution'. General construction of multi-indexed (q-)Racah polynomials through multiple Darboux transformations is presented. Explicit examples of multi-indexed (q-)Racah polynomials are exhibited. The final section is for a summary and comments.

2 New orthogonal polynomials in ordinary QM

For the construction of the non-classical orthogonal polynomials, the fundamental knowledge of the corresponding classical counterparts is essential; the complete sets of the eigenvalues, eigenfunctions, discrete symmetries and forms of Darboux transformations, etc. The passage from the classical to non-classical orthogonal polynomials is basically the same for the ordinary and discrete QM. Here we show the derivation and some explicit examples of the non-classical orthogonal polynomials for the familiar examples from the ordinary QM, *i.e.* the Hermite, Laguerre and Jacobi.

2.1 Classical polynomials: the Hermite, Laguerre and Jacobi

We begin with the summary of fundamental properties of the classical orthogonal polynomials in 1-d QM formulation. The eigenvalue problem is defined in a finite or (semi-)infinite interval $x_1 < x < x_2$,

$$\mathcal{H}\phi_n(x) = \mathcal{E}(n)\phi_n(x), \quad (n \in \mathbb{Z}_{\geq 0}), \quad (\phi_n, \phi_m) \stackrel{\text{def}}{=} \int_{x_1}^{x_2} \phi_n^*(x)\phi_m(x)dx = h_n\delta_{n\,m}, \tag{2.1}$$

with the Hamiltonian or the Schrödinger operator

$$\mathcal{H} = -\frac{d^2}{dx^2} + V(x), \quad V(x) \in \mathbb{R}, \quad V(x) \in C^\infty. \tag{2.2}$$

Throughout this section we consider the real eigenfunctions and wavefunctions, $\phi_n^*(x) = \phi_n(x)$. The properties of the Hermite (H), Laguerre (L) and Jacobi (J) systems are summarised as follows. The first is the Hermite system:

$$\text{H:} \qquad V(x) = x^2 - 1, \quad -\infty < x < \infty, \quad \mathcal{E}(n) = 2n \quad (n \in \mathbb{Z}_{\geq 0}), \tag{2.3}$$

$$\phi_n(x) = \phi_0(x)H_n(x), \quad \phi_0(x) = e^{-x^2/2}, \quad H_n(x) : \text{Hermite poly.} \tag{2.4}$$

The constant (-1) term in the potential is added to make the groundstate energy vanishing $\mathcal{E}(0) = 0$. The same convention is adopted for the L and J systems shown below. The square of the ground state eigenfunction $\phi_0^2(x) = e^{-x^2}$ provides the orthogonality weight function for the Hermite polynomials:

$$(\!(H_n, H_m)\!) = \int_{-\infty}^{\infty} e^{-x^2} H_n(x)H_m(x)dx = h_n\delta_{n\,m}, \quad h_n = 2^n n!\sqrt{\pi}. \tag{2.5}$$

The Hamiltonian without the constant term $\mathcal{H}' \stackrel{\text{def}}{=} \mathcal{H} + 1$ has a discrete symmetry

$$x \to ix \Rightarrow \mathcal{H}' \to -\mathcal{H}'. \tag{2.6}$$

By acting on the eigenfunctions, it generates square non-integrable seed solutions of *negative energy*

$$\varphi_n(x) \stackrel{\text{def}}{=} i^n\phi_n(ix), \quad \mathcal{H}\varphi_n(x) = \widetilde{\mathcal{E}}_n\varphi_n(x), \quad \widetilde{\mathcal{E}}_n = -2(n+1),\ (n \in \mathbb{Z}_{\geq 0}). \tag{2.7}$$

The second is the Laguerre system with $g > 1/2$:

$$\text{L: } V(x) = x^2 + \frac{g(g-1)}{x^2} - (1+2g),\ 0 < x < \infty,\ \mathcal{E}(n) = 4n\ (n \in \mathbb{Z}_{\geq 0}), \tag{2.8}$$

$$\phi_n(x;g) = \phi_0(x;g)L_n^{(g-1/2)}(x^2), \quad \phi_0(x;g) = e^{-x^2/2}x^g, \tag{2.9}$$

in which $L_n^{(\alpha)}(\eta)$ is the Laguerre polynomial and its weight function is given by $\phi_0^2(x;g)$ with $\alpha \stackrel{\text{def}}{=} g - 1/2$,

$$(\!(L_n^{(\alpha)}, L_m^{(\alpha)})\!) = \int_0^\infty e^{-x^2}x^{2g}L_n^{(\alpha)}(x^2)L_m^{(\alpha)}(x^2)dx = h_n\delta_{n\,m}, \tag{2.10}$$

$$= \frac{1}{2}\int_0^\infty e^{-\eta}\eta^\alpha L_n^{(\alpha)}(\eta)L_m^{(\alpha)}(\eta)d\eta, \quad h_n = \frac{\Gamma(n+g+1/2)}{2n!}. \tag{2.11}$$

The lower end point $x = 0$ is a regular singular point with the characteristic exponents g and $1-g$. The Hamiltonian without the constant term $\mathcal{H}' \stackrel{\text{def}}{=} \mathcal{H} + 1 + 2g$ has the same discrete symmetry as the Hermite system

$$\text{L1:} \qquad x \to ix \Rightarrow \mathcal{H}' \to -\mathcal{H}',$$

called L1 symmetry transformation. By acting on the eigenfunctions it generates square non-integrable seed solutions of *negative energy*, called type I *virtual state solutions*,

$$\varphi_n^{\mathrm{I}}(x) \stackrel{\text{def}}{=} |\phi_n(ix;g)| = e^{x^2/2}x^gL_n^{(g-1/2)}(-x^2), \tag{2.12}$$

$$\mathcal{H}\varphi_n^{\mathrm{I}}(x) = \widetilde{\mathcal{E}}_n^{\mathrm{I}}\varphi_n^{\mathrm{I}}(x), \quad \widetilde{\mathcal{E}}_n^{\mathrm{I}} = -4(n+g+1/2), \quad (n \in \mathbb{Z}_{\geq 0}). \tag{2.13}$$

It is obvious that $\varphi_n^{\mathrm{I}}(x)$ has no zero in $0 < x < \infty$. It is easy to see that the Hamiltonian $\mathcal{H}' \stackrel{\text{def}}{=} \mathcal{H} + 1 + 2g$ is invariant under the exchange of the characteristic exponents at $x = 0$,

$$\text{L2:} \quad g \leftrightarrow 1-g \Rightarrow \mathcal{H}' \Leftrightarrow \mathcal{H}', \tag{2.14}$$

which is called L2 symmetry transformation. By acting on the lower lying eigenfunctions it generates square non-integrable seed solutions of *negative energy* called type II virtual state solutions,

$$\varphi_n^{\mathrm{II}}(x) \stackrel{\text{def}}{=} \phi_n(x;1-g) = e^{-x^2/2}x^{1-g}L_n^{(1/2-g)}(x^2), \tag{2.15}$$

$$\mathcal{H}\varphi_n^{\mathrm{II}}(x) = \widetilde{\mathcal{E}}_n^{\mathrm{II}}\varphi_n^{\mathrm{II}}(x),\ \widetilde{\mathcal{E}}_n^{\mathrm{II}} = -4(n-g-1/2),\ n = 0, 1, \ldots, [g-1/2]'. \tag{2.16}$$

For the above range of n, $\varphi_n^{\mathrm{II}}(x)$ has no zero in $0 < x < \infty$, [32]. Here $[a]'$ denotes the greatest integer less than a. By applying type I and II transformations on the eigenfunctions, type III virtual state solutions are obtained:

$$\varphi_n^{\mathrm{III}}(x) \stackrel{\text{def}}{=} |\phi_n(ix;1-g)| = e^{x^2/2}x^{1-g}L_n^{(1/2-g)}(-x^2), \tag{2.17}$$

$$\mathcal{H}\varphi_n^{\mathrm{III}}(x) = \widetilde{\mathcal{E}}_n^{\mathrm{III}}\varphi_n^{\mathrm{III}}(x),\ \widetilde{\mathcal{E}}_n^{\mathrm{III}} = -4(n+1),\ n \in \mathbb{Z}_{\geq 0}. \tag{2.18}$$

The third is the Jacobi system with $g > 1/2$, $h > 1/2$:

$$\text{J:} \qquad V(x) = \frac{g(g-1)}{\sin^2 x} + \frac{h(h-1)}{\cos^2 x} - (g+h)^2, \quad 0 < x < \pi/2, \tag{2.19}$$

$$\mathcal{E}(n) = 4n(n+g+h) \ (n \in \mathbb{Z}_{\geq 0}), \tag{2.20}$$

$$\phi_n(x;g,h) = \phi_0(x;g,h) P_n^{(\alpha,\beta)}(\cos 2x), \quad \alpha \stackrel{\text{def}}{=} g - 1/2, \ \beta \stackrel{\text{def}}{=} h - 1/2, \tag{2.21}$$

$$\phi_0(x;g,h) = (\sin x)^g (\cos x)^h, \tag{2.22}$$

in which $P_n^{(\alpha,\beta)}(\eta)$ is the Jacobi polynomial and its weight function is $\phi_0^2(x;g,h)$,

$$(\!(P_n^{(\alpha,\beta)}, P_m^{(\alpha,\beta)})\!) = \int_0^{\pi/2} (\sin x)^{2g} (\cos x)^{2h} P_n^{(\alpha,\beta)}(\cos 2x) P_m^{(\alpha,\beta)}(\cos 2x) dx \tag{2.23}$$

$$= \frac{1}{2^{(2+\alpha+\beta)}} \int_{-1}^{1} (1-\eta)^\alpha (1+\eta)^\beta P_n^{(\alpha,\beta)}(\eta) P_m^{(\alpha,\beta)}(\eta) d\eta \tag{2.24}$$

$$= h_n \delta_{nm}, \quad h_n = \frac{\Gamma(n+g+\frac{1}{2})\Gamma(n+h+\frac{1}{2})}{2n!(2n+g+h)\Gamma(n+g+h)}. \tag{2.25}$$

The two end points $x = \pi/2$ and $x = 0$ are regular singular points with the characteristic exponents $\{h, 1-h\}$ and $\{g, 1-g\}$, respectively. The Hamiltonian without the constant term $\mathcal{H}' \stackrel{\text{def}}{=} \mathcal{H} + (g+h)^2$ has two discrete symmetry transformations, exchanging the characteristic exponents at $x = \pi/2$ and $x = 0$, respectively:

$$\text{J1: } h \leftrightarrow 1-h, \qquad \text{J2: } g \leftrightarrow 1-g \quad \Longrightarrow \mathcal{H}' \Leftrightarrow \mathcal{H}', \tag{2.26}$$

which are called J1 and J2 symmetry transformations, respectively. By acting on the lower lying eigenfunctions they generate square non-integrable seed solutions of *negative energy* called type I and type II virtual state solutions, respectively:

$$\varphi_n^{\mathrm{I}}(x) \stackrel{\text{def}}{=} \phi_n(x;g,1-h) = (\sin x)^g (\cos x)^{1-h} P_n^{(g-1/2,1/2-h)}(\cos 2x), \tag{2.27}$$

$$\mathcal{H}\varphi_n^{\mathrm{I}}(x) = \tilde{\mathcal{E}}_n^{\mathrm{I}} \varphi_n^{\mathrm{I}}(x), \ \ \tilde{\mathcal{E}}_n^{\mathrm{I}} = -4(n+g+1/2)(h-n-1/2),$$
$$n = 0, 1, \ldots, [h-1/2]', \tag{2.28}$$

$$\varphi_n^{\mathrm{II}}(x) \stackrel{\text{def}}{=} \phi_n(x;1-g,h) = (\sin x)^{1-g} (\cos x)^h P_n^{(1/2-g,h-1/2)}(\cos 2x), \tag{2.29}$$

$$\mathcal{H}\varphi_n^{\mathrm{II}}(x) = \tilde{\mathcal{E}}_n^{\mathrm{II}} \varphi_n^{\mathrm{II}}(x), \ \ \tilde{\mathcal{E}}_n^{\mathrm{II}} = -4(g-n-1/2)(n+h+1/2),$$
$$n = 0, 1, \ldots, [g-1/2]'. \tag{2.30}$$

These virtual state solutions have no nodes in $0 < x < \pi/2$ [26, 32]. By applying type I and II transformations on the eigenfunctions, type III virtual state solutions are obtained:

$$\varphi_n^{\mathrm{III}}(x) \stackrel{\text{def}}{=} \phi_n(x;1-g,1-h) = (\sin x)^{1-g} (\cos x)^{1-h} P_n^{(1/2-g,1/2-h)}(\cos 2x),$$
$$\mathcal{H}\varphi_n^{\mathrm{III}}(x) = \tilde{\mathcal{E}}_n^{\mathrm{III}} \varphi_n^{\mathrm{III}}(x), \ \ \tilde{\mathcal{E}}_n^{\mathrm{III}} = -4(n+1)(g+h-n-1).$$

In the above three systems, H, L, and J, the constant parts of the potential function $V(x)$ are so chosen as to achieve the *zero ground state energy* $\mathcal{E}(0)=0$. That is, the Hamiltonians or the Schrödinger operators $\mathcal{H}$ are *positive semi-definite* and they have a factorised expression, remiscenct of the well-known theorem in Linear Algebra:

$$\mathcal{H}=\mathcal{A}^\dagger\mathcal{A},\quad \mathcal{A}\stackrel{\text{def}}{=}\frac{d}{dx}-\partial_x\log|\phi_0(x)|,\quad \mathcal{A}^\dagger=-\frac{d}{dx}-\partial_x\log|\phi_0(x)|,\quad \mathcal{A}\phi_0(x)=0. \tag{2.31}$$

This expression is valid for any one-dimensional ordinary QM system having zero ground state energy $\mathcal{E}(0)=0$, as the ground state wavefunction $\phi_0(x)$ has no node. Thus we obtain a non-singular expression of the potential function $V(x)$

$$V(x)=\frac{\partial_x^2\phi_0(x)}{\phi_0(x)}=\partial_x\left(\frac{\partial_x\phi_0(x)}{\phi_0(x)}\right)+\left(\frac{\partial_x\phi_0(x)}{\phi_0(x)}\right)^2, \tag{2.32}$$

By similarity transforming $\mathcal{H}$ in terms of the ground state eigenfunction $\phi_0(x)$, we obtain the second order differential operator $\widetilde{\mathcal{H}}$

$$\widetilde{\mathcal{H}}\stackrel{\text{def}}{=}\phi_0(x)^{-1}\circ\mathcal{H}\circ\phi_0(x)=-\frac{d^2}{dx^2}-2\partial_x\log|\phi_0(x)|\cdot\frac{d}{dx}, \tag{2.33}$$

which governs the classical orthogonal polynomials H, L and J.
For H, it is

$$\text{H:}\qquad -H_n''(x)+2xH_n'(x)=2nH_n(x). \tag{2.34}$$

For L and J they read

$$\text{L:}\qquad -\eta\partial_\eta^2L_n^{(\alpha)}(\eta)-(\alpha+1-\eta)\partial_\eta L_n^{(\alpha)}(\eta)=n\,L_n^{(\alpha)}(\eta), \tag{2.35}$$

$$\begin{aligned}\text{J:}\qquad &-(1-\eta^2)\partial_\eta^2P_n^{(\alpha,\beta)}(\eta)-[\beta-\alpha+(\alpha+\beta+2)\eta]\partial_\eta P_n^{(\alpha,\beta)}(\eta)\\ &\qquad\qquad=n(n+\alpha+\beta+1)P_n^{(\alpha,\beta)}(\eta),\end{aligned} \tag{2.36}$$

after the change of the independent variables $\eta(x)=x^2$ and $\eta(x)=\cos 2x$, respectively.

2.2 Darboux transformation

Darboux transformations are essential for the derivation of non-classical orthogonal polynomials. In its original form, a Darboux transformation maps one solution $\psi(x)$ of a Schrödinger operator $\mathcal{H}$, to another $\psi^{(1)}(x)$ with the same energy $\mathcal{E}$ of a deformed Schrödinger operator $\mathcal{H}^{(1)}$ in terms of a seed solution $\varphi(x)$. Explicitly the transformation reads

$$\mathcal{H}\psi(x)=\mathcal{E}\psi(x),\quad \mathcal{H}\varphi(x)=\widetilde{\mathcal{E}}\varphi(x),\quad \psi(x),\varphi(x),\mathcal{E},\widetilde{\mathcal{E}}\in\mathbb{C}, \tag{2.37}$$

$$\mathcal{H}^{(1)}\psi^{(1)}(x)=\mathcal{E}\psi^{(1)}(x), \tag{2.38}$$

$$\psi^{(1)}(x)\stackrel{\text{def}}{=}\frac{\varphi(x)\psi'(x)-\varphi'(x)\psi(x)}{\varphi(x)},\quad \mathcal{H}^{(1)}\stackrel{\text{def}}{=}\mathcal{H}-2\partial_x^2\log|\varphi(x)|. \tag{2.39}$$

Exercise Verify by direct calculation. Let us prepare one solution $\psi(x)$ and M distinct seed solutions $\{\varphi_j(x),\tilde{\mathcal{E}}_j\}$ of $\mathcal{H}$:

$$\mathcal{H}\psi(x)=\mathcal{E}\psi(x),\quad \mathcal{H}\varphi_j(x)=\tilde{\mathcal{E}}_j\varphi_j(x),\ \mathcal{E},\tilde{\mathcal{E}}_j\in\mathbb{C},\ j=1,\dots,M. \tag{2.40}$$

Applying Darboux transformations to $\psi(x)$ successively by using $\{\varphi_j(x)\}$ in turn, we arrive at:

Theorem 2.1 (Darboux [17]) *An isospectral solution* $\psi^{(M)}(x)$ *of a deformed Hamiltonian* $\mathcal{H}^{(M)}$*,*

$$\mathcal{H}^{(M)}\psi^{(M)}(x)=\mathcal{E}\psi^{(M)}(x),\quad \psi^{(M)}(x)\stackrel{\textit{def}}{=}\frac{\mathrm{W}[\varphi_1,\ldots,\varphi_M,\psi](x)}{\mathrm{W}[\varphi_1,\ldots,\varphi_M](x)}, \tag{2.41}$$

$$\mathcal{H}^{(M)}\stackrel{\textit{def}}{=}\mathcal{H}-2\frac{d^2\log|\mathrm{W}[\varphi_1,\ldots,\varphi_M](x)|}{dx^2}. \tag{2.42}$$

Here the Wronskian of n functions $\{f_1(x),\ldots,f_n(x)\}$ is defined by

$$\mathrm{W}\,[f_1,\ldots,f_n](x)\stackrel{\text{def}}{=}\det\Bigl(\frac{d^{j-1}f_k(x)}{dx^{j-1}}\Bigr)_{1\le j,k\le n}. \tag{2.43}$$

The theorem applies to any Schrödinger equation even with a complex potential.

Exercise Verify the above Theorem by induction using the following identity of the Wronskians.

$$\begin{aligned}&\mathrm{W}\bigl[\mathrm{W}[f_1,f_2,\ldots,f_n,g],\mathrm{W}[f_1,f_2,\ldots,f_n,h]\,\bigr](x)\\ &=\mathrm{W}[f_1,f_2,\ldots,f_n](x)\,\mathrm{W}[f_1,f_2,\ldots,f_n,g,h](x)\qquad(n\ge 0).\end{aligned} \tag{2.44}$$

2.3 Krein-Adler polynomials

The Krein-Adler polynomials [21, 22] are obtained as the main parts of the eigenfunctions of the system obtained by deforming the complete set of eigenfunctions $\{\phi_n(x)\}$ (H, L or J) through Darboux transformations by choosing a part of the eigenfunctions as the seed solutions. Let $\mathcal{D}$ be a set of distinct non-negative integers, $\mathcal{D}=\{d_1,d_2,\ldots,d_M\}$ which specifies the set of seed eigenfunctions $\{\phi_{d_1}(x),\ldots,\phi_{d_M}(x)\}$. The deformed system reads:

$$\mathcal{H}_{\mathcal{D}}\stackrel{\text{def}}{=}\mathcal{H}-2\partial_x^2\Bigl(\log|\mathrm{W}\,[\phi_{d_1},\phi_{d_2},\ldots,\phi_{d_M}](x)|\Bigr), \tag{2.45}$$

$$\mathcal{H}_{\mathcal{D}}\phi_{\mathcal{D};n}(x)=\mathcal{E}(n)\phi_{\mathcal{D};n}(x), \tag{2.46}$$

$$\phi_{\mathcal{D};n}(x)\stackrel{\text{def}}{=}\frac{\mathrm{W}\,[\phi_{d_1},\phi_{d_2},\ldots,\phi_{d_M},\phi_n](x)}{\mathrm{W}\,[\phi_{d_1},\phi_{d_2},\ldots,\phi_{d_M}](x)},\quad (n\in\mathbb{Z}_{\ge 0}\backslash\mathcal{D}). \tag{2.47}$$

The norms of the deformed eigenfunctions are

$$(\phi_{\mathcal{D};n},\phi_{\mathcal{D};m})=\prod_{j=1}^{M}\bigl(\mathcal{E}(n)-\mathcal{E}(d_j)\bigr)\cdot(\phi_n,\phi_m)\quad (n,m\in\mathbb{Z}_{\ge 0}\backslash\mathcal{D}). \tag{2.48}$$

It is necessary and sufficient for the set $\mathcal{D}$ to satisfy the conditions

$$\prod_{j=1}^{M}(m-d_j)\ge 0,\quad \forall m\in\mathbb{Z}_{\ge 0}, \tag{2.49}$$

for the positivity of the norms and non-singularity of the potential [22]. The Darboux-Crum [18] transformation is the case when $\mathcal{D}$ consists of consecutive integers from zero, $\mathcal{D}=\{0,1,\ldots,M-1\}$, then the above conditions (2.49) are simply satisfied.

Let us denote the eigenfunctions of the (H, L, J) system generically as

$$\phi_n(x) = \phi_0(x) P_n\big(\eta(x)\big), \quad \eta(x) = x,\ x^2,\ \cos 2x \text{ for H, L, J.} \tag{2.50}$$

By using the following properties of the Wronskian

$$\mathrm{W}[gf_1, gf_2, \ldots, gf_n](x) = g(x)^n \mathrm{W}[f_1, f_2, \ldots, f_n](x), \tag{2.51}$$

$$\begin{aligned} &\mathrm{W}[f_1(y), f_2(y), \ldots, f_n(y)](x) \\ &\qquad = y'(x)^{n(n-1)/2} \mathrm{W}[f_1, f_2, \ldots, f_n](y), \end{aligned} \tag{2.52}$$

we arrive at

$$\phi_{\mathcal{D};n}(x) = \frac{\phi_0(x)\eta'(x)^M}{\mathrm{W}[P_{d_1}, P_{d_2}, \ldots, P_{d_M}](\eta)} \mathrm{W}[P_{d_1}, P_{d_2}, \ldots, P_{d_M}, P_n](\eta),$$

which gives the explicit expressions of the Krein-Adler polynomials

$$\mathrm{W}[P_{d_1}, P_{d_2}, \ldots, P_{d_M}, P_n](\eta), \qquad (n \in \mathbb{Z}_{\geq 0} \backslash \mathcal{D}), \tag{2.53}$$

with the degree $\ell'_{\mathcal{D}} + n$ and the orthogonality weight function

$$\ell'_{\mathcal{D}} = \sum_{j=1}^{M} d_j - M(M+1)/2, \quad \frac{\phi_0^2(x)\eta'(x)^{2M}}{\big(\mathrm{W}[P_{d_1}, P_{d_2}, \ldots, P_{d_M}](\eta)\big)^2}. \tag{2.54}$$

This means that infinitely many families of *complete set of orthogonal rational functions having the same orthogonality weight functions with shifted parameters* can be generated.

Let us consider a simple explicit example of H and $\mathcal{D} = \{1, 2\}$ [29, 22]. The deformed Hamiltonian

$$\mathcal{H}_{\mathcal{D}} = -\frac{d^2}{dx^2} + x^2 + 3 + \frac{32x^2}{(2x^2+1)^2} - \frac{8}{2x^2+1}, \quad -\infty < x < \infty, \tag{2.55}$$

has an eigenpolynomial of degree n, $\mathrm{W}[H_1, H_2, H_n](x)$, $n \in \mathbb{Z}_{\geq 0} \backslash \{1, 2\}$, with the orthogonality weight function $e^{-x^2}/(2x^2+1)^2$. Obviously three term recurrence relations do not hold but they form a complete set. Essentially the same deformation is achieved by using the seed solution $\varphi_2(x) = e^{x^2/2} H_2(ix)$ obtained by the discrete symmetry transformation (2.6) acting on $\phi_2(x)$. More generally, using an appropriate set of these seed solutions for H has the same effects as certain Krein-Adler transformations [36]. A similar theorem holds for L/J system when the type III virtual state solutions are used [36].

2.4 Multi-indexed Laguerre and Jacobi polynomials

The multi-indexed Laguerre/Jacobi polynomials are obtained by deforming the L/J system by multiple Darboux transformations in terms of type I and II virtual state solutions. In this subsection we assume that the couplings g and h are generic real numbers. Here we emphasise the logical structure [27] rather than following the historical developments. Let us denote, for simplicity of presentation, the type I/II virtual state polynomials as $\xi^{\mathrm{I}}_n(\eta)$ and $\xi^{\mathrm{II}}_n(\eta)$:

$$
\begin{aligned}
&\mathrm{L}:\ \xi^{\mathrm{I}}_n(\eta)\stackrel{\text{def}}{=}L_n^{(g-1/2)}(-\eta),\qquad \xi^{\mathrm{II}}_n(\eta)\stackrel{\text{def}}{=}L_n^{(1/2-g)}(\eta),\\
&\mathrm{J}:\ \xi^{\mathrm{I}}_n(\eta)\stackrel{\text{def}}{=}P_n^{(g-1/2,1/2-h)}(\eta),\ \ \xi^{\mathrm{II}}_n(\eta)\stackrel{\text{def}}{=}P_n^{(1/2-g,h-1/2)}(\eta).
\end{aligned}
$$

Let us prepare two sets of distinct positive integers which specify the degrees of type I and II virtual state solutions:

$$
\mathcal{D}=\mathcal{D}^{\mathrm{I}}\cup\mathcal{D}^{\mathrm{II}},\qquad \mathcal{D}^{\mathrm{I}}=\{d^{\mathrm{I}}_1,d^{\mathrm{I}}_2,\ldots,d^{\mathrm{I}}_M\},\quad \mathcal{D}^{\mathrm{II}}=\{d^{\mathrm{II}}_1,d^{\mathrm{II}}_2,\ldots,d^{\mathrm{II}}_N\}. \tag{2.56}
$$

The multiple Darboux transformations using these seed solutions produce a deformed system:

$$
\mathcal{H}_{\mathcal{D}}\stackrel{\text{def}}{=}\mathcal{H}-2\partial_x^2\Big(\log\big|\mathrm{W}\,[\varphi^{\mathrm{I}}_{d_1},\ldots,\varphi^{\mathrm{I}}_{d_M},\varphi^{\mathrm{II}}_{d_1},\ldots,\varphi^{\mathrm{II}}_{d_N}](x)\big|\Big), \tag{2.57}
$$

$$
\mathcal{H}_{\mathcal{D}}\phi_{\mathcal{D},n}(x;\boldsymbol{\lambda})=\mathcal{E}(n)\phi_{\mathcal{D},n}(x;\boldsymbol{\lambda})\quad(n\in\mathbb{Z}_{\geq 0}\backslash\mathcal{D}), \tag{2.58}
$$

$$
\phi_{\mathcal{D},n}(x;\boldsymbol{\lambda})\stackrel{\text{def}}{=}\frac{\mathrm{W}\,[\varphi^{\mathrm{I}}_{d_1},\ldots,\varphi^{\mathrm{I}}_{d_M},\varphi^{\mathrm{II}}_{d_1},\ldots,\varphi^{\mathrm{II}}_{d_N},\phi_n](x)}{\mathrm{W}\,[\varphi^{\mathrm{I}}_{d_1},\ldots,\varphi^{\mathrm{I}}_{d_M},\varphi^{\mathrm{II}}_{d_1},\ldots,\varphi^{\mathrm{II}}_{d_N}](x)}, \tag{2.59}
$$

in which $\boldsymbol{\lambda}$ specify the coupling(s) dependence, $\boldsymbol{\lambda}=g$ for L and $\boldsymbol{\lambda}=\{g,h\}$ for J. The nodeless property of each seed solution $\varphi^{\mathrm{I,II}}_{d_j}$ conspires to achieve the nodelessness of the denominator function of $\phi_{\mathcal{D},n}(x;\boldsymbol{\lambda})$. Similar to the corresponding expressions of the Krein-Adler polynomials (2.48), we obtain the norms of the deformed eigenfunctions $\phi_{\mathcal{D},n}(x)$:

$$
(\phi_{\mathcal{D},n},\phi_{\mathcal{D},m})=\prod_{j=1}^{M}\big(\mathcal{E}(n)-\tilde{\mathcal{E}}^{\mathrm{I}}_{d_j}\big)\prod_{j=1}^{N}\big(\mathcal{E}(n)-\tilde{\mathcal{E}}^{\mathrm{II}}_{d_j}\big)\cdot(\phi_n,\phi_m)\quad(n,m\in\mathbb{Z}_{\geq 0}). \tag{2.60}
$$

This clearly shows the necessity of the *negative* virtual state energies $\{\tilde{\mathcal{E}}^{\mathrm{I,II}}_{d_j}<0\}$.

The multi-indexed Laguerre/Jacobi polynomials are extracted by factorising the deformed eigenfunction $\phi_{\mathcal{D},n}(x;\boldsymbol{\lambda})$ into the ground state eigenfunction and the polynomial part by using the Wronskian formulas (2.51), (2.52):

$$
\phi_{\mathcal{D},n}(x;\boldsymbol{\lambda})=c_{\mathcal{F}}^{M+N}\psi_{\mathcal{D}}(x;\boldsymbol{\lambda})P_{\mathcal{D},n}(\eta(x);\boldsymbol{\lambda}),\quad \psi_{\mathcal{D}}(x;\boldsymbol{\lambda})\stackrel{\text{def}}{=}\frac{\phi_0(x;\boldsymbol{\lambda}^{[M,N]})}{\Xi_{\mathcal{D}}(\eta(x);\boldsymbol{\lambda})}, \tag{2.61}
$$

in which $c_{\mathcal{F}}=2$ for L and $c_{\mathcal{F}}=-4$ for J. The coupling $\boldsymbol{\lambda}$ is shifted to $\boldsymbol{\lambda}^{[M,N]}$:

$$
\boldsymbol{\lambda}^{[M,N]}=g+M-N\ \text{ for L},\quad \boldsymbol{\lambda}^{[M,N]}=\{g+M-N,h-M+N\}\ \text{ for J}. \tag{2.62}
$$

The general formulas for the multi-indexed polynomial $P_{\mathcal{D},n}(\eta(x);\boldsymbol{\lambda})$ and the denominator polynomial $\Xi_{\mathcal{D}}(\eta(x);\boldsymbol{\lambda})$ are:

$$P_{\mathcal{D},n}(\eta;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \mathrm{W}[\mu_1,\ldots,\mu_M,\nu_1,\ldots,\nu_N,P_n](\eta) \times \begin{cases} e^{-M\eta}\,\eta^{(M+g+\frac{1}{2})N} & :\mathrm{L} \\ \big(\frac{1-\eta}{2}\big)^{(M+g+\frac{1}{2})N}\big(\frac{1+\eta}{2}\big)^{(N+h+\frac{1}{2})M} & :\mathrm{J} \end{cases}, \tag{2.63}$$

$$\Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \mathrm{W}[\mu_1,\ldots,\mu_M,\nu_1,\ldots,\nu_N](\eta) \times \begin{cases} e^{-M\eta}\,\eta^{(M+g-\frac{1}{2})N} & :\mathrm{L} \\ \big(\frac{1-\eta}{2}\big)^{(M+g-\frac{1}{2})N}\big(\frac{1+\eta}{2}\big)^{(N+h-\frac{1}{2})M} & :\mathrm{J} \end{cases}, \tag{2.64}$$

$$\mu_j \stackrel{\text{def}}{=} \begin{cases} e^{\eta}\xi^{\mathrm{I}}_{d_j}(\eta) & :\mathrm{L} \\ \big(\frac{1+\eta}{2}\big)^{\frac{1}{2}-h}\xi^{\mathrm{I}}_{d_j}(\eta) & :\mathrm{J} \end{cases}, \quad \nu_j \stackrel{\text{def}}{=} \begin{cases} \eta^{\frac{1}{2}-g}\xi^{\mathrm{II}}_{d_j}(\eta) & :\mathrm{L} \\ \big(\frac{1-\eta}{2}\big)^{\frac{1}{2}-g}\xi^{\mathrm{II}}_{d_j}(\eta) & :\mathrm{J} \end{cases}, \tag{2.65}$$

in which P_n in (2.63) denotes the original polynomial for L/J. The multi-indexed polynomial $P_{\mathcal{D},n}$ is of degree $\ell_{\mathcal{D}}+n$ and the denominator polynomial $\Xi_{\mathcal{D}}$ is of degree $\ell_{\mathcal{D}}$ in η, in which $\ell_{\mathcal{D}}$ is given by

$$\ell_{\mathcal{D}} \stackrel{\text{def}}{=} \sum_{j=1}^{M} d^{\mathrm{I}}_j + \sum_{j=1}^{N} d^{\mathrm{II}}_j - \frac{1}{2}M(M-1) - \frac{1}{2}N(N-1) + MN \geq 1. \tag{2.66}$$

Here the label n specifies the energy eigenvalue $\mathcal{E}(n)$ of $\phi_{\mathcal{D},n}$ and it also counts the nodes due to the oscillation theorem. Since the degrees $0,1,\ldots,\ell_{\mathcal{D}}-1$ are missing, the multi-indexed polynomials $\{P_{\mathcal{D},n}\}$ do not satisfy three term recurrence relations but they form a complete set in L^2 with the orthogonality relations:

$$\begin{aligned}&\int d\eta\,\frac{\mathrm{W}(\eta;\boldsymbol{\lambda}^{[M,N]})}{\Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda})^2}P_{\mathcal{D},n}(\eta;\boldsymbol{\lambda})P_{\mathcal{D},m}(\eta;\boldsymbol{\lambda})\\ &= h_n\delta_{nm}\times\begin{cases} \prod_{j=1}^{M}(n+g+d^{\mathrm{I}}_j+\frac{1}{2})\cdot\prod_{j=1}^{N}(n+g-d^{\mathrm{II}}_j-\frac{1}{2}) & :\mathrm{L} \\ 4^{-M-N}\prod_{j=1}^{M}(n+g+d^{\mathrm{I}}_j+\frac{1}{2})(n+h-d^{\mathrm{I}}_j-\frac{1}{2}) & \\ \qquad\times\prod_{j=1}^{N}(n+g-d^{\mathrm{II}}_j-\frac{1}{2})(n+h+d^{\mathrm{II}}_j+\frac{1}{2}) & :\mathrm{J} \end{cases}.\end{aligned} \tag{2.67}$$

The weight function of the original polynomials $\mathrm{W}(\eta;\boldsymbol{\lambda})d\eta = \phi_0(x;\boldsymbol{\lambda})^2dx$ reads explicitly, see (2.11) and (2.24):

$$\mathrm{W}(\eta;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \begin{cases} \frac{1}{2}e^{-\eta}\eta^{g-\frac{1}{2}} & :\mathrm{L} \\ \frac{1}{2^{g+h+1}}(1-\eta)^{g-\frac{1}{2}}(1+\eta)^{h-\frac{1}{2}} & :\mathrm{J} \end{cases}. \tag{2.68}$$

The very form of the deformed eigenfunctions (2.61) suggests that the system can be regarded as *orthogonal rational functions system* $\{P_{\mathcal{D},n}(\eta)/\Xi_{\mathcal{D}}(\eta)\}$, $n\in\mathbb{Z}_{\geq 0}$ with the same orthogonality weight function as the L/J system but parameter(s) are shifted $\mathrm{W}(\eta,\boldsymbol{\lambda}^{[M,N]})$. It is important to note that the lowest degree polynomial $P_{\mathcal{D},0}(\eta;\boldsymbol{\lambda})$ is related to the denominator polynomial $\Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda})$ by the parameter shift $\boldsymbol{\lambda}\to\boldsymbol{\lambda}+\boldsymbol{\delta}$ ($\boldsymbol{\delta}=1$ (L), $\boldsymbol{\delta}=\{1,1\}$ (J), *i.e.* $g\to g+1$ for L and $\{g,h\}\to\{g+1,h+1\}$ for J):

$$P_{\mathcal{D},0}(\eta;\boldsymbol{\lambda}) \propto \Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda}+\boldsymbol{\delta}). \tag{2.69}$$

The above formulas (2.63) and (2.64) are drastically simplified when type I (II) seed solutions only are used.

By similarity transforming the deformed Hamiltonian $\mathcal{H}_{\mathcal{D}}$ in terms of the ground state eigenfunction $\psi_{\mathcal{D}}(x;\boldsymbol{\lambda})$, we obtain the second order differential operator $\widetilde{\mathcal{H}}_{\mathcal{D}}$ governing the multi-indexed polynomials:

$$\begin{aligned}\widetilde{\mathcal{H}}_{\mathcal{D}} &\stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x;\boldsymbol{\lambda})^{-1}\circ\mathcal{H}_{\mathcal{D}}\circ\psi_{\mathcal{D}}(x;\boldsymbol{\lambda})\\ &= -4\biggl(c_2(\eta)\frac{d^2}{d\eta^2}+\Bigl(c_1(\eta,\boldsymbol{\lambda}^{[M,N]})-2c_2(\eta)\frac{\partial_\eta\Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda})}{\Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda})}\Bigr)\frac{d}{d\eta}\\ &\qquad\quad +c_2(\eta)\frac{\partial_\eta^2\Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda})}{\Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda})}-c_1(\eta,\boldsymbol{\lambda}^{[M,N]}-\boldsymbol{\delta})\frac{\partial_\eta\Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda})}{\Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda})}\biggr), \qquad (2.70)\\ \widetilde{\mathcal{H}}_{\mathcal{D}}P_{\mathcal{D},n}(\eta;\boldsymbol{\lambda}) &= \mathcal{E}(n)P_{\mathcal{D},n}(\eta;\boldsymbol{\lambda}), \qquad (2.71)\end{aligned}$$

in which

$$c_1(\eta,\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \begin{cases} g+\frac{1}{2}-\eta & : \mathrm{L} \\ h-g-(g+h+1)\eta & : \mathrm{J}\end{cases}, \quad c_2(\eta) \stackrel{\text{def}}{=} \begin{cases} \eta & : \mathrm{L} \\ 1-\eta^2 & : \mathrm{J}\end{cases}. \qquad (2.72)$$

The above differential equation (2.71) is Fuchsian for the J case, since the $\ell_{\mathcal{D}}$ zeros of $\Xi_{\mathcal{D}}(\eta;\boldsymbol{\lambda})$ are all simple with the same characteristic exponents, 0 and 3. The L case is obtained as a confluent limit.

The first examples of multi-indexed polynomials were the simplest ones with $\mathcal{D}=\{1\}$ for L and J by Gomez-Ullate et al. [23] and Quesne [24] and they were called exceptional orthogonal polynomials. In this case type I seed solutions define the same polynomials as those of type II seed solutions by a shift of parameters. The general $\mathcal{D}=\{\ell\}$, $\forall\ell\geq 1$ cases for type I and II were derived in [26], [33]. The present derivation of $P_{\mathcal{D},n}(\eta;\boldsymbol{\lambda})$ is due to [27].

2.4.1 Explicit examples of multi-indexed Laguerre polynomials

We present two explicit examples of multi-indexed Laguerre polynomials specified by (i) $\mathcal{D}=\{\ell^{\mathrm{I}}\}$, (ii) $\mathcal{D}=\{\ell^{\mathrm{II}}\}$.

(i) $\mathcal{D}=\{\ell^{\mathbf{I}}\}$ In this case $\xi_\ell^{\mathrm{I}}(\eta)=L_\ell^{(g-1/2)}(-\eta)$, $\eta=x^2$ and the potential and the eigenfunctions of the deformed QM system are:

$$\begin{aligned}&V_\ell^{\mathrm{I}}(x)=x^2+\frac{g(g+1)}{x^2}-(3+2g)-2\partial_x^2\log|\xi_\ell^{\mathrm{I}}(\eta)|,\\ &\phi_{\ell,n}^{\mathrm{I}}(x)=2\psi_\ell^{\mathrm{I}}(x)P_{\ell,n}^{\mathrm{I}}(\eta),\quad \psi_\ell^{\mathrm{I}}(x)=\frac{e^{-x^2/2}x^{g+1}}{\xi_\ell^{\mathrm{I}}(\eta)},\\ &P_{\ell,n}^{\mathrm{I}}(\eta)=-\left(\partial_\eta\xi_\ell^{\mathrm{I}}(\eta)+\xi_\ell^{\mathrm{I}}(\eta)\right)L_n^{(g-1/2)}(\eta)+\xi_\ell^{\mathrm{I}}(\eta)\partial_\eta L_n^{(g-1/2)}(\eta).\end{aligned}$$

The second order differential operator $\widetilde{\mathcal{H}}_\ell^{\mathrm{I}}$ governing $P_{\ell,n}^{\mathrm{I}}(\eta)$ is

$$\widetilde{\mathcal{H}}_\ell^{\mathrm{I}} P_{\ell,n}^{\mathrm{I}}(\eta) = n P_{\ell,n}^{\mathrm{I}}(\eta),$$
$$\widetilde{\mathcal{H}}_\ell^{\mathrm{I}} = -\Bigg[\eta\frac{d^2}{d\eta^2} + \left(L_1^{(g+1/2)}(\eta) - 2\eta\frac{\partial_\eta \xi_\ell^{\mathrm{I}}(\eta)}{\xi_\ell^{\mathrm{I}}(\eta)}\right)\frac{d}{d\eta} + \eta\frac{\partial_\eta^2 \xi_\ell^{\mathrm{I}}(\eta)}{\xi_\ell^{\mathrm{I}}(\eta)} - L_1^{(g-1/2)}(\eta)\frac{\partial_\eta \xi_\ell^{\mathrm{I}}(\eta)}{\xi_\ell^{\mathrm{I}}(\eta)}\Bigg].$$

(ii) $\mathcal{D} = \{\ell^{\mathbf{II}}\}$ In this case $\xi_\ell^{\mathrm{II}}(\eta) = L_\ell^{(1/2-g)}(\eta)$, $\eta = x^2$ and the potential and the eigenfunctions of the deformed QM system are:

$$V_\ell^{\mathrm{I}}(x) = x^2 + \frac{(g-1)(g-2)}{x^2} + (1-2g) - 2\partial_x^2 \log|\xi_\ell^{\mathrm{II}}(\eta)|,$$
$$\phi_{\ell,n}^{\mathrm{II}}(x) = 2\psi_\ell^{\mathrm{II}}(x) P_{\ell,n}^{\mathrm{II}}(\eta), \quad \psi_\ell^{\mathrm{II}}(x) = \frac{e^{-x^2/2}x^{g-1}}{\xi_\ell^{\mathrm{II}}(\eta)},$$
$$P_{\ell,n}^{\mathrm{II}}(\eta) = \left(-\eta\partial_\eta \xi_\ell^{\mathrm{II}}(\eta) + (g-1/2)\xi_\ell^{\mathrm{II}}(\eta)\right) L_n^{(g-1/2)}(\eta) + \eta\xi_\ell^{\mathrm{II}}(\eta)\partial_\eta L_n^{(g-1/2)}(\eta).$$

The second order differential operator $\widetilde{\mathcal{H}}_\ell^{\mathrm{II}}$ governing $P_{\ell,n}^{\mathrm{II}}(\eta)$ is

$$\widetilde{\mathcal{H}}_\ell^{\mathrm{II}} P_{\ell,n}^{\mathrm{II}}(\eta) = n P_{\ell,n}^{\mathrm{II}}(\eta),$$
$$\widetilde{\mathcal{H}}_\ell^{\mathrm{II}} = -\Bigg[\eta\frac{d^2}{d\eta^2} + \left(L_1^{(g-3/2)}(\eta) - 2\eta\frac{\partial_\eta \xi_\ell^{\mathrm{II}}(\eta)}{\xi_\ell^{\mathrm{II}}(\eta)}\right)\frac{d}{d\eta} + \eta\frac{\partial_\eta^2 \xi_\ell^{\mathrm{II}}(\eta)}{\xi_\ell^{\mathrm{II}}(\eta)} - L_1^{(g-5/2)}(\eta)\frac{\partial_\eta \xi_\ell^{\mathrm{II}}(\eta)}{\xi_\ell^{\mathrm{II}}(\eta)}\Bigg].$$

2.4.2 Explicit examples of multi-indexed Jacobi polynomials

We present two explicit examples of multi-indexed Jacobi polynomials,
(i) $\mathcal{D} = \{\ell^{\mathrm{I}}\}$, (ii) $\mathcal{D} = \{\ell^{\mathrm{II}}\}$. In this subsection we use the abbreviation $P_n(\eta) \equiv P_n^{(g-1/2,h-1/2)}(\eta)$.

(i) $\mathcal{D} = \{\ell^{\mathbf{I}}\}$ In this case $\xi_\ell^{\mathrm{I}}(\eta) = P_\ell^{(g-1/2,1/2-h)}(\eta)$, $\eta = \cos 2x$ and the potential and the eigenfunctions of the deformed QM system are:

$$V_\ell^{\mathrm{I}}(x) = \frac{g(g+1)}{\sin^2 x} + \frac{(h-1)(h-2)}{\cos^2 x} - 2\partial_x^2 \log|\xi_\ell^{\mathrm{I}}(\eta)| - (g+h)^2,$$
$$\phi_{\ell,n}^{\mathrm{I}}(x) = -4\psi_\ell^{\mathrm{I}}(x) P_{\ell,n}^{\mathrm{I}}(\eta), \quad \psi_\ell^{\mathrm{I}}(x) = \frac{(\sin x)^{g+1}(\cos x)^{h-1}}{\xi_\ell^{\mathrm{I}}(\eta)},$$
$$P_{\ell,n}^{\mathrm{I}}(\eta) = -\tfrac{1}{4}\big(2(1+\eta)\partial_\eta \xi_\ell^{\mathrm{I}}(\eta) + (1-2h)\xi_\ell^{\mathrm{I}}(\eta)\big)P_n(\eta) + \tfrac{1}{2}(1+\eta)\xi_\ell^{\mathrm{I}}(\eta)\partial_\eta P_n(\eta).$$

The second order differential operator $\widetilde{\mathcal{H}}_\ell^{\mathrm{I}}$ governing $P_{\ell,n}^{\mathrm{I}}(\eta)$ is

$$
\begin{aligned}
&\widetilde{\mathcal{H}}_\ell^{\mathrm{I}} P_{\ell,n}^{\mathrm{I}}(\eta) = n(n+g+h)P_{\ell,n}^{\mathrm{I}}(\eta),\\
&\widetilde{\mathcal{H}}_\ell^{\mathrm{I}} = -\Bigg[(1-\eta^2)\frac{d^2}{d\eta^2} + \left(h-g-2-(g+h+1)\eta - 2(1-\eta^2)\frac{\partial_\eta \xi_\ell^{\mathrm{I}}(\eta)}{\xi_\ell^{\mathrm{I}}(\eta)}\right)\frac{d}{d\eta}\\
&\qquad\qquad + (1-\eta^2)\frac{\partial_\eta^2 \xi_\ell^{\mathrm{I}}(\eta)}{\xi_\ell^{\mathrm{I}}(\eta)} - (h-g-2-(g+h-1)\eta)\frac{\partial_\eta \xi_\ell^{\mathrm{I}}(\eta)}{\xi_\ell^{\mathrm{I}}(\eta)}\Bigg].
\end{aligned}
$$

(ii) $\mathcal{D} = \{\ell^{\mathbf{II}}\}$ In this case $\xi_\ell^{\mathrm{II}}(\eta) = P_\ell^{(1/2-g,h-1/2)}(\eta)$, $\eta = \cos 2x$ and the potential and the eigenfunctions of the deformed QM system are

$$
\begin{aligned}
&V_\ell^{\mathrm{II}}(x) = \frac{(g-1)(g-2)}{\sin^2 x} + \frac{h(h+1)}{\cos^2 x} - 2\partial_x^2 \log|\xi_\ell^{\mathrm{II}}(\eta)| - (g+h)^2,\\
&\phi_{\ell,n}^{\mathrm{II}}(x) = -4\psi_\ell^{\mathrm{II}}(x)P_{\ell,n}^{\mathrm{II}}(\eta), \quad \psi_\ell^{\mathrm{II}}(x) = \frac{(\sin x)^{g-1}(\cos x)^{h+1}}{\xi_\ell^{\mathrm{II}}(\eta)},\\
&P_{\ell,n}^{\mathrm{II}}(\eta) = -\tfrac{1}{4}\left(2(1-\eta)\partial_\eta \xi_\ell^{\mathrm{II}}(\eta) + (2g-1)\xi_\ell^{\mathrm{II}}(\eta)\right)P_n(\eta) + \tfrac{1}{2}(1-\eta)\xi_\ell^{\mathrm{II}}(\eta)\partial_\eta P_n(\eta).
\end{aligned}
$$

The second order differential operator $\widetilde{\mathcal{H}}_\ell^{\mathrm{II}}$ governing $P_{\ell,n}^{\mathrm{II}}(\eta)$ is

$$
\begin{aligned}
&\widetilde{\mathcal{H}}_\ell^{\mathrm{II}} P_{\ell,n}^{\mathrm{II}}(\eta) = n(n+g+h)P_{\ell,n}^{\mathrm{II}}(\eta),\\
&\widetilde{\mathcal{H}}_\ell^{\mathrm{I}} = -\Bigg[(1-\eta^2)\frac{d^2}{d\eta^2} + \left(h-g+2-(g+h+1)\eta - 2(1-\eta^2)\frac{\partial_\eta \xi_\ell^{\mathrm{II}}(\eta)}{\xi_\ell^{\mathrm{II}}(\eta)}\right)\frac{d}{d\eta}\\
&\qquad\qquad + (1-\eta^2)\frac{\partial_\eta^2 \xi_\ell^{\mathrm{II}}(\eta)}{\xi_\ell^{\mathrm{II}}(\eta)} - (h-g+2-(g+h-1)\eta)\frac{\partial_\eta \xi_\ell^{\mathrm{II}}(\eta)}{\xi_\ell^{\mathrm{II}}(\eta)}\Bigg].
\end{aligned}
$$

3 Overview of the simplest quantum mechanics

Let us introduce 'Simplest Quantum Mechanics' by following the similarity and parallelism between the eigenvalue problems in Quantum Mechanics (QM) and those of hermitian matrices;

$$
\text{QM:} \quad \mathcal{H}\psi(x) = \mathcal{E}\psi(x), \tag{3.1}
$$

$$
\mathcal{H}: \ \text{self-adjoint } \mathcal{H} = \mathcal{H}^\dagger \quad (f,g) \stackrel{\text{def}}{=} \int f^*(x)g(x)dx, \quad (f,\mathcal{H}g) = (\mathcal{H}f,g), \tag{3.2}
$$

$$
\text{Matrix:} \quad \mathcal{H}v = \lambda v, \quad \sum_j \mathcal{H}_{i,j}v_j = \lambda v_i, \tag{3.3}
$$

$$
\mathcal{H}: \ \text{hermitian} \quad \mathcal{H}_{i,j} = \mathcal{H}_{j,i}^*, \quad (u,v) \stackrel{\text{def}}{=} \sum_j u_j^* v_j, \quad (f,\mathcal{H}g) = (\mathcal{H}f,g). \tag{3.4}
$$

Their eigenvalues are real and eigenfunctions (vectors) belonging to distinct eigenvalues are orthogonal:

$$
\lambda \in \mathbb{R}, \quad \mathcal{H}\psi_1(x) = \lambda_1\psi_1(x), \ \mathcal{H}\psi_2(x) = \lambda_2\psi_2(x), \ \lambda_1 \neq \lambda_2, (\psi_1,\psi_2) = 0. \tag{3.5}
$$

3.1 Problem Setting:1-d QM

QM is based upon a very special type of self-adjoint operators. For simplicity, let us focus on the simplest case of *one dimensional* QM. The Hamiltonian is a second order differential operator corresponding to Newtonian mechanics:

$$\mathcal{H} = -\frac{d^2}{dx^2} + V(x), \qquad V(x) \in \mathbb{R}.$$

Many *exactly solvable potentials* and their eigenvalues, eigenfunctions are known [1, 2]. The three well-known examples of exactly solvable QM discussed in the previous section define the *classical orthogonal polynomials*, the Hermite, Laguerre and Jacobi. For these polynomials the square of the groundstate eigenfunction $\phi_0^2(x)$, having no zero, provides the orthogonality weight function

$$(\phi_n, \phi_m) = (\!(P_n, P_m)\!) \stackrel{\text{def}}{=} \int \phi_0^2(x) P_n(\eta(x)) P_m(\eta(x)) dx = h_n \delta_{n\,m}, \quad h_n > 0. \tag{3.6}$$

At this point very naive and natural questions arise:

Q1: Is there a special class of hermitian matrices corresponding to the ordinary one-dimensional QM (2.2)?
Q2: Are there many *exactly solvable* ones whose eigenfunctions (vectors) define orthogonal polynomials?

The answer to both questions is **Yes**. For Q1, it is called *Jacobi matrices*, which are tri-diagonal and real symmetric matrices of finite or infinite dimensions. For Q2, they are *classical orthogonal polynomials of a discrete variable* [10] whose orthogonality measures consist of discrete point sets. They belong to the Askey scheme of hypergeometric orthogonal polynomials [3, 5]. In the rest of this note we will explore the Simplest Quantum Mechanics, which is also called discrete Quantum Mechanics with real shifts (rdQM).

3.2 Factorised Hamiltonian

In order to pursue the similarity with the one-dimensional QM, let us denote the indices of the matrices by $x, y = 0, 1, \ldots x_{\max}$ and the vector component by v_x or $v(x)$. The matrix eigenvalue equation (3.3) is rewritten as

$$\sum_{y=0}^{x_{\max}} \mathcal{H}_{x,y} v_y = \lambda v_x, \quad \text{or} \quad \mathcal{H} v(x) = \lambda v(x), \quad \sum_{y=0}^{x_{\max}} \mathcal{H}_{x,y} v(y) = \lambda v(x),$$

in which $x_{\max} = N$, a positive integer, for finite dimensional matrices and $x_{\max} = \infty$ for infinite matrices. For finite matrices, there are $N + 1$ eigenvalues. For infinite matrices we restrict to those matrices having discrete eigenvalues only and their spectrum is bounded from below. In other words, there is a lowest eigenvalue. Thus we denote the eigenvalue problem as

$$\mathcal{H}\phi_n(x) = \mathcal{E}(n)\phi_n(x), \quad \sum_{y=0} \mathcal{H}_{x,y}\phi_n(y) = \mathcal{E}(n)\phi_n(x), \quad n = 0, 1, 2, \ldots, \tag{3.7}$$

in which the eigenvalues are numbered in the increasing order. We can always make the lowest eigenvalue to be vanishing by subtracting $\mathcal{E}(0)\times$ Identity Matrix from the Hamiltonian $\mathcal{H}$:

$$0=\mathcal{E}(0)\leq\mathcal{E}(1)\leq\mathcal{E}(2)\leq\cdots.$$

Now the Hamiltonian, an hermitian matrix, is *positive semi-definite*. A linear algebra theorem tells that a positive semi-definite hermitian matrix can always be expressed in a *factorised form*:

$$\mathcal{H}=\mathcal{A}^\dagger\mathcal{A},\quad 0=\det(\mathcal{A})=\det(\mathcal{A}^\dagger)=\det(\mathcal{H}),\tag{3.8}$$

in which matrix $\mathcal{A}$ can be multiplied by any unitary matrix U, $\mathcal{A}\to\mathcal{A}'=U\mathcal{A}$.

This is also the case for the positive semi-definite ($\mathcal{E}(0)=0$) Hamiltonian $\mathcal{H}$ in the ordinary QM in one dimension (2.2) as discussed in (2.31).

We expect that the Hamiltonian $\mathcal{H}$ (3.8) is a *second order difference operator* consisting of a positive unit shift $\psi(x)\to\psi(x+1)$ and the negative unit shift $\psi(x)\to\psi(x-1)$ operators. For a continuous function $f(x)$, Taylor expansion reads

$$f(x+a)=\left(e^{a\partial_x}f\right)(x)=\sum_{n=0}^{\infty}\frac{a^n}{n!}\partial_x^nf(x).$$

This suggests the following simplified notation for the unit shift operators

$$e^{\pm\partial}\equiv e^{\pm\partial_x};\quad \left(e^{\pm\partial}f\right)(x)=f(x\pm1),\quad (e^{\partial})^\dagger=e^{-\partial},\tag{3.9}$$

which will be *abused* for the present case of discrete variables $x=0,1,2,\ldots$,

$$f(x\pm1)=\left(e^{\pm\partial}f\right)(x)=\sum_y(e^{\pm\partial})_{x,y}f(y)\ \Rightarrow (e^{\pm\partial})_{x,y}=\delta_{x\pm1,y}.$$

As a matrix the positive (negative) unit shift operator e^{∂} ($e^{-\partial}$) is a *super* (*sub*) *diagonal* matrix.

The factorisation operators $\mathcal{A}$, $\mathcal{A}^\dagger$ in the ordinary 1-d QM case are a function plus a first order differential operator. This suggests that $\mathcal{A}$, $\mathcal{A}^\dagger$ in matrix QM (3.8) be a function plus a first order difference operator $e^{\pm\partial}$, either positive e^{∂} or negative $e^{-\partial}$ shift operator, but not both. Otherwise, the Hamiltonian would be a fourth order difference operator containing $e^{\pm2\partial}$ as well as $e^{\pm\partial}$.

A simple guesswork would lead to the form

$$\mathcal{A}=\sqrt{B(x)}-e^{\partial}\sqrt{D(x)},\quad \mathcal{A}^\dagger=\sqrt{B(x)}-\sqrt{D(x)}\,e^{-\partial},\quad B(x),D(x)>0,\tag{3.10}$$

$$\mathcal{A}_{x,y}=\sqrt{B(x)}\,\delta_{x,y}-\sqrt{D(x+1)}\,\delta_{x+1,y},\quad (\mathcal{A}^\dagger)_{x,y}=\sqrt{B(x)}\,\delta_{x,y}-\sqrt{D(x)}\,\delta_{x-1,y},\tag{3.11}$$

with two positive potential functions $B(x)$ and $D(x)$. Obviously a 'function' $f(x)$ corresponds to a diagonal matrix:

$$f(x)\ \leftrightarrow\ \text{diag}\big(f(0),f(1),\ldots,f(x_{\max})\big),\tag{3.12}$$

which could be expressed by $f(x)\mathbf{1}$. However, here and hereafter we suppress the identity matrix $\mathbf{1}=(\delta_{x,y})$, $\sqrt{B(x)}\mathbf{1}\to\sqrt{B(x)}$. The resulting Hamiltonian is

$$\mathcal{H}=B(x)+D(x)-\sqrt{B(x)}\,e^{\partial}\sqrt{D(x)}-\sqrt{D(x)}\,e^{-\partial}\sqrt{B(x)}, \tag{3.13}$$

$$\mathcal{H}_{x,y}=\big(B(x)+D(x)\big)\delta_{x,y}-\sqrt{B(x)D(x+1)}\,\delta_{x+1,y}-\sqrt{B(x-1)D(x)}\,\delta_{x-1,y}. \tag{3.14}$$

In order that $(\mathcal{H}\psi)(x)$ does not contain undefined quantities $\psi(-1)$ or $\psi(N+1)$ for the finite case, the positive potential functions must vanish at the boundary

$$B(x),D(x)>0,\quad D(0)=0,\quad B(N)=0. \tag{3.15}$$

As seen clearly from the two types of equivalent expressions for the Hamiltonian $\mathcal{H}$ (3.13), (3.14) or $\mathcal{A}$, $\mathcal{A}^\dagger$ (3.10), (3.11), one can treat them either as matrices (3.14), (3.11) or as difference operators (3.13), (3.10) acting on functions. For actual calculations, however, the difference operators are much easier to handle than explicit matrix forms.

Thus the Hamiltonian $\mathcal{H}$ is a *tri-diagonal real symmetric* matrix:

$$\mathcal{H}=\begin{pmatrix} B(0) & -\sqrt{B(0)D(1)} & 0 & \cdots & \cdots & 0\\ -\sqrt{B(0)D(1)} & B(1)+D(1) & -\sqrt{B(1)D(2)} & 0 & \cdots & \vdots\\ 0 & -\sqrt{B(1)D(2)} & B(2)+D(2) & -\sqrt{B(2)D(3)} & \cdots & \vdots\\ \vdots & \cdots & \cdots & \cdots & \cdots & \vdots\\ \vdots & \cdots & \cdots & \cdots & \cdots & 0\\ 0 & \cdots & \cdots & -\sqrt{B(N-2)D(N-1)} & B(N-1)+D(N-1) & -\sqrt{B(N-1)D(N)}\\ 0 & \cdots & \cdots & 0 & -\sqrt{B(N-1)D(N)} & D(N) \end{pmatrix}.$$

This type of matrices are called *Jacobi* matrices. It is known that the first components of its eigenvectors are non-vanishing and that all the eigenvalues are *simple*:

$$\phi_n(0)\neq 0,\qquad 0=\mathcal{E}(0)<\mathcal{E}(1)<\mathcal{E}(2)<\cdots<\mathcal{E}(N)\ (<\cdots). \tag{3.16}$$

Exercise Verify these simple facts.
This guarantees the orthogonality of all eigenvectors. The factorisation matrices $\mathcal{A}$ and $\mathcal{A}^\dagger$ read explicitly

$$\mathcal{A}=\begin{pmatrix} \sqrt{B(0)} & -\sqrt{D(1)} & 0 & \cdots & \cdots & 0\\ 0 & \sqrt{B(1)} & -\sqrt{D(2)} & 0 & \cdots & \vdots\\ 0 & 0 & \sqrt{B(2)} & -\sqrt{D(3)} & \cdots & \vdots\\ \vdots & \cdots & \cdots & \cdots & \cdots & \vdots\\ \vdots & \cdots & \cdots & \cdots & \cdots & 0\\ 0 & \cdots & \cdots & 0 & \sqrt{B(N-1)} & -\sqrt{D(N)}\\ 0 & \cdots & \cdots & 0 & 0 & 0 \end{pmatrix}, \tag{3.17}$$

$$\mathcal{A}^\dagger=\begin{pmatrix}\sqrt{B(0)}&0&0&\cdots&\cdots&0\\ -\sqrt{D(1)}&\sqrt{B(1)}&0&0&\cdots&\vdots\\ 0&-\sqrt{D(2)}&\sqrt{B(2)}&0&\cdots&\vdots\\ \vdots&\cdots&\cdots&\cdots&\cdots&\vdots\\ \vdots&\cdots&\cdots&\cdots&\cdots&0\\ 0&\cdots&\cdots&-\sqrt{D(N-1)}&\sqrt{B(N-1)}&0\\ 0&\cdots&\cdots&0&-\sqrt{D(N)}&0\end{pmatrix}. \tag{3.18}$$

From these it is obvious $0=\det(\mathcal{A})=\det(\mathcal{A}^\dagger)=\det(\mathcal{H})$ for the finite case. For the infinite dimensional case, $\prod_{x=0}^\infty B(x)=0$ is needed.

The groundstate eigenfunction (vector) $\phi_0(x)$, $\mathcal{H}\phi_0(x)=0$, is easily obtained as the zero mode of the operator $\mathcal{A}$, $\mathcal{A}\phi_0(x)=0$, as in the ordinary QM (2.31):

$$\mathcal{A}\phi_0(x)=0\Rightarrow\sqrt{B(x)}\phi_0(x)-\sqrt{D(x+1)}\phi_0(x+1)=0, \tag{3.19}$$

$$\Rightarrow\phi_0(x)=\prod_{y=0}^{x-1}\sqrt{\frac{B(y)}{D(y+1)}},\quad x=1,2,\ldots, \tag{3.20}$$

with the boundary condition

$$\phi_0(0)=1. \tag{3.21}$$

As in the ordinary QM, the groundstate wavefunction has no zero.

We look for the solution of the matrix eigenvalue problem (3.7) by assuming the factorised form

$$\phi_n(x)=\phi_0(x)\check{P}_n(x), \tag{3.22}$$

as in the exactly solvable examples in ordinary QM (2.4),(2.9),(2.21),(2.50). In the simplest QM, one can interpret $\check{P}_n(x)$ either as a function or a vector with the x component $\check{P}_n(x)$. In the latter interpretation, $\phi_0(x)$ in (3.22) is understood as a diagonal matrix. The matrix eigenvalue problem $\mathcal{H}\phi_n(x)=\mathcal{E}(n)\phi_n(x)$ (3.7) is now rewritten as

$$\begin{aligned}(B(x)+D(x))\,\phi_0(x)\check{P}_n(x)-\sqrt{B(x)D(x+1)}\phi_0(x+1)\check{P}_n(x+1)&\\ -\sqrt{B(x-1)D(x)}\phi_0(x-1)\check{P}_n(x-1)=\mathcal{E}(n)\phi_0(x)\check{P}_n(x).&\end{aligned}$$

By using the zero mode equation for $\phi_0(x)$ (3.19) and dividing by $\phi_0(x)$, we arrive at a simple difference equation for $\check{P}_n(x)$:

$$B(x)\left(\check{P}_n(x)-\check{P}_n(x+1)\right)+D(x)\left(\check{P}_n(x)-\check{P}_n(x-1)\right)=\mathcal{E}(n)\check{P}_n(x), \tag{3.23}$$

$$\Rightarrow\widetilde{\mathcal{H}}\check{P}_n(x)=\mathcal{E}(n)\check{P}_n(x),\qquad\widetilde{\mathcal{H}}1=0, \tag{3.24}$$

$$\widetilde{\mathcal{H}}\stackrel{\text{def}}{=}\phi_0(x)^{-1}\cdot\mathcal{H}\cdot\phi_0(x)=B(x)(\mathbf{1}-e^{\partial})+D(x)(\mathbf{1}-e^{-\partial}). \tag{3.25}$$

This result justifies the rather oddly looking $\sqrt{B(x)}$ and $\sqrt{D(x)}$ in the definitions of $\mathcal{A}$ and $\mathcal{A}^\dagger$ (3.10). For the matrix interpretation of $\widetilde{\mathcal{H}}$ (3.25), $\phi_0(x)$ is a diagonal matrix,

$\phi_0(x) = \text{diag}\{\phi_0(0), \phi_0(1), \cdots, \phi_0(N)\}$, instead of a groundstate eigenvector. For the difference operator interpretation of $\widetilde{\mathcal{H}}$ (3.25), $\phi_0(x)$ is a function and it would be suitable to rewrite (3.25)

$$\widetilde{\mathcal{H}} \stackrel{\text{def}}{=} \phi_0(x)^{-1} \circ \mathcal{H} \circ \phi_0(x), \tag{3.26}$$

as in the ordinary QM (2.33).

A simple sufficient condition for the solvability of the similarity transformed Hamiltonian $\widetilde{\mathcal{H}}$ is the *triangularity* with respect to a special basis

$$1,\ \eta(x),\ \eta(x)^2,\ \ldots, \eta(x)^n,\ \ldots, \tag{3.27}$$

spanned by a certain function $\eta(x)$ which is called *sinusoidal coordinate* [6]:

$$\widetilde{\mathcal{H}}\eta(x)^n = \mathcal{E}(n)\eta(x)^n + \text{lower degrees in } \eta(x). \tag{3.28}$$

This property is preserved under the affine transformation of $\eta(x)$, $\eta(x) \to a\eta(x) + b$ (a, b: constants). We choose the boundary condition

$$\eta(0) = 0. \tag{3.29}$$

The triangularity (3.28) implies that the eigenvectors can be obtained as polynomials in $\eta(x)$ ($\check{P}_n(x) \equiv P_n(\eta(x))$) by *finite linear algebra* up to normalisation:

$$\left.\begin{array}{l} \widetilde{\mathcal{H}}P_n(\eta(x)) = \mathcal{E}(n)P_n(\eta(x)), \\ \mathcal{H}\phi_n(x) = \mathcal{E}(n)\phi_n(x), \quad \phi_n(x) = \phi_0(x)P_n(\eta(x)), \end{array}\right. \quad n = 0, 1, 2, \ldots, (N)\ , \ldots. \tag{3.30}$$

We choose a simple *universal normalisation* of $P_n(\eta(x))$

$$P_n(0) = 1\ \Leftrightarrow \check{P}_n(0) = 1, \quad n = 0, 1, 2, \ldots, (N)\ , \ldots, \tag{3.31}$$

which also means

$$P_0 = 1. \tag{3.32}$$

The above normalisation is always possible due to the property of the eigenvectors of the Jacobi matrices $\phi_n(0) \neq 0$, (3.16). Here are five known forms of the sinusoidal coordinates in rdQM [6] ($0 < q < 1$):

$$\begin{array}{l} \text{(i) } \eta(x) = x, \qquad \text{(ii) } \eta(x) = \epsilon' x(x + d), \quad (\epsilon' = 1 \text{ for } d > -1,\ \epsilon' = -1 \text{ for } d < -N) \\ \text{(iii) } \eta(x) = 1 - q^x, \qquad \text{(iv) } \eta(x) = q^{-x} - 1, \\ \text{(v) } \eta(x) = \epsilon'(q^{-x} - 1)(1 - dq^x), \quad (\epsilon' = 1 \text{ for } d < q^{-1},\ \epsilon' = -1 \text{ for } d > q^{-N}). \end{array} \tag{3.33}$$

3.2.1 Explicit Examples

Here are some examples of simplest QM [6], which are called by the name of the eigenpolynomials [5]. One finite dimensional example is the Krawtchouk and two from infinite ones are the Meixner and the Charlier.

Krawtchouk The potential functions are

$$B(x)=p(N-x),\quad D(x)=(1-p)x,\quad 0<p<1,\quad \eta(x)=x. \tag{3.34}$$

The triangularity reads

$$\begin{aligned}\widetilde{\mathcal{H}}x^n&=p(N-x)\big(x^n-(x+1)^n\big)+(1-p)x\big(x^n-(x-1)^n\big)\\&=nx^n+\text{lower degrees},\quad \mathcal{E}(n)=n.\end{aligned}$$

The eigenpolynomials are (see (A.3))

$$\begin{aligned}P_n(x;p,N)&={}_2F_1\Big(\begin{matrix}-n,\,-x\\-N\end{matrix}\;\Big|\;\frac{1}{p}\Big),\quad P_0=1,\;P_1=\frac{pN-x}{pN},\\P_2&=\frac{p^2N(N-1)+(2p(1-N)-1)x+x^2}{p^2N(N-1)},\ldots.\end{aligned}\tag{3.35}$$

The orthogonality weight function is the *binomial distribution*:

$$\phi_0^2(x)=\prod_{y=0}^{x-1}\frac{p}{1-p}\frac{N-y}{y+1}=\Big(\frac{p}{1-p}\Big)^x\frac{N!}{x!(N-x)!}=\Big(\frac{p}{1-p}\Big)^x\frac{N!}{\Gamma(x+1)\Gamma(N+1-x)}. \tag{3.36}$$

The trace formula is easy to verify:

$$\frac{N}{2}(N+1)=\sum_{n=0}^{N}\mathcal{E}(n)=\mathrm{Tr}(\mathcal{H})=\sum_{x=0}^{N}\left(B(x)+D(x)\right). \tag{3.37}$$

Meixner The potential functions are

$$B(x)=\frac{c}{1-c}(x+\beta),\quad D(x)=\frac{x}{1-c},\quad \beta>0,\quad 0<c<1,\quad \eta(x)=x. \tag{3.38}$$

The triangularity reads

$$\begin{aligned}(1-c)\widetilde{\mathcal{H}}x^n&=c(x+\beta)\big(x^n-(x+1)^n\big)+x\big(x^n-(x-1)^n\big)\\&=(1-c)nx^n+\text{lower degrees},\quad \mathcal{E}(n)=n.\end{aligned}$$

The eigenpolynomials are

$$\begin{aligned}P_n(x;\beta,c)&={}_2F_1\Big(\begin{matrix}-n,\,-x\\\beta\end{matrix}\;\Big|\;1-\frac{1}{c}\Big),\quad P_0=1,\;P_1=\frac{\beta c-(1-c)x}{\beta c},\\P_2&=\frac{\beta(\beta+1)c^2+(-1+c)(1+c+2\beta c)x+(-1+c)^2x^2}{\beta(\beta+1)c^2},\ldots.\end{aligned}\tag{3.39}$$

The orthogonality weight function is square summable:

$$\begin{aligned}\phi_0^2(x)&=\prod_{y=0}^{x-1}\frac{c(y+\beta)}{y+1}=\frac{(\beta)_xc^x}{x!}=\frac{\Gamma(\beta+x)\,c^x}{\Gamma(\beta)\Gamma(x+1)},\\\sum_{x=0}^{\infty}\phi_0^2(x)&=\sum_{x=0}^{\infty}\frac{(\beta)_xc^x}{x!}={}_1F_0\Big(\begin{matrix}\beta\\-\end{matrix}\;\Big|\;c\Big)=\frac{1}{(1-c)^\beta},\end{aligned}\tag{3.40}$$

in which $(a)_n$ is the shifted factorial (Pochhammer symbol) (A.1).

Charlier The potential functions are

$$B(x) = a, \quad D(x) = x, \quad 0 < a, \quad \eta(x) = x. \tag{3.41}$$

The triangularity is trivial

$$\begin{aligned}\widetilde{\mathcal{H}} x^n &= a\big(x^n - (x+1)^n\big) + x\big(x^n - (x-1)^n\big)\\ &= n x^n + \text{lower degrees}, \quad \mathcal{E}(n) = n.\end{aligned}$$

The eigenpolynomials are

$$\begin{aligned} P_n(x;a) &= {}_2F_0\Big(\begin{matrix}-n,\,-x\\ -\end{matrix}\,\Big|\,-\frac{1}{a}\Big), \quad P_0 = 1,\ P_1 = \frac{a-x}{a},\\ P_2 &= \frac{a^2 - (1+2a)x + x^2}{a^2}, \ldots . \end{aligned} \tag{3.42}$$

The orthogonality weight function is *Poisson distribution*, which is square summable:

$$\phi_0^2(x) = \prod_{y=0}^{x-1} \frac{a}{y+1} = \frac{a^x}{x!} = \frac{a^x}{\Gamma(x+1)}, \quad \sum_{x=0}^{\infty} \phi_0^2(x) = \sum_{x=0}^{\infty} \frac{a^x}{x!} = e^a. \tag{3.43}$$

In all these examples $\phi_0^2(x)$ is a *meromorphic function* of x and it vanishes on the integer points outside of the domain:

$$\phi_0^2(x) = 0, \quad x \in \mathbb{Z}\backslash\{0, 1, \ldots, N\}, \quad \text{or} \quad x \in \mathbb{Z}_{<0}. \tag{3.44}$$

3.2.2 Other Examples

Here are some other examples [5] without specifying the parameter ranges. The triangularity of the polynomial equations (3.28) is *purely algebraic* and independent of the parameter ranges. As shown in the examples, $B(x)$, $D(x)$ are rational functions of x or $q^{\pm x}$ and the polynomial solutions are well defined in the whole complex plane $x \in \mathbb{C}$. The parameter ranges are restricted by the positivity of the potential $B(x)$, $D(x)$, the sinusoidal coordinate $\eta(x)$ and the eigenvalues $\mathcal{E}(n)$. The positivity of the orthogonality weight function $\phi_0^2(x)$ is not guaranteed for the parameters outside of the ranges.

Finite dimensional examples are followed by infinite dimensional ones. Within each group, the most generic one is followed by simpler examples. The q-polynomials come after non q-polynomials. We use the naming of the orthogonal polynomials used in [5]. The parametrisation of some polynomials (Racah, (dual) Hahn and their q-versions) are different from the conventional ones. We advocate using the present parametrisations for their obvious symmetries. For the shifted q-factorials $(a;q)_n$, $(a_1, \ldots, a_r; q)_n$, etc., see Appendix A (A.2).

Finite dimensional examples. The most generic ones, the Racah and q-Racah are skipped here, as they are discussed in detail in section 8 in the corse of non-classical polynomials.

Hahn

$$\begin{aligned} B(x) &= (x+a)(N-x), \quad D(x) = x(b+N-x), \quad \eta(x) = x,\\ \mathcal{E}(n) &= n(n+a+b-1), \quad \phi_0^2(x) = \frac{N!}{x!\,(N-x)!}\,\frac{(a)_x\,(b)_{N-x}}{(b)_N}. \end{aligned} \tag{3.45}$$

dual Hahn

$$
\begin{aligned}
B(x)&=\frac{(x+a)(x+a+b-1)(N-x)}{(2x-1+a+b)(2x+a+b)},\quad D(x)=\frac{x(x+b-1)(x+a+b+N-1)}{(2x-2+a+b)(2x-1+a+b)},\\
&\eta(x)=x(x+a+b-1),\qquad \mathcal{E}(n)=n,\\
&\phi_0^2(x)=\frac{N!}{x!\,(N-x)!}\,\frac{(a)_x\,(2x+a+b-1)(a+b)_N}{(b)_x\,(x+a+b-1)_{N+1}}.
\end{aligned}
\tag{3.46}
$$

q-Hahn

$$
\begin{aligned}
B(x)&=(1-aq^x)(q^{x-N}-1),\quad D(x)=aq^{-1}(1-q^x)(q^{x-N}-b),\\
\eta(x)&=q^{-x}-1,\quad \mathcal{E}(n)=(q^{-n}-1)(1-abq^{n-1}),\\
\phi_0^2(x)&=\frac{(q\,;q)_N}{(q\,;q)_x\,(q\,;q)_{N-x}}\,\frac{(a;q)_x\,(b\,;q)_{N-x}}{(b\,;q)_N\,a^x}.
\end{aligned}
\tag{3.47}
$$

dual q-Hahn

$$
\begin{aligned}
B(x)&=\frac{(q^{x-N}-1)(1-aq^x)(1-abq^{x-1})}{(1-abq^{2x-1})(1-abq^{2x})},\\
D(x)&=aq^{x-N-1}\frac{(1-q^x)(1-abq^{x+N-1})(1-bq^{x-1})}{(1-abq^{2x-2})(1-abq^{2x-1})},\\
\eta(x)&=(q^{-x}-1)(1-abq^{x-1}),\quad \mathcal{E}(n)=q^{-n}-1,\\
\phi_0^2(x)&=\frac{(q\,;q)_N}{(q\,;q)_x\,(q\,;q)_{N-x}}\,\frac{(a,abq^{-1}\,;q)_x}{(abq^N,b\,;q)_x\,a^x}\,\frac{1-abq^{2x-1}}{1-abq^{-1}}.
\end{aligned}
\tag{3.48}
$$

quantum q-Krawtchouk

$$
\begin{aligned}
&B(x)=p^{-1}q^x(q^{x-N}-1),\quad D(x)=(1-q^x)(1-p^{-1}q^{x-N-1}),\\
&\eta(x)=q^{-x}-1,\quad \mathcal{E}(n)=1-q^n,\quad \phi_0^2(x)=\frac{(q\,;q)_N}{(q\,;q)_x(q\,;q)_{N-x}}\,\frac{p^{-x}q^{x(x-1-N)}}{(p^{-1}q^{-N}\,;q)_x}.
\end{aligned}
\tag{3.49}
$$

q-Krawtchouk

$$
\begin{aligned}
&B(x)=q^{x-N}-1,\quad D(x)=p(1-q^x),\quad \eta(x)=q^{-x}-1,\\
&\mathcal{E}(n)=(q^{-n}-1)(1+pq^n),\quad \phi_0^2(x)=\frac{(q\,;q)_N}{(q\,;q)_x(q\,;q)_{N-x}}\,p^{-x}q^{\frac12 x(x-1)-xN}.
\end{aligned}
\tag{3.50}
$$

dual q-Krawtchouk

$$
\begin{aligned}
B(x)&=\frac{(q^{x-N}-1)(1+pq^x)}{(1+pq^{2x})(1+pq^{2x+1})},\quad D(x)=pq^{2x-N-1}\frac{(1-q^x)(1+pq^{x+N})}{(1+pq^{2x-1})(1+pq^{2x})},\\
\eta(x)&=(q^{-x}-1)(1+pq^x),\quad \mathcal{E}(n)=q^{-n}-1,\\
\phi_0^2(x)&=\frac{(q\,;q)_N}{(q;q)_x(q;q)_{N-x}}\,\frac{(-p\,;q)_x}{(-pq^{N+1}\,;q)_x\,p^xq^{\frac12 x(x+1)}}\,\frac{1+pq^{2x}}{1+p}.
\end{aligned}
\tag{3.51}
$$

affine q-Krawtchouk

$$\begin{aligned} &B(x)=(q^{x-N}-1)(1-pq^{x+1}),\quad D(x)=pq^{x-N}(1-q^x),\\ &\qquad\eta(x)=q^{-x}-1,\quad \mathcal{E}(n)=q^{-n}-1,\quad \phi_0^2(x)=\frac{(q\,;q)_N}{(q\,;q)_x(q\,;q)_{N-x}}\frac{(pq\,;q)_x}{(pq)^x}. \end{aligned} \tag{3.52}$$

Infinite dimensional examples.

little q-Jacobi

$$\begin{aligned} &B(x)=a(q^{-x}-bq),\quad D(x)=q^{-x}-1,\quad \eta(x)=1-q^x,\\ &\qquad \mathcal{E}(n)=(q^{-n}-1)(1-abq^{n+1}),\quad \phi_0^2(x)=\frac{(bq\,;q)_x}{(q\,;q)_x}(aq)^x. \end{aligned} \tag{3.53}$$

little q-Laguerre This is obtained by setting $b=0$ of the little q-Jacobi (3.53).

$$B(x)=aq^{-x},\quad D(x)=q^{-x}-1,\quad \eta(x)=1-q^x,\quad \mathcal{E}(n)=q^{-n}-1,\quad \phi_0^2(x)=\frac{(aq)^x}{(q\,;q)_x}. \tag{3.54}$$

Al-Salam-Carlitz II

$$\begin{aligned} &B(x)=a(q^{-x}-bq),\quad D(x)=(q^{-x}-1)(1-aq^x),\quad \eta(x)=q^{-x}-1,\\ &\qquad \mathcal{E}(n)=1-q^n,\quad \phi_0^2(x)=\frac{a^xq^{x^2}}{(q,aq\,;q)_x}. \end{aligned} \tag{3.55}$$

alternative q-Charlier

$$\begin{aligned} &B(x)=a,\quad D(x)=q^{-x}-1,\quad \eta(x)=1-q^x,\\ &\qquad \mathcal{E}(n)=(q^{-n}-1)(1+aq^n),\quad \phi_0^2(x)=\frac{a^xq^{x(x+1)/2}}{(q\,;q)_x}. \end{aligned} \tag{3.56}$$

The absence of the q-Meixner and q-Charlier

$$\begin{aligned} &q\text{-Meixner;}\quad B(x)=cq^x(1-bq^{x+1}),\quad D(x)=(1-q^x)(1+bcq^x),\\ &\qquad\qquad \eta(x)=q^{-x}-1,\ \mathcal{E}(n)=1-q^n, \end{aligned} \tag{3.57}$$

$$q\text{-Charlier;}\quad B(x)=aq^x,\quad D(x)=1-q^x,\quad \eta(x)=q^{-x}-1,\quad \mathcal{E}(n)=1-q^n, \tag{3.58}$$

in the above list must be stressed, although their orthogonality weight functions in references do not contain Jackson integrals. This is because the set of eigenvectors of the difference Schrödinger equation (3.7) is not *complete* for these two polynomials [9].

3.2.3 Exercise

1. Verify the triangularity, $\mathcal{E}(n)$ and $\phi_0^2(x)$ for the other examples in §3.2.2.
2. Calculate the lower members of the eigenpolynomials P_1 and P_2 explicitly for some examples.
3. Verify the trace formula (3.37) for the finite dimensional examples.
4. Derive the meromorphic expressions of $\phi_0^2(x)$ and confirm that they vanish outside of the domain (3.44). For q-polynomials use the formula $(a\,;q)_n = (a\,;q)_\infty/(aq^n\,;q)_\infty$ (A.2).

4 Dual Polynomials

The orthogonality of the eigenvectors of the Jacobi matrix $\mathcal{H}$ (3.13), (3.14) implies

$$\sum_x \phi_0^2(x)P_n(\eta(x))P_m(\eta(x)) = \frac{1}{d_n^2}\,\delta_{n,m}, \tag{4.1}$$

in which we choose the normalisation constants $\{d_n > 0\}$ to be in the denominator. In terms of the normalised eigenvectors

$$\hat{\phi}_0(x) = d_0\phi_0(x), \quad \hat{\phi}_n(x) = d_n\phi_0(x)P_n(\eta(x)) = \hat{\phi}_0(x)\frac{d_n}{d_0}P_n(\eta(x)),$$

the orthonormality relation reads

$$\sum_x d_n\phi_0(x)P_n(\eta(x))\cdot d_m\phi_0(x)P_m(\eta(x)) = \delta_{n,m}.$$

For the complete set of eigenvectors this means

$$\sum_n d_n\phi_0(x)P_n(\eta(x))\cdot d_n\phi_0(y)P_n(\eta(y)) = \delta_{x,y},$$

which states the simplest duality that the row eigenvectors are also orthogonal. When written slightly differently

$$\sum_n d_n^2 P_n(\eta(x))P_n(\eta(y)) = \frac{1}{\phi_0^2(x)}\,\delta_{x,y}, \tag{4.2}$$

it displays the duality with (4.1) explicitly.

As $P_n(\eta)$ is an orthogonal polynomial, it satisfies three term recurrence relations (see Appendix B)

$$\eta P_n(\eta) = A_nP_{n+1}(\eta) + B_nP_n(\eta) + C_nP_{n-1}(\eta), \quad n = 0, 1, \ldots, \tag{4.3}$$

with real coefficients A_n, B_n and C_n ($C_0 = 0$). With the relation

$$B_n = -(A_n + C_n), \tag{4.4}$$

which is a consequence of the universal normalisation (boundary) condition $P_n(0)=1$ (3.31), the above three term recurrence relation takes the same form as the $\widetilde{\mathcal{H}}$ equation (3.23) *in the n-variable*:

$$
\begin{aligned}
&-A_n\big(P_n(\eta)-P_{n+1}(\eta)\big)-C_n\big(P_n(\eta)-P_{n-1}(\eta)\big)=\eta P_n(\eta),\\
&\big[-A_n(1-e^{\partial_n})-C_n(1-e^{-\partial_n})\big]\,P_n(\eta)=\eta P_n(\eta),
\end{aligned}
\tag{4.5}
$$

in which η is the eigenvalue.

The *dual* polynomial is an important concept in the theory of orthogonal polynomials of a discrete variable [3, 4, 5, 10, 11, 12]. They arise naturally as the solution of the original eigenvalue problem (3.7) or (3.23) obtained in a different way. Let us rewrite the similarity transformed eigenvalue problem $\widetilde{\mathcal{H}}\,\psi(x)=\mathcal{E}\,\psi(x)$ (3.24) into an explicit matrix form with the change of the notation $\psi(x)\to{}^t(Q_0,Q_1,\ldots,Q_x,\ldots)$

$$
\sum_y \widetilde{\mathcal{H}}_{x,y}Q_y=\mathcal{E}Q_x,\quad x,y=0,1,\ldots,(N),\ldots. \tag{4.6}
$$

Because of the tri-diagonality of $\widetilde{\mathcal{H}}$, it is in fact a three term recurrence relation for Q_x as a polynomial in $\mathcal{E}$:

$$
\begin{aligned}
\mathcal{E}Q_x(\mathcal{E})=B(x)\big(Q_x(\mathcal{E})-Q_{x+1}(\mathcal{E})\big)+D(x)\big(Q_x(\mathcal{E})-Q_{x-1}(\mathcal{E})\big),&\\
x=0,1,\ldots,(N),\ldots.&
\end{aligned}
\tag{4.7}
$$

Starting with the boundary (initial) condition

$$
Q_0=1, \tag{4.8}
$$

we determine $Q_x(\mathcal{E})$ as a degree x polynomial in $\mathcal{E}$. It is easy to see that $Q_x(\mathcal{E})$ also satisfies the universal normalisation condition (3.31),

$$
Q_x(0)=1,\quad x=0,1,\ldots,(N),\ldots. \tag{4.9}
$$

Replacing $\mathcal{E}$ by the actual value of the n-th eigenvalue $\mathcal{E}(n)$ (3.28) in $Q_x(\mathcal{E})$, we obtain the explicit form of the eigenfunction (vector)

$$
\sum_y \widetilde{\mathcal{H}}_{x,y}Q_y(\mathcal{E}(n))=\mathcal{E}(n)Q_x(\mathcal{E}(n)),\quad x=0,1,\ldots,(N),\ldots. \tag{4.10}
$$

In the finite dimensional case, $\{Q_0(\mathcal{E}),\ldots,Q_x(\mathcal{E}),\ldots,Q_N(\mathcal{E})\}$ as degree x polynomials in $\mathcal{E}$ are determined by (4.7) for $x=0,\ldots,N-1$. The last equation

$$
\mathcal{E}Q_N(\mathcal{E})=D(N)\big(Q_N(\mathcal{E})-Q_{N-1}(\mathcal{E})\big), \tag{4.11}
$$

is a degree $N+1$ algebraic equation (characteristic equation) of $\mathcal{E}$ for the determination of all the eigenvalues $\{\mathcal{E}(n)\}$.

Here are five known forms of the eigenvalues in rdQM, which are essentially of the same forms as the sinusoidal coordinates (3.33) ($0<q<1$):

$$\begin{aligned}&\text{(i)}: \ \mathcal{E}(n)=n, \qquad \text{(ii)}: \ \mathcal{E}(n)=\epsilon n(n+\alpha), \ (\epsilon=1 \text{ for } \ \alpha>-1, -1 \text{ for } \ \alpha<-N)\\ &\text{(iii)}: \ \mathcal{E}(n)=1-q^n, \qquad \text{(iv)}: \ \mathcal{E}(n)=q^{-n}-1,\\ &\text{(v)}: \ \mathcal{E}(n)=\epsilon(q^{-n}-1)(1-\alpha q^n), \quad (\epsilon=1 \text{ for } \ \alpha<q^{-1}, \ -1 \text{ for } \ \alpha>q^{-N}).\end{aligned} \tag{4.12}$$

Convince yourself that all the eigenvalues of the examples in §3.2.1, §3.2.2 are of these forms.

In subsequent sections we will provide further two independent algebraic methods of the determination of the eigenvalues $\{\mathcal{E}(n)\}$ based on the shape-invariance (in §6) and the exact Heisenberg operator solution in §7.

We now have two expressions (polynomials) for the eigenvectors of the problem (3.23) belonging to the eigenvalue $\mathcal{E}(n)$; $P_n(\eta(x))$ and $Q_x(\mathcal{E}(n))$. Due to the simplicity of the spectrum of the Jacobi matrix (3.16), they must be equal up to a multiplicative factor α_n,

$$P_n(\eta(x))=\alpha_n Q_x(\mathcal{E}(n)), \quad x=0,1,\ldots,(N),\ldots, \tag{4.13}$$

which turns out to be unity because of the boundary (initial) condition at $x=0$ (3.29), (3.31), (4.8) (or at $n=0$ (3.21), (3.32), (4.9));

$$P_n(\eta(0))=P_n(0)=1=Q_0(\mathcal{E}(n)), \qquad n=0,1,\ldots,(N),\ldots, \tag{4.14}$$

$$P_0(\eta(x))=1=Q_x(0)=Q_x(\mathcal{E}(0)), \quad x=0,1,\ldots,(N),\ldots. \tag{4.15}$$

We have established that the two polynomials, $\{P_n(\eta)\}$ and its *dual* polynomial $\{Q_x(\mathcal{E})\}$, coincide at the integer lattice points:

$$P_n(\eta(x))=Q_x(\mathcal{E}(n)), \quad n=0,1,\ldots,(N),\ldots, \quad x=0,1,\ldots,(N),\ldots. \tag{4.16}$$

The completeness relation (4.2)

$$\sum_n d_n^2 P_n(\eta(x))P_n(\eta(y))=\sum_n d_n^2 Q_x(\mathcal{E}(n))Q_y(\mathcal{E}(n))=\frac{1}{\phi_0^2(x)}\,\delta_{x,y}, \tag{4.17}$$

is now the orthogonality relation of the dual polynomial $Q_x(\mathcal{E}(n))$, and the previous normalisation constant d_n^2 is now the orthogonality weight function.

The real symmetric (hermitian) matrix $\mathcal{H}_{x,y}$ (3.14) can be expressed in terms of the complete set of the eigenvalues and the corresponding normalised eigenvectors (spectral representation)

$$\mathcal{H}_{x,y}=\sum_n \mathcal{E}(n)\hat{\phi}_n(x)\hat{\phi}_n(y), \tag{4.18}$$

$$\hat{\phi}_n(x)=d_n\phi_0(x)P_n(\eta(x))=d_n\phi_0(x)Q_x(\mathcal{E}(n)). \tag{4.19}$$

The very fact that it is tri-diagonal can be easily verified by using the difference equation for the polynomial $P_n(\eta(x))$ (3.23) or the three term recurrence relation for $Q_x(\mathcal{E}(n))$ (4.7).

Here is a list of the dual correspondence:

$$\begin{aligned}
&x \leftrightarrow n, \quad \eta(x) \leftrightarrow \mathcal{E}(n), \quad \eta(0)=0 \leftrightarrow \mathcal{E}(0)=0,\\
&B(x) \leftrightarrow -A_n, \quad D(x) \leftrightarrow -C_n, \quad \frac{\phi_0(x)}{\phi_0(0)} \leftrightarrow \frac{d_n}{d_0}.
\end{aligned} \tag{4.20}$$

In the last expression, we have inserted $\phi_0(0)=1$ (3.20) for symmetry. It should be remarked that $B(x)$ and $D(x)$ govern the difference equation for the polynomial $P_n(\eta)$, the solution of which requires the knowledge of the sinusoidal coordinate $\eta(x)$. The same quantities $B(x)$ and $D(x)$ specify the three term recurrence of the dual polynomial $Q_x(\mathcal{E})$ without the knowledge of the spectrum $\mathcal{E}(n)$. The explicit forms of $\eta(x)$ and $\mathcal{E}(n)$ are required for the polynomials $P_n(\eta)$ and $Q_x(\mathcal{E})$ to be the eigenvectors of the eigenvalue problem (3.7). Likewise, A_n and C_n in (4.3) specify the polynomial $P_n(\eta)$ without the knowledge of the sinusoidal coordinate. As for the dual polynomial $Q_x(\mathcal{E}(n))$, A_n and C_n provide the difference equation (in n) (4.5), the solution of which needs the explicit form of $\mathcal{E}(n)$. Let us stress that it is the eigenvalue problem (3.7) with the specific Hamiltonian (3.13) that determines the polynomial $P_n(\eta)$ and its dual $Q_x(\mathcal{E})$, the spectrum $\mathcal{E}(n)$, the sinusoidal coordinate $\eta(x)$ and the orthogonality measures $\phi_0^2(x)$ and d_n^2.

The three explicit examples in §3.2.1, the Krawtchouk (3.34), Meixner (3.38) and Charlier (3.41) are self-dual, as the explicit forms of the polynomials ${}_2F_1\Bigl(\begin{smallmatrix}-n,\,-x\\ -N\end{smallmatrix}\Bigm|\frac{1}{p}\Bigr)$ (3.35), ${}_2F_1\Bigl(\begin{smallmatrix}-n,\,-x\\ \beta\end{smallmatrix}\Bigm|1-\frac{1}{c}\Bigr)$ (3.39), and ${}_2F_0\Bigl(\begin{smallmatrix}-n,\,-x\\ -\end{smallmatrix}\Bigm|-\frac{1}{a}\Bigr)$ (3.42) are invariant under the exchange $x \leftrightarrow n$.

5 Fundamental Structure of Solution Space

Let us explore the structure of the solution space of the eigenvalue problem for the positive semi-definite Jacobi matrices:

$$\mathcal{H}\phi_n(x) = \mathcal{E}(n)\phi_n(x), \quad n=0,1,2,\ldots, \tag{5.1}$$

$$\mathcal{H} \equiv \mathcal{H}^{[0]} = \mathcal{A}^\dagger\mathcal{A}, \quad \mathcal{H}^{[0]}\phi_0(x)=0, \quad \mathcal{A}\phi_0(x)=0, \quad \mathcal{E}(0)=0. \tag{5.2}$$

By changing the order of $\mathcal{A}^\dagger$ and $\mathcal{A}$, a new hermitian matrix $\mathcal{H}^{[1]}$ is defined:

$$\mathcal{H}^{[1]} \stackrel{\text{def}}{=} \mathcal{A}\mathcal{A}^\dagger, \quad \mathcal{H}^{[0]} = \mathcal{A}^\dagger\mathcal{A}, \quad \phi_n^{[0]}(x) \equiv \phi_n(x), \quad n=0,1,\ldots,. \tag{5.3}$$

It is again a tri-diagonal symmetric matrix. If the original Hamiltonian $\mathcal{H}^{[0]}$ is an $(N+1)\times(N+1)$ matrix, the new one $\mathcal{H}^{[1]}$ is an $N\times N$ matrix, as seen clearly from the explicit forms of $\mathcal{A}$ (3.17) and $\mathcal{A}^\dagger$ (3.18). This is due to the boundary condition $B(N)=0$. The new one $\mathcal{H}^{[1]}$ is called the *partner* or the *associated* Hamiltonian.

These two Hamiltonians are connected by the following *intertwining relations*:

$$\mathcal{A}\mathcal{H}^{[0]} = \mathcal{A}\mathcal{A}^\dagger\mathcal{A} = \mathcal{H}^{[1]}\mathcal{A}, \qquad \mathcal{A}^\dagger\mathcal{H}^{[1]} = \mathcal{A}^\dagger\mathcal{A}\mathcal{A}^\dagger = \mathcal{H}^{[0]}\mathcal{A}^\dagger. \tag{5.4}$$

The *iso-spectrality* of the Hamiltonians $\mathcal{H}^{[0]}$ and $\mathcal{H}^{[1]}$ *except for the groundstate* $\phi_0^{[0]}(x)$,

$$\mathcal{H}^{[0]}\phi_n^{[0]}(x)=\mathcal{E}(n)\phi_n^{[0]}(x)\quad(n=0,1,\ldots),\quad \mathcal{A}\phi_0^{[0]}(x)=0, \tag{5.5}$$
$$\mathcal{H}^{[1]}\phi_n^{[1]}(x)=\mathcal{E}(n)\phi_n^{[1]}(x)\quad(n=1,2,\ldots), \tag{5.6}$$
$$\phi_n^{[1]}(x)\stackrel{\text{def}}{=}\mathcal{A}\phi_n^{[0]}(x),\quad \phi_n^{[0]}(x)=\frac{\mathcal{A}^\dagger}{\mathcal{E}(n)}\phi_n^{[1]}(x)\quad(n=1,2,\ldots), \tag{5.7}$$
$$(\phi_n^{[1]},\phi_m^{[1]})=\mathcal{E}(n)(\phi_n^{[0]},\phi_m^{[0]})\quad(n,m=1,2,\ldots). \tag{5.8}$$

is a simple consequence of the intertwining relations. The groundstate energy of the partner Hamiltonian $\mathcal{H}^{[1]}$ is $\mathcal{E}(1)$ as the original $\phi_0(x)$ is *deleted*, $\mathcal{A}\phi_0(x)=0$.

By subtracting the groundstate energy $\mathcal{E}(1)$ from the diagonal part of $\mathcal{H}^{[1]}$, another positive semi-definite Hamiltonian $\mathcal{H}^{[1]}-\mathcal{E}(1)$ is obtained, which is again factorised

$$\mathcal{H}^{[1]}={\mathcal{A}^{[1]}}^\dagger\mathcal{A}^{[1]}+\mathcal{E}(1),\quad B^{[1]}(x),D^{[1]}(x)>0,\quad D^{[1]}(0)=0,\quad B^{[1]}(N-1)=0, \tag{5.9}$$
$$\mathcal{A}^{[1]}=\sqrt{B^{[1]}(x)}-e^{\partial}\sqrt{D^{[1]}(x)},\quad {\mathcal{A}^{[1]}}^\dagger=\sqrt{B^{[1]}(x)}-\sqrt{D^{[1]}(x)}\,e^{-\partial},$$

in the same manner as the original Hamiltonian

$$\mathcal{A}^{[1]}\phi_1^{[1]}(x)=0. \tag{5.10}$$

By changing the order of ${\mathcal{A}^{[1]}}^\dagger$ and $\mathcal{A}^{[1]}$, a new tri-diagonal Hamiltonian $\mathcal{H}^{[2]}$ is defined:

$$\mathcal{H}^{[2]}\stackrel{\text{def}}{=}\mathcal{A}^{[1]}{\mathcal{A}^{[1]}}^\dagger+\mathcal{E}(1). \tag{5.11}$$

The two Hamiltonians $\mathcal{H}^{[1]}-\mathcal{E}(1)$ and $\mathcal{H}^{[2]}-\mathcal{E}(1)$ are intertwined by $\mathcal{A}^{[1]}$ and $\mathcal{A}^{[1]\dagger}$:

$$\mathcal{A}^{[1]}\big(\mathcal{H}^{[1]}-\mathcal{E}(1)\big)=\mathcal{A}^{[1]}\mathcal{A}^{[1]\dagger}\mathcal{A}^{[1]}=\big(\mathcal{H}^{[2]}-\mathcal{E}(1)\big)\mathcal{A}^{[1]},$$
$$\mathcal{A}^{[1]\dagger}\big(\mathcal{H}^{[2]}-\mathcal{E}(1)\big)=\mathcal{A}^{[1]\dagger}\mathcal{A}^{[1]}\mathcal{A}^{[1]\dagger}=\big(\mathcal{H}^{[1]}-\mathcal{E}(1)\big)\mathcal{A}^{[1]\dagger}.$$

The iso-spectrality of $\mathcal{H}^{[1]}$ and $\mathcal{H}^{[2]}$ and the relations of their eigenvectors are obtained as before:

$$\mathcal{H}^{[2]}\phi_n^{[2]}(x)=\mathcal{E}(n)\phi_n^{[2]}(x)\qquad(n=2,3,\ldots),$$
$$\phi_n^{[2]}(x)\stackrel{\text{def}}{=}\mathcal{A}^{[1]}\phi_n^{[1]}(x),\quad \phi_n^{[1]}(x)=\frac{\mathcal{A}^{[1]\dagger}}{\mathcal{E}(n)-\mathcal{E}(1)}\phi_n^{[2]}(x)\qquad(n=2,3,\ldots),$$
$$(\phi_n^{[2]},\phi_m^{[2]})=\big(\mathcal{E}(n)-\mathcal{E}(1)\big)(\phi_n^{[1]},\phi_m^{[1]})\qquad(n,m=2,3,\ldots),$$
$$\mathcal{H}^{[2]}=\mathcal{A}^{[2]\dagger}\mathcal{A}^{[2]}+\mathcal{E}(2),\quad \mathcal{A}^{[2]}\phi_2^{[2]}(x)=0.$$

By the transformation $\mathcal{H}^{[1]}\to\mathcal{H}^{[2]}$, the groundstate corresponding to $\mathcal{E}(1)$ is deleted, $\mathcal{A}^{[1]}\phi_1^{[1]}(x)=0$.

This process of deleting the lowest energy state goes successively:

$$\mathcal{H}^{[s]} \stackrel{\text{def}}{=} \mathcal{A}^{[s-1]}\mathcal{A}^{[s-1]\dagger} + \mathcal{E}(s-1) = \mathcal{A}^{[s]\dagger}\mathcal{A}^{[s]} + \mathcal{E}(s), \tag{5.12}$$

$$\mathcal{H}^{[s]}\phi_n^{[s]}(x) = \mathcal{E}(n)\phi_n^{[s]}(x) \ (n = s, s+1, \ldots), \ \mathcal{A}^{[s]}\phi_s^{[s]}(x) = 0, \tag{5.13}$$

$$\phi_n^{[s]}(x) \stackrel{\text{def}}{=} \mathcal{A}^{[s-1]}\phi_n^{[s-1]}(x), \quad \phi_n^{[s-1]}(x) = \frac{\mathcal{A}^{[s-1]\dagger}}{\mathcal{E}(n) - \mathcal{E}(s-1)}\phi_n^{[s]}(x) \quad (n = s, s+1, \ldots), \tag{5.14}$$

$$(\phi_n^{[s]}, \phi_m^{[s]}) = \big(\mathcal{E}(n) - \mathcal{E}(s-1)\big)(\phi_n^{[s-1]}, \phi_m^{[s-1]}) \quad (n, m = s, s+1, \ldots). \tag{5.15}$$

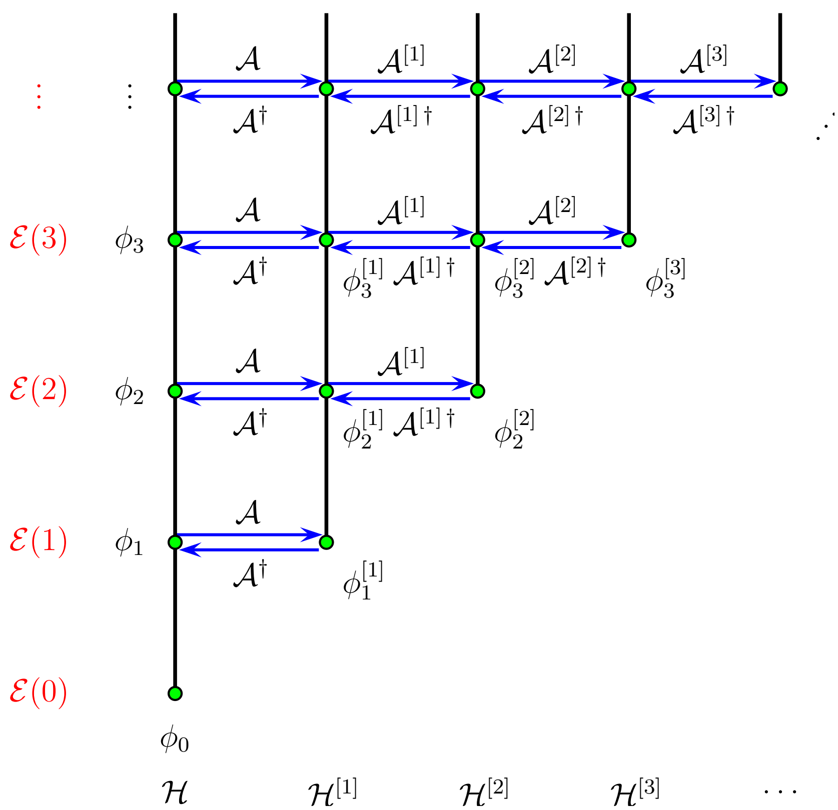

Figure 1: Fundamental structure of the solution space of 1-d QM.

Summarising these results we arrive at the following

Theorem 5.1 (Crum [18]) *For a given Hamiltonian system* $\{\mathcal{H}^{[0]}, \mathcal{E}(n), \phi_n^{[0]}(x)\}$ *there exist as many associated Hamiltonian systems* $\{\mathcal{H}^{[1]}, \mathcal{E}(n), \phi_n^{[1]}(x)\}$, $\{\mathcal{H}^{[2]}, \mathcal{E}(n), \phi_n^{[2]}(x)\}$, $\ldots$, *as the number of discrete eigenvalues. They share the eigenvalues* $\{\mathcal{E}(n)\}$ *of the original Hamiltonian and the eigenvectors of* $\mathcal{H}^{[j]}$ *and* $\mathcal{H}^{[j+1]}$ *are related by* $\mathcal{A}^{[j]}$ *and* $\mathcal{A}^{[j]\dagger}$.

It should be stressed that Crum's theorem is the consequence of the factorisation of positive semi-definite Hamiltonians. It holds equally well in ordinary 1-d QM and in simplest QM.

6 Shape Invariance: Sufficient Condition of Exact Solvability

The structure of the solution space gives a key to understand the solvability. That is *shape invariance*, which is a sufficient condition for exact solvability. In most cases Hamiltonians depend on several parameters, $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \ldots)$. Let us symbolically express the parameter dependence of various quantities as $\mathcal{H}(\boldsymbol{\lambda})$, $\mathcal{A}(\boldsymbol{\lambda})$, $\mathcal{E}(n;\boldsymbol{\lambda})$, $\phi_n(x;\boldsymbol{\lambda})$, $\eta(x;\boldsymbol{\lambda})$, $P_n(\eta(x;\boldsymbol{\lambda});\boldsymbol{\lambda})$ etc.

The system is exactly solvable if the matrix $\mathcal{A}^{[1]}$ of the partner Hamiltonian $\mathcal{H}^{[1]}$ has the same form as $\mathcal{A} \equiv \mathcal{A}^{[0]}$ with a certain parameter shift:

$$\mathcal{A}^{[1]}(\boldsymbol{\lambda}) \propto \mathcal{A}^{[0]}(\boldsymbol{\lambda} + \boldsymbol{\delta}),$$

in which $\boldsymbol{\delta}$ is the shift of the parameters. This can be rephrased as

$$\mathcal{A}(\boldsymbol{\lambda})\mathcal{A}(\boldsymbol{\lambda})^\dagger = \kappa\mathcal{A}(\boldsymbol{\lambda} + \boldsymbol{\delta})^\dagger\mathcal{A}(\boldsymbol{\lambda} + \boldsymbol{\delta}) + \mathcal{E}(1;\boldsymbol{\lambda}), \tag{6.1}$$

in which $\kappa > 0$ is a parameter corresponding to the overall scale change of the Hamiltonians. From Fig. 1, we find that the eigenvalues and the corresponding eigenvectors are expressed by the first excited energy $\mathcal{E}(1;\boldsymbol{\lambda})$, $\mathcal{A}(\boldsymbol{\lambda})$, $\mathcal{A}(\boldsymbol{\lambda})^\dagger$ and the groundstate vector $\phi_0(x;\boldsymbol{\lambda})$ at variously shifted values of $\boldsymbol{\lambda}$ [6]:

$$\mathcal{E}(n;\boldsymbol{\lambda}) = \sum_{s=0}^{n-1} \kappa^s \mathcal{E}(1;\boldsymbol{\lambda}^{[s]}), \qquad \boldsymbol{\lambda}^{[s]} \stackrel{\text{def}}{=} \boldsymbol{\lambda} + s\boldsymbol{\delta}, \tag{6.2}$$

$$\phi_n(x;\boldsymbol{\lambda}) \propto \mathcal{A}(\boldsymbol{\lambda}^{[0]})^\dagger\mathcal{A}(\boldsymbol{\lambda}^{[1]})^\dagger\mathcal{A}(\boldsymbol{\lambda}^{[2]})^\dagger \cdots \mathcal{A}(\boldsymbol{\lambda}^{[n-1]})^\dagger\phi_0(x;\boldsymbol{\lambda}^{[n]}). \tag{6.3}$$

As we will see shortly, the eigenvector formula (6.3) is the generalised *Rodrigues formula*. In terms of the potential functions the shape invariance condition (6.1) is rewritten as

$$B(x+1;\boldsymbol{\lambda})D(x+1;\boldsymbol{\lambda}) = \kappa^2\, B(x;\boldsymbol{\lambda}+\boldsymbol{\delta})D(x+1;\boldsymbol{\lambda}+\boldsymbol{\delta}), \tag{6.4}$$

$$B(x;\boldsymbol{\lambda}) + D(x+1;\boldsymbol{\lambda}) = \kappa\big(B(x;\boldsymbol{\lambda}+\boldsymbol{\delta}) + D(x;\boldsymbol{\lambda}+\boldsymbol{\delta})\big) + \mathcal{E}(1;\boldsymbol{\lambda}). \tag{6.5}$$

The size of the matrix N is also a part of $\boldsymbol{\lambda}$ and the corresponding shift is -1.

6.1 Shape Invariance Data

Here are the shape invariance data of various polynomials [6].

1. Krawtchouk (3.34); $\boldsymbol{\lambda} = (p, N)$,$\boldsymbol{\delta} = (0, -1)$, $\kappa = 1$, $\mathcal{E}(1;\boldsymbol{\lambda}) = 1 \Rightarrow \mathcal{E}(n;\boldsymbol{\lambda}) = n$.

2. Meixner (3.38); $\boldsymbol{\lambda} = (\beta, c)$, $\boldsymbol{\delta} = (1, 0)$, $\kappa = 1$, $\mathcal{E}(1;\boldsymbol{\lambda}) = 1 \Rightarrow \mathcal{E}(n;\boldsymbol{\lambda}) = n$.

3. Charlier (3.41); $\boldsymbol{\lambda} = (a)$, $\boldsymbol{\delta} = (0)$, $\kappa = 1$, $\mathcal{E}(1;\boldsymbol{\lambda}) = 1 \Rightarrow \mathcal{E}(n;\boldsymbol{\lambda}) = n$.

4. Racah (8.3), (8.4); $\boldsymbol{\lambda} = (a, b, c, d)$, $\boldsymbol{\delta} = (1, 1, 1, 1)$, $\kappa = 1$, $\mathcal{E}(1\,;\boldsymbol{\lambda}) = 1 + \tilde{d} \Rightarrow \mathcal{E}(n\,;\boldsymbol{\lambda}) = n(n + \tilde{d})$.

5. Hahn (3.45); $\boldsymbol{\lambda} = (a, b, N)$, $\boldsymbol{\delta} = (1, 1, -1)$, $\kappa = 1$, $\mathcal{E}(1; \boldsymbol{\lambda}) = a + b \Rightarrow \mathcal{E}(n; \boldsymbol{\lambda}) = n(n + a + b - 1)$.

6. dual Hahn (3.46); $\boldsymbol{\lambda} = (a, b, N)$, $\boldsymbol{\delta} = (1, 0, -1)$, $\kappa = 1$, $\mathcal{E}(1; \boldsymbol{\lambda}) = 1 \Rightarrow \mathcal{E}(n; \boldsymbol{\lambda}) = n$.

7. q-Racah (8.3), (8.4); $q^{\boldsymbol{\lambda}} = (a, b, c, d)$, $\boldsymbol{\delta} = (1, 1, 1, 1)$, $\kappa = q^{-1}$, $\mathcal{E}(1\,; \boldsymbol{\lambda}) = (q^{-1}-1)(1-\tilde{d}q)$ $\Rightarrow \mathcal{E}(n; \boldsymbol{\lambda}) = (q^{-n} - 1)(1 - \tilde{d}q^n)$.

8. q-Hahn (3.47); $q^{\boldsymbol{\lambda}} = (a, b, q^N)$, $\boldsymbol{\delta} = (1, 1, -1)$, $\kappa = q^{-1}$, $\mathcal{E}(1; \boldsymbol{\lambda}) = (q^{-1} - 1)(1 - ab)$ $\Rightarrow \mathcal{E}(n; \boldsymbol{\lambda}) = (q^{-n} - 1)(1 - abq^{n-1})$.

9. dual q-Hahn (3.48); $q^{\boldsymbol{\lambda}} = (a, b, q^N)$, $\boldsymbol{\delta} = (1, 0, -1)$, $\kappa = q^{-1}$, $\mathcal{E}(1\,; \boldsymbol{\lambda}) = q^{-1} - 1$ $\Rightarrow \mathcal{E}(n\,; \boldsymbol{\lambda}) = q^{-n} - 1$.

10. quantum q-Krawtchouk (3.49); $q^{\boldsymbol{\lambda}} = (p, q^N)$, $\boldsymbol{\delta} = (1, -1)$, $\kappa = q$, $\mathcal{E}(1\,; \boldsymbol{\lambda}) = 1 - q$ $\Rightarrow \mathcal{E}(n\,; \boldsymbol{\lambda}) = 1 - q^n$.

11. q-Krawtchouk (3.50); $q^{\boldsymbol{\lambda}} = (p, q^N)$, $\boldsymbol{\delta} = (2, -1)$, $\kappa = q^{-1}$, $\mathcal{E}(1\,; \boldsymbol{\lambda}) = (q^{-1} - 1)(1 + pq)$ $\Rightarrow \mathcal{E}(n\,; \boldsymbol{\lambda}) = (q^{-n} - 1)(1 + pq^n)$.

12. dual q-Krawtchouk (3.51); $q^{\boldsymbol{\lambda}} = (p, q^N)$, $\boldsymbol{\delta} = (1, -1)$, $\kappa = q^{-1}$, $\mathcal{E}(1\,; \boldsymbol{\lambda}) = q^{-1} - 1$ $\Rightarrow\Rightarrow \mathcal{E}(n\,; \boldsymbol{\lambda}) = q^{-n} - 1$.

13. affine q-Krawtchouk (3.52); $q^{\boldsymbol{\lambda}} = (p, q^N)$, $\boldsymbol{\delta} = (1, -1)$, $\kappa = q^{-1}$, $\mathcal{E}(1\,; \boldsymbol{\lambda}) = q^{-1} - 1$ $\Rightarrow \mathcal{E}(n\,; \boldsymbol{\lambda}) = q^{-n} - 1$.

14. little q-Jacobi (3.53); $q^{\boldsymbol{\lambda}} = (a, b)$, $\boldsymbol{\delta} = (1, 1)$, $\kappa = q^{-1}$, $\mathcal{E}(1\,; \boldsymbol{\lambda}) = (q^{-1} - 1)(1 - abq^2)$ $\Rightarrow \mathcal{E}(n\,; \boldsymbol{\lambda}) = (q^{-n} - 1)(1 - abq^{n+1})$.

15. little q-Laguerre (3.54); $q^{\boldsymbol{\lambda}} = a$, $\boldsymbol{\delta} = 1$, $\kappa = q^{-1}$, $\mathcal{E}(1\,; \boldsymbol{\lambda}) = q^{-1}-1 \Rightarrow \mathcal{E}(n\,; \boldsymbol{\lambda}) = q^{-n}-1$.

16. Al-Salam Carlitz II (3.55); $q^{\boldsymbol{\lambda}} = a$, $\boldsymbol{\delta} = 0$, $\kappa = q$, $\mathcal{E}(1\,; \boldsymbol{\lambda}) = 1 - q \Rightarrow \mathcal{E}(n\,; \boldsymbol{\lambda}) = 1 - q^n$.

17. alternative q-Charlier (3.56); $q^{\boldsymbol{\lambda}} = a$, $\boldsymbol{\delta} = 2$, $\kappa = q^{-1}$, $\mathcal{E}(1\,; \boldsymbol{\lambda}) = (q^{-1} - 1)(1 + aq)$ $\Rightarrow \mathcal{E}(n\,; \boldsymbol{\lambda}) = (q^{-n} - 1)(1 + aq^n)$.

For various q-polynomials, *e.g.* (dual) q-Hahn, q-Racah, etc. the shifts of the parameters a, b, c, etc, are multiplicative. For example, in the q-Hahn case $a \to aq$, $b \to bq$. It should be noted that some dual pairs, *e.g.* the q-Hahn and dual q-Hahn, q-Krawtchouk and dual q-Krawtchouk, etc, have the identical parameter set $\boldsymbol{\lambda}$ but the shifts $\boldsymbol{\delta}$ are different.

6.1.1 Exercise

Verify the above shape invariance (6.1) and the universal eigenvalue formula (6.2) for the examples in §3.2.1, §3.2.2 with the data given above.

6.2 Auxiliary Function $\varphi(x)$

In the potential functions $B(x;\boldsymbol{\lambda})$, $D(x;\boldsymbol{\lambda})$ the parameter shift $\boldsymbol{\lambda}\to\boldsymbol{\lambda}+\boldsymbol{\delta}$ is closely related with the coordinate shift $x\to x+1$. But they are not the same for systems having the sinusoidal coordinate $\eta(x)\neq x$. Let us introduce an *auxiliary function* $\varphi(x;\boldsymbol{\lambda})$ by

$$\varphi(x;\boldsymbol{\lambda})\stackrel{\text{def}}{=}\frac{\eta(x+1;\boldsymbol{\lambda})-\eta(x;\boldsymbol{\lambda})}{\eta(1;\boldsymbol{\lambda})},\quad \varphi(0;\boldsymbol{\lambda})=1, \tag{6.6}$$

which connects potential functions $B(x;\boldsymbol{\lambda}+\boldsymbol{\delta})$, $D(x;\boldsymbol{\lambda}+\boldsymbol{\delta})$ with $B(x+1;\boldsymbol{\lambda})$, $D(x;\boldsymbol{\lambda})$ in systems with $\eta(x)\neq x$:

$$B(x;\boldsymbol{\lambda}+\boldsymbol{\delta})=\kappa^{-1}\frac{\varphi(x+1;\boldsymbol{\lambda})}{\varphi(x;\boldsymbol{\lambda})}B(x+1;\boldsymbol{\lambda}), \tag{6.7}$$

$$D(x;\boldsymbol{\lambda}+\boldsymbol{\delta})=\kappa^{-1}\frac{\varphi(x-1;\boldsymbol{\lambda})}{\varphi(x;\boldsymbol{\lambda})}D(x;\boldsymbol{\lambda}). \tag{6.8}$$

Likewise the groundstate eigenvector $\phi_0(x)$ with $\boldsymbol{\lambda}$ and $\boldsymbol{\lambda}+\boldsymbol{\delta}$ are related

$$\sqrt{B(0\,;\boldsymbol{\lambda})}\phi_0(x\,;\boldsymbol{\lambda}+\boldsymbol{\delta})=\varphi(x\,;\boldsymbol{\lambda})\sqrt{B(x\,;\boldsymbol{\lambda})}\phi_0(x\,;\boldsymbol{\lambda}), \tag{6.9}$$

$$\sqrt{B(0\,;\boldsymbol{\lambda})}\phi_0(x\,;\boldsymbol{\lambda}+\boldsymbol{\delta})=\varphi(x\,;\boldsymbol{\lambda})\sqrt{D(x+1\,;\boldsymbol{\lambda})}\phi_0(x+1\,;\boldsymbol{\lambda}). \tag{6.10}$$

Crum's theorem tells that the eigenvectors $\phi_n(x\,;\boldsymbol{\lambda})$ and $\phi_{n-1}(x\,;\boldsymbol{\lambda}+\boldsymbol{\delta})$ are related by $\mathcal{A}(\boldsymbol{\lambda})$ and $\mathcal{A}(\boldsymbol{\lambda})^\dagger$:

$$\mathcal{A}(\boldsymbol{\lambda})\phi_n(x;\boldsymbol{\lambda})=\mathcal{E}(n)(\boldsymbol{\lambda})\phi_{n-1}\big(x;\boldsymbol{\lambda}+\boldsymbol{\delta}\big)/\sqrt{B(0;\boldsymbol{\lambda})} \tag{6.11}$$

$$\mathcal{A}(\boldsymbol{\lambda})^\dagger\phi_{n-1}\big(x;\boldsymbol{\lambda}+\boldsymbol{\delta}\big)=\phi_n(x;\boldsymbol{\lambda})\times\sqrt{B(0;\boldsymbol{\lambda})}, \tag{6.12}$$

in which the factor $\sqrt{B(0;\boldsymbol{\lambda})}$ is introduced for convenience.

6.2.1 Exercise

1. Verify the relations among potential functions (6.7), (6.8) for various systems listed in §3.2.1, §3.2.2.

2. Show that the relations satisfied by the groundstate vector $\phi_0(x)$ (6.9), (6.10) are the consequences of (6.7), (6.8) and (3.20).

6.3 Universal Rodrigues Formula

Let us introduce the *forward and backward shift operators* $\mathcal{F}(\boldsymbol{\lambda})$ and $\mathcal{B}(\boldsymbol{\lambda})$ acting on the polynomial eigenfunctions $\{\check{P}_n(x\,;\boldsymbol{\lambda})\}$:

$$\begin{aligned}
\mathcal{F}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta})^{-1}\cdot\mathcal{A}(\boldsymbol{\lambda})\cdot\phi_0(x;\boldsymbol{\lambda})\times\sqrt{B(0;\boldsymbol{\lambda})}\\
&= B(0;\boldsymbol{\lambda})\varphi(x;\boldsymbol{\lambda})^{-1}(1-e^{\partial}), \qquad (6.13)\\
\mathcal{B}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \phi_0(x;\boldsymbol{\lambda})^{-1}\cdot\mathcal{A}(\boldsymbol{\lambda})^{\dagger}\cdot\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta})\times\frac{1}{\sqrt{B(0;\boldsymbol{\lambda})}}\\
&= \frac{1}{B(0;\boldsymbol{\lambda})}\bigl(B(x;\boldsymbol{\lambda})-D(x;\boldsymbol{\lambda})e^{-\partial}\bigr)\varphi(x;\boldsymbol{\lambda}), \qquad (6.14)\\
\widetilde{\mathcal{H}} &= \mathcal{B}(\boldsymbol{\lambda})\mathcal{F}(\boldsymbol{\lambda}) = B(x\,;\boldsymbol{\lambda})(1-e^{\partial})+D(x\,;\boldsymbol{\lambda})(1-e^{-\partial}), \qquad (6.15)\\
\mathcal{F}(\boldsymbol{\lambda})\check{P}_n(x\,;\boldsymbol{\lambda}) &= \mathcal{E}(n;\boldsymbol{\lambda})\check{P}_{n-1}(x\,;\boldsymbol{\lambda}+\boldsymbol{\delta}), \qquad (6.16)\\
\mathcal{B}(\boldsymbol{\lambda})\check{P}_{n-1}(x\,;\boldsymbol{\lambda}+\boldsymbol{\delta}) &= \check{P}_n(x\,;\boldsymbol{\lambda}). \qquad (6.17)
\end{aligned}$$

By taking the hermitian conjugate of the forward shift operator $\mathcal{F}(\boldsymbol{\lambda})$ (6.13), we obtain

$$\mathcal{A}(\boldsymbol{\lambda})^{\dagger} \propto \phi_0(x;\boldsymbol{\lambda})^{-1}\cdot\mathcal{D}(\boldsymbol{\lambda})\cdot\phi_0(x;\boldsymbol{\lambda}+\boldsymbol{\delta}), \qquad (6.18)$$

$$\mathcal{D}(\boldsymbol{\lambda}) \stackrel{\text{def}}{=} (1-e^{-\partial})\varphi(x;\boldsymbol{\lambda})^{-1}. \qquad (6.19)$$

By applying the above formula to the shape invariance formula (6.3) and imposing the universal normalisation (3.31), we obtain *universal Rodrigues formula* for all the orthogonal polynomials of a discrete variable in the Askey scheme:

$$P_n(\eta(x;\boldsymbol{\lambda});\boldsymbol{\lambda}) = \phi_0(x;\boldsymbol{\lambda})^{-2}\cdot\prod_{j=0}^{n-1}\mathcal{D}(\boldsymbol{\lambda}+j\boldsymbol{\delta})\cdot\phi_0^2(x;\boldsymbol{\lambda}+n\boldsymbol{\delta}). \qquad (6.20)$$

This is especially simple for the systems with $\eta(x)=x$, $P_n(x;\boldsymbol{\lambda})=\phi_0(x;\boldsymbol{\lambda})^{-2}\cdot(1-e^{-\partial})^n\cdot\phi_0(x;\boldsymbol{\lambda}+n\boldsymbol{\delta})^2$, which holds *e.g.* for the Krawtchouk (3.34), Meixner (3.38) and Charlier (3.41). It is easy to convince that the universal normalisation $P_n(0)=1$ is satisfied. In (6.20), the term involving $e^{-m\partial}$ $(1\le m\le n)$ all vanish at $x=0$ because of $\phi_0^2(-m;\boldsymbol{\lambda}+n\boldsymbol{\delta})=0$ due to (3.44). The rest is simply $\phi_0(0;\boldsymbol{\lambda})^{-2}\phi_0^2(0;\boldsymbol{\lambda}+n\boldsymbol{\delta})=1$ due to the boundary condition of $\phi_0(x)$ at $x=0$, (3.21).

6.3.1 Exercise

Calculate explicitly P_1 and P_2 of the Krawtchouk (3.34), Meixner (3.38) and Charlier (3.41) by using the universal Rodrigues formula (6.20).

7 Solvability in Heisenberg Picture

In QM the Schrödinger picture and the Heisenberg picture are known. So far we have discussed exactly solvable simplest QM in the Schrödinger picture. In this section we show that the same systems are solvable in the Heisenberg picture, too.

In the Heisenberg picture, the observables depend on time and the states are fixed. Heisenberg equation for the observable $\hat{\mathbf{A}}(t)$ read

$$\frac{\partial}{\partial t}\hat{\mathbf{A}}(t) = i\,[\mathcal{H}, \hat{\mathbf{A}}(t)]. \tag{7.1}$$

By picking up an arbitrary normalised orthogonal functions $\{\hat{\phi}_n(x)\}$, one can rewrite the above equation in matrix form:

$$\frac{\partial}{\partial t}\hat{\mathbf{A}}_{n,m}(t) = i\sum_{k=0}^{\infty}\Big(\mathcal{H}_{n,k}\hat{\mathbf{A}}_{k,m}(t) - \hat{\mathbf{A}}_{n,k}(t)\mathcal{H}_{k,m}\Big),$$
$$\hat{\mathbf{A}}_{n,m}(t) \stackrel{\text{def}}{=} \int \hat{\phi}_n(x)^*\hat{\mathbf{A}}(t)\hat{\phi}_m(x)dx, \quad \mathcal{H}_{n,m} \stackrel{\text{def}}{=} \int \hat{\phi}_n(x)^*\mathcal{H}\hat{\phi}_m(x)dx.$$

The formal solution of the Heisenberg equation (7.1)

$$\hat{\mathbf{A}}(t) = e^{it\mathcal{H}}\hat{\mathbf{A}}(0)e^{-it\mathcal{H}} = \sum_{n=0}^{\infty}\frac{(it)^n}{n!}(\mathrm{ad}\,\mathcal{H})^n\hat{\mathbf{A}}(0),$$

is expressed concisely in terms of adjoint operator $(\mathrm{ad}\,\mathcal{H})X \stackrel{\text{def}}{=} [\mathcal{H}, X]$. As seen from the Heisenberg equation (7.1) $(\mathrm{ad}\,\mathcal{H})^n\hat{\mathbf{A}}(0)$ corresponds to the n-th time derivative of $\hat{\mathbf{A}}(t)$ at $t = 0$. For explicit closed form result one has to calculate multiple commutators

$$[\mathcal{H}, [\mathcal{H}, \cdots, [\mathcal{H}, \hat{\mathbf{A}}(0)]]\cdots]$$

and evaluate the infinite sum. This is why the Heisenberg equations are considered intractable for most of the observables.

Here we show that the Heisenberg operator solution for the sinusoidal coordinate $\eta(x)$

$$e^{it\mathcal{H}}\eta(x)e^{-it\mathcal{H}}$$

can be obtained explicitly in a closed form for all the exactly solvable simplest QM [6]. The sinusoidal coordinate $\eta(x)$ is the argument of the eigenpolynomial $P_n(\eta(x))$ in the factorised form of the eigenvector $\phi_n(x)$ (3.22). As shown in the preceding sections, for the matrix interpretation of the Hamiltonian $\mathcal{H}$, $\eta(x)$ is a diagonal matrix. For the difference operator interpretation, it is just a function.

7.1 Closure Relation

It is easy to see that the following *closure relation* is a sufficient condition for the exact solvability of the Heisenberg equation for the sinusoidal coordinate,

$$\begin{aligned}[][\mathcal{H}, [\mathcal{H}, \eta(x)]\,] &= \eta(x)\,R_0(\mathcal{H}) + [\mathcal{H}, \eta(x)]\,R_1(\mathcal{H}) + R_{-1}(\mathcal{H}),\\ (\mathrm{ad}\,\mathcal{H})^2\eta(x) &= \eta(x)\,R_0(\mathcal{H}) + (\mathrm{ad}\,\mathcal{H})\eta(x)\,R_1(\mathcal{H}) + R_{-1}(\mathcal{H}),\end{aligned} \tag{7.2}$$

in which $R_i(y)$, $(i=0,\pm1)$ is a polynomial in y. By similarity transformation in terms of $\phi_0(x\,;\boldsymbol{\lambda})$ (3.20), (7.2) reads

$$\begin{aligned}
[\widetilde{\mathcal{H}},[\widetilde{\mathcal{H}},\eta(x)]\,]&=\eta(x)\,R_0(\widetilde{\mathcal{H}})+[\widetilde{\mathcal{H}},\eta(x)]\,R_1(\widetilde{\mathcal{H}})+R_{-1}(\widetilde{\mathcal{H}}),\\
(\mathrm{ad}\,\widetilde{\mathcal{H}})^2\eta(x)&=\eta(x)\,R_0(\widetilde{\mathcal{H}})+(\mathrm{ad}\,\widetilde{\mathcal{H}})\eta(x)\,R_1(\widetilde{\mathcal{H}})+R_{-1}(\widetilde{\mathcal{H}}),
\end{aligned}\tag{7.3}$$

The l.h.s. consists of the operators $e^{2\partial}$, e^{∂}, 1, $e^{-\partial}$, $e^{-2\partial}$ and $\mathcal{H}$ contains $e^{\pm\partial}$. Thus R_i can be parametrised as

$$R_1(z)=r_1^{(1)}z+r_1^{(0)},\quad R_0(z)=r_0^{(2)}z^2+r_0^{(1)}z+r_0^{(0)},\quad R_{-1}(z)=r_{-1}^{(2)}z^2+r_{-1}^{(1)}z+r_{-1}^{(0)}.\tag{7.4}$$

The coefficients $r_i^{(j)}$ depend on the overall normalisation of the Hamiltonian and the sinusoidal coordinate: $r_1^{(j)}\propto B(0)^{1-j}$, $r_0^{(j)}\propto B(0)^{2-j}$, $r_{-1}^{(j)}\propto\eta(1)B(0)^{2-j}$.

Based on the closure relation (7.2), the triple commutator $[\mathcal{H},[\mathcal{H},[\mathcal{H},\eta(x)]]]\equiv(\mathrm{ad}\,\mathcal{H})^3\eta(x)$ is expressed as a linear combination of $\eta(x)$ and $[\mathcal{H},\eta(x)]$ with polynomial coefficients in $\mathcal{H}$,

$$\begin{aligned}
&(\mathrm{ad}\,\mathcal{H})^3\eta(x)=[\mathcal{H},\eta(x)]R_0(\mathcal{H})+[\mathcal{H},[\mathcal{H},\eta(x)]]\,R_1(\mathcal{H})\\
&\quad=\eta(x)\,R_0(\mathcal{H})R_1(\mathcal{H})+(\mathrm{ad}\,\mathcal{H})\eta(x)\,\big(R_1(\mathcal{H})^2+R_0(\mathcal{H})\big)+R_{-1}(\mathcal{H})R_1(\mathcal{H}).
\end{aligned}$$

The closure relation (7.2) can be understood as the Cayley-Hamilton theorem for the operator ad$\mathcal{H}$ acting on $\eta(x)$. The fact that the closure occurs at the second order reflects that the Schrödinger equation is second order. Thus the higher order commutator $(\mathrm{ad}\,\mathcal{H})^n\eta(x)$ is also expressed as a linear combination of $\eta(x)$ and $[\mathcal{H},\eta(x)]$ with polynomial coefficients in $\mathcal{H}$. We arrive at the desired result

$$\begin{aligned}
e^{it\mathcal{H}}\eta(x)e^{-it\mathcal{H}}&=\sum_{n=0}^{\infty}\frac{(it)^n}{n!}(\mathrm{ad}\,\mathcal{H})^n\eta(x)\\
&=[\mathcal{H},\eta(x)]\frac{e^{i\alpha_+(\mathcal{H})t}-e^{i\alpha_-(\mathcal{H})t}}{\alpha_+(\mathcal{H})-\alpha_-(\mathcal{H})}-R_{-1}(\mathcal{H})R_0(\mathcal{H})^{-1}\\
&\quad+\big(\eta(x)+R_{-1}(\mathcal{H})R_0(\mathcal{H})^{-1}\big)\frac{-\alpha_-(\mathcal{H})e^{i\alpha_+(\mathcal{H})t}+\alpha_+(\mathcal{H})e^{i\alpha_-(\mathcal{H})t}}{\alpha_+(\mathcal{H})-\alpha_-(\mathcal{H})}.
\end{aligned}\tag{7.5}$$

This simply means that $\eta(x)$ undergoes a sinusoidal motion with two frequencies $\alpha_\pm(\mathcal{H})$ depending on the energy:

$$\alpha_\pm(\mathcal{H})\stackrel{\text{def}}{=}\tfrac12\Big(R_1(\mathcal{H})\pm\sqrt{R_1(\mathcal{H})^2+4R_0(\mathcal{H})}\,\Big),\tag{7.6}$$

$$\alpha_+(\mathcal{H})+\alpha_-(\mathcal{H})=R_1(\mathcal{H}),\quad \alpha_+(\mathcal{H})\alpha_-(\mathcal{H})=-R_0(\mathcal{H}).\tag{7.7}$$

The explanation is simple. The general solution of a three term recurrence relation with constant coefficients

$$\alpha a_{n+2}+\beta a_{n+1}+\gamma a_n=0,\quad n=0,1,\ldots,\quad \alpha,\beta,\gamma\in\mathbb{C},$$

is given by the roots of the corresponding quadratic equation,

$$\begin{aligned}
&\alpha x^2+\beta x+\gamma=0,\quad x_\pm\stackrel{\text{def}}{=}\frac{-\beta\pm\sqrt{\beta^2-4\alpha\gamma}}{2\alpha},\\
&a_n=A(x_+)^n+B(x_-)^n,\quad A+B=a_0,\quad Ax_++Bx_-=a_1.
\end{aligned}$$

The closure relation (7.2) becomes a three term recurrence relation by shifting $\eta(x)$,

$$(\mathrm{ad}\,\mathcal{H})^2\tilde{\eta}(x) - (\mathrm{ad}\,\mathcal{H})\tilde{\eta}(x)R_1(\mathcal{H}) - \tilde{\eta}(x)\,R_0(\mathcal{H}) = 0,$$
$$\tilde{\eta}(x) \stackrel{\text{def}}{=} \eta(x) + R_{-1}(\mathcal{H})R_0(\mathcal{H})^{-1},$$

giving rise to the solution

$$(\mathrm{ad}\,\mathcal{H})^n\tilde{\eta}(x) = A\alpha_+(\mathcal{H})^n + B\alpha_-(\mathcal{H})^n,$$
$$A = -\tilde{\eta}(x)\frac{\alpha_-(\mathcal{H})}{\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})} + [\mathcal{H}, \eta(x)]\frac{1}{\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})},$$
$$B = \tilde{\eta}(x)\frac{\alpha_+(\mathcal{H})}{\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})} - [\mathcal{H}, \eta(x)]\frac{1}{\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})}.$$

Summing them up produces $e^{i\alpha_\pm(\mathcal{H})t}$ in the solution (7.5).

The energy spectrum (eigenvalues) are determined by the overdetermined equations ($\mathcal{E}(0) = 0$)

$$\mathcal{E}(n+1;\boldsymbol{\lambda}) - \mathcal{E}(n;\boldsymbol{\lambda}) = \alpha_+(\mathcal{E}(n;\boldsymbol{\lambda})) = \mathcal{E}(1;\boldsymbol{\lambda} + n\boldsymbol{\delta}), \tag{7.8}$$
$$\mathcal{E}(n-1;\boldsymbol{\lambda}) - \mathcal{E}(n;\boldsymbol{\lambda}) = \alpha_-(\mathcal{E}(n;\boldsymbol{\lambda})) = -\mathcal{E}(1;\boldsymbol{\lambda} + (n-1)\boldsymbol{\delta}). \tag{7.9}$$

It is interesting to verify that the quantity $R_1(\mathcal{E}(n))^2 + 4R_0(\mathcal{E}(n))$ inside of the square root in $\alpha_\pm(\mathcal{H})$ (7.6) is a complete square for exactly solvable systems.

7.2 Creation and Annihilation Operators

By combining the three term recurrence relation for $P_n(\eta)$ (4.3) and the factorised form of the eigenvectors (3.22), we obtain

$$\eta(x)\phi_n(x) = A_n\phi_{n+1}(x) + B_n\phi_n(x) + C_n\phi_{n-1}(x) \quad (n \geq 0). \tag{7.10}$$

When the Heisenberg operator solution (7.5) is applied to the eigenvector $\phi_n(x)$, we obtain

$$\begin{aligned} &e^{it\mathcal{H}}\eta(x)e^{-it\mathcal{H}}\phi_n(x) \\ &= e^{it(\mathcal{E}(n+1)-\mathcal{E}(n))}A_n\phi_{n+1}(x) + B_n\phi_n(x) + e^{it(\mathcal{E}(n-1)-\mathcal{E}(n))}C_n\phi_{n-1}(x) \\ &= e^{it\alpha_+(\mathcal{E}(n))}A_n\phi_{n+1}(x) + B_n\phi_n(x) + e^{it\alpha_-(\mathcal{E}(n))}C_n\phi_{n-1}(x) \end{aligned} \tag{7.11}$$

We find out creation $a^{(+)}$ and the annihilation $a^{(-)}$ operators as the coefficients of $e^{i\alpha_\pm(\mathcal{H})t}$:

$$\begin{aligned} &e^{it\mathcal{H}}\eta(x)e^{-it\mathcal{H}} \\ &\quad = a^{(+)}e^{i\alpha_+(\mathcal{H})t} + a^{(-)}e^{i\alpha_-(\mathcal{H})t} - R_{-1}(\mathcal{H})R_0(\mathcal{H})^{-1}, \end{aligned} \tag{7.12}$$

$$\begin{aligned} a^{(\pm)} &\stackrel{\text{def}}{=} \pm\Big([\mathcal{H}, \eta(x)] - \tilde{\eta}(x)\alpha_\mp(\mathcal{H})\Big)\big(\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})\big)^{-1} \\ &\quad = \pm\big(\alpha_+(\mathcal{H}) - \alpha_-(\mathcal{H})\big)^{-1}\Big([\mathcal{H}, \eta(x)] + \alpha_\pm(\mathcal{H})\tilde{\eta}(x)\Big), \end{aligned} \tag{7.13}$$

$$a^{(+)\dagger} = a^{(-)}, \tag{7.14}$$

$$a^{(+)}\phi_n(x) = A_n\phi_{n+1}(x), \quad a^{(-)}\phi_n(x) = C_n\phi_{n-1}(x), \tag{7.15}$$

$$B_n = -R_{-1}(\mathcal{E}(n))R_0(\mathcal{E}(n))^{-1} = -(A_n + C_n). \tag{7.16}$$

The above B_n formula (7.16) is quite interesting. It is independent of the normalisation of the polynomials. The coefficients R_0, R_{-1} are independent of the eigenpolynomial, as they are determined by the Hamiltonian and the sinusoidal coordinate. But they are related with the eigenpolynomial through the spectrum $\mathcal{E}(n)$. The eigenvectors of the excited states $\{\phi_n(x)\}$ are obtained by multiple application of the creation operators on the groundstate eigenvector $\phi_0(x)$, $\phi_n(x) \propto (a^{(+)})^n\phi_0(x)$. This is the exact solvability in the Heisenberg picture.

The eigenvector of the annihilation operator is the *coherent state*. It is interesting to calculate the coherent states explicitly for various systems.

7.3 Determination of A_n and C_n

The starting point is the three term recurrence relations of the polynomial $P_n(\eta)$ and its dual $Q_x(\mathcal{E})$:

$$\eta(x)P_n(\eta(x)) = A_n\big(P_{n+1}(\eta(x)) - P_n(\eta(x))\big) + C_n\big(P_{n-1}(\eta(x)) - P_n(\eta(x))\big), \tag{7.17}$$

$$\mathcal{E}(n)Q_x(\mathcal{E}(n)) = B(x)\big(Q_x(\mathcal{E}(n)) - Q_{x+1}(\mathcal{E}(n))\big) + D(x)\big(Q_x(\mathcal{E}(n)) - Q_{x-1}(\mathcal{E}(n))\big). \tag{7.18}$$

By putting $x = 0$ in (7.18) and using $Q_0 = 1$, $D(0) = 0$, we obtain

$$P_n(\eta(1)) = Q_1(\mathcal{E}(n)) = \frac{\mathcal{E}(n) - B(0)}{-B(0)}, \tag{7.19}$$

in which the first equality is due to the duality (4.16). Next, by putting $x = 1$ in (7.17) and using (7.19), we obtain

$$\eta(1)(\mathcal{E}(n) - B(0)) = A_n(\mathcal{E}(n+1) - \mathcal{E}(n)) + C_n(\mathcal{E}(n-1) - \mathcal{E}(n)). \tag{7.20}$$

The two equations (7.16) and (7.20) for $n \geq 1$ give

$$A_n = \frac{\frac{R_{-1}(\mathcal{E}(n))}{R_0(\mathcal{E}(n))}\big(\mathcal{E}(n) - \mathcal{E}(n-1)\big) + \eta(1)\big(\mathcal{E}(n) - B(0)\big)}{\mathcal{E}(n+1) - \mathcal{E}(n-1)}, \tag{7.21}$$

$$C_n = \frac{\frac{R_{-1}(\mathcal{E}(n))}{R_0(\mathcal{E}(n))}\big(\mathcal{E}(n) - \mathcal{E}(n+1)\big) + \eta(1)\big(\mathcal{E}(n) - B(0)\big)}{\mathcal{E}(n-1) - \mathcal{E}(n+1)}, \tag{7.22}$$

and for $n = 0$ we obtain from (7.16)

$$A_0 = R_{-1}(0)R_0(0)^{-1}, \quad C_0 = 0. \tag{7.23}$$

They are simplified ($n \geq 1$) in terms of $\alpha_\pm$:

$$A_n = \frac{R_{-1}(\mathcal{E}(n)) + \eta(1)\big(\mathcal{E}(n) - B(0)\big)\alpha_+(\mathcal{E}(n))}{\alpha_+(\mathcal{E}(n))\big(\alpha_+(\mathcal{E}(n)) - \alpha_-(\mathcal{E}(n))\big)}, \tag{7.24}$$

$$C_n = \frac{R_{-1}(\mathcal{E}(n)) + \eta(1)\big(\mathcal{E}(n) - B(0)\big)\alpha_-(\mathcal{E}(n))}{\alpha_-(\mathcal{E}(n))\big(\alpha_-(\mathcal{E}(n)) - \alpha_+(\mathcal{E}(n))\big)}. \tag{7.25}$$

Note that (7.20) for $n=0$ gives another important relation

$$A_0\mathcal{E}(1)+B(0)\eta(1)=0. \tag{7.26}$$

This relation ensures that the expression for C_n (7.25) vanishes for $n=0$. Written differently, the above relation (7.26) means another dual relation

$$\frac{B(0)}{\mathcal{E}(1)}=\frac{-A_0}{\eta(1)}, \tag{7.27}$$

between the two intensive quantities. That is they are independent of the overall normalisation of the Hamiltonian $\mathcal{H}$ of the polynomial system.

7.4 Closure Relation Data and A_n, C_n

It is straightforward to calculate the closure relation (7.2), (7.3) for simpler systems. For the Krawtchouk (3.34), Meixner (3.38) and Charlier (3.41), $R_1=0$ and $R_0=1$, $R_{-1}\neq 0$, meaning $\alpha_\pm=\pm 1$. This leads to the linear spectrum $\mathcal{E}(n)=n$ (7.8), (7.9) and simple expressions of the creation/annihilation operators (7.13), the coefficients of the three term recurrence relation A_n, C_n (7.24), (7.25).

1. Krawtchouk (3.34); $R_1=0$, $R_0=1$, $R_{-1}(z)=(2p-1)z-pN \Rightarrow A_n=-p(N-n)$, $C_n=-(1-p)n$. This polynomial is *self-dual*. That is, $-A_n$, $-C_n$ are obtained from $B(x)$, $D(x)$ by the replacement $x\to n$. The dual Krawtchouk polynomial is exactly the same as the Krawtchouk polynomial.

2. Meixner (3.38); $R_1=0$, $R_0=1$, $R_{-1}(z)=-\frac{1+c}{1-c}z-\frac{\beta c}{1-c} \Rightarrow A_n=-\frac{c}{1-c}(n+\beta)$, $C_n=-\frac{1}{1-c}$. The Meixner is also self-dual.

3. Charlier (3.41); $R_1=0$, $R_0=1$, $R_{-1}(z)=-z-a \Rightarrow A_n=-a$, $C_n=-n$. The Charlier is self-dual, too.

It is interesting to calculate the closure relation (7.2) and derive the coefficients of the three term recurrence A_n, C_n explicitly (7.24), (7.25).

4. Hahn (3.45); $R_1=2$, $R_0(z)=4z+(a+b-2)(a+b)$,
   $$R_{-1}(z)=-(2N-a+b)z-a(a+b-2)N,$$
   $$\Rightarrow\ -A_n=\frac{(n+a)(n+a+b-1)(N-n)}{(2n-1+a+b)(2n+a+b)},\quad -C_n=\frac{n(n+b-1)(n+a+b+N-1)}{(2n-2+a+b)(2n-1+a+b)}.$$

   These are the same as $B(x)$, $D(x)$ of the dual Hahn (3.46) with x replaced by n.

5. dual Hahn (3.46); $R_1=0$, $R_0=1$, $R_{-1}(z)=2z^2-(2N-a+b)z-\ aN$,
   $$\Rightarrow\ -A_n=(n+a)(N-n),\quad -C_n=-n(b+N-n).$$

   These are the same as $B(x)$, $D(x)$ of the Hahn (3.45) with x replaced by n.

6. q-Hahn (3.47); $R_1(z)=(q^{-\frac12}-q^{\frac12})^2z',\quad z'\stackrel{\text{def}}{=}z+(1+abq^{-1})$,
$$R_0(z)=(q^{-\frac12}-q^{\frac12})^2\bigl(z'^2-ab(1+q^{-1})^2\bigr),$$
$$\begin{aligned}R_{-1}(z)=(q^{-\frac12}-q^{\frac12})^2\Bigl(z'^2&-\bigl(a(1+bq^{-1})+(1+aq^{-1})q^{-N}\bigr)z'\\&+a(1+q^{-1})\bigl((a-1)bq^{-1}+(1+bq^{-1})q^{-N}\bigr)\Bigr),\end{aligned}$$
$$\Rightarrow -A_n=\frac{(q^{n-N}-1)(1-aq^n)(1-abq^{n-1})}{(1-abq^{2n-1})(1-abq^{2n})},$$
$$-C_n=aq^{n-N-1}\,\frac{(1-q^n)(1-abq^{n+N-1})(1-bq^{n-1})}{(1-abq^{2n-2})(1-abq^{2n-1})}.$$
These are the same as $B(x)$, $D(x)$ of the dual q-Hahn (3.48) with x replaced by n.

7. dual q-Hahn (3.48); $R_1(z)=(q^{-\frac12}-q^{\frac12})^2z',\quad z'\stackrel{\text{def}}{=}z+1,\quad R_0(z)=(q^{-\frac12}-q^{\frac12})^2z'^2$,
$$\begin{aligned}R_{-1}(z)=(q^{-\frac12}-q^{\frac12})^2\Bigl((1+abq^{-1})z'^2&-\bigl(a(1+bq^{-1})+(1+aq^{-1})q^{-N}\bigr)z'\\&+a(1+q^{-1})q^{-N}\Bigr),\end{aligned}$$
$$\Rightarrow -A_n=(1-aq^n)(q^{n-N}-1),\quad -C_n=aq^{-1}(1-q^n)(q^{n-N}-b).$$
These are the same as $B(x)$, $D(x)$ of the q-Hahn (3.47) with x replaced by n.

8. Quantum q-Krawtchouk (3.49); $R_1(z)=(q^{-\frac12}-q^{\frac12})^2z',\quad z'\stackrel{\text{def}}{=}z-1$,
$$R_0(z)=(q^{-\frac12}-q^{\frac12})^2z'^2,$$
$$R_{-1}(z)=(q^{-\frac12}-q^{\frac12})^2\bigl(z'^2+p^{-1}(1+p+q^{-N-1})z'+p^{-1}(1+q^{-1})\bigr),$$
$$\Rightarrow -A_n=p^{-1}q^{-n-N-1}(1-q^{N-n}),\quad -C_n=(q^{-n}-1)(1-p^{-1}q^{-n}).$$

9. q-Krawtchouk (3.50); $R_1(z)=(q^{-\frac12}-q^{\frac12})^2z',\quad z'\stackrel{\text{def}}{=}z+1-p$,
$$R_0(z)=(q^{-\frac12}-q^{\frac12})^2\bigl(z'^2+p(q^{-\frac12}+q^{\frac12})^2\bigr),$$
$$R_{-1}(z)=(q^{-\frac12}-q^{\frac12})^2\bigl(z'^2+(p-q^{-N})z'+p(1+q^{-1})(1-q^{-N})\bigr),$$
$$\Rightarrow -A_n=\frac{(q^{n-N}-1)(1+pq^n)}{(1+pq^{2n})(1+pq^{2n+1})},\quad -C_n=pq^{2n-N-1}\frac{(1-q^n)(1+pq^{n+N})}{(1+pq^{2n-1})(1+pq^{2n})}.$$

10. affine q-Krawtchouk (3.52); $R_1(z)=(q^{-\frac12}-q^{\frac12})^2z',\quad z'\stackrel{\text{def}}{=}z+1$,
$$R_0(z)=(q^{-\frac12}-q^{\frac12})^2z'^2,$$
$$R_{-1}(z)=(q^{-\frac12}-q^{\frac12})^2\bigl(z'^2-(pq+(1+p)q^{-N})z'+p(1+q)q^{-N}\bigr),$$
$$\Rightarrow -A_n=(q^{n-N}-1)(1-pq^{n+1}),\quad -C_n=pq^{n-N}(1-q^n).$$

11. little q-Jacobi (3.53); $R_1(z)=(q^{-\frac12}-q^{\frac12})^2z',\quad z'\stackrel{\text{def}}{=}z+1+abq$,
$$R_0(z)=(q^{-\frac12}-q^{\frac12})^2\bigl(z'^2-ab(1+q)^2\bigr),$$
$$R_{-1}(z)=(q^{-\frac12}-q^{\frac12})^2\bigl(-z'^2+(1+a)z'-a(1+q)(1-bq)\bigr),$$
$$\Rightarrow -A_n=aq^{2n+1}\frac{(1-bq^{n+1})(1-abq^{n+1})}{(1-abq^{2n+1})(1-abq^{2n+2})},\quad -C_n=\frac{(1-q^n)(1-aq^n)}{(1-abq^{2n})(1-abq^{2n+1})}.$$

12. little q-Laguerre (3.54); $R_1(z)=(q^{-\frac12}-q^{\frac12})^2z'$, $\quad z'\stackrel{\text{def}}{=}z+1$, $\quad R_0(z)=(q^{-\frac12}-q^{\frac12})^2z'^2$,
$$R_{-1}(z)=(q^{-\frac12}-q^{\frac12})^2\big(-z'^2+(1+a)z'-a(1+q)\big),$$
$$\Rightarrow -A_n=aq^{2n+1},\quad -C_n=(1-q^n)(1-aq^n).$$

These are the same as $B(x)$, $D(x)$ of the Al-Salam Carlitz II (3.55) with x replaced by n.

13. Al-Salam Carlitz II (3.55); $R_1(z)=(q^{-\frac12}-q^{\frac12})^2z'$, $\quad z'\stackrel{\text{def}}{=}z-1$, $\quad R_0(z)=(q^{-\frac12}-q^{\frac12})^2z'^2$,
$$R_{-1}(z)=(q^{-\frac12}-q^{\frac12})^2\big(z'^2+(1+a)z'\big),$$
$$\Rightarrow -A_n=aq^{-n},\quad -C_n=(q^{-n}-1).$$

These are the same as $B(x)$, $D(x)$ of the little q-Laguerre (3.54) with x replaced by n.

14. alternative q-Charlier (3.56); $R_1(z)=(q^{-\frac12}-q^{\frac12})^2z'$, $\quad z'\stackrel{\text{def}}{=}z+1-a$,
$$R_0(z)=(q^{-\frac12}-q^{\frac12})^2\big(z'^2+a(q^{-\frac12}+q^{\frac12})^2\big),$$
$$R_{-1}(z)=(q^{-\frac12}-q^{\frac12})^2\big(-z'^2+z'-a(1+q)\big),$$
$$\Rightarrow -A_n=aq^{3n+1}\frac{1+aq^n}{(1+aq^{2n})(1+aq^{2n+1})},\quad -C_n=\frac{1-q^n}{(1+aq^{2n-1})(1+aq^{2n})}.$$

7.4.1 Exercise

Based on the above data of $R_j(z)$, $j=0,\pm1$, determine the eigenvalues $\{\mathcal{E}(n)\}$ as solutions of the overdetermined equations (7.8), (7.9) for various systems.

8 New orthogonal polynomials in Simplest QM (rdQM)

In this section we will present new orthogonal polynomials obtained by deforming those polynomials constituting the eigenpolynomials of the Simplest QM. As the the most generic members in this group we choose the Racah and q-Racah polynomials [35]. For the others, *e.g.* the multi-indexed Meixner or little q-Jacobi, etc., see [37].

8.1 Classical polynomials: the Racah and q-Racah

The Racah (R) and q-Racah (qR) systems contain four real parameters a, b, c, d and q for qR, which are symbolically denoted by $\boldsymbol{\lambda}$:

$$\text{R}:\ \boldsymbol{\lambda}=(a,b,c,d),\quad \boldsymbol{\delta}=(1,1,1,1),\quad \kappa=1, \tag{8.1}$$
$$q\text{R}:\ q^{\boldsymbol{\lambda}}=(a,b,c,d),\quad \boldsymbol{\delta}=(1,1,1,1),\quad \kappa=q^{-1},\quad 0<q<1, \tag{8.2}$$

where $q^{\boldsymbol{\lambda}}$ stands for $q^{(\lambda_1,\lambda_2,\ldots)}=(q^{\lambda_1},q^{\lambda_2},\ldots)$. The potential functions $B(x)$ and $D(x)$ are:

$$B(x;\boldsymbol{\lambda})=\begin{cases} -\dfrac{(x+a)(x+b)(x+c)(x+d)}{(2x+d)(2x+1+d)} & :\mathrm{R} \\ -\dfrac{(1-aq^x)(1-bq^x)(1-cq^x)(1-dq^x)}{(1-dq^{2x})(1-dq^{2x+1})} & :q\mathrm{R} \end{cases}, \tag{8.3}$$

$$D(x;\boldsymbol{\lambda})=\begin{cases} -\dfrac{(x+d-a)(x+d-b)(x+d-c)x}{(2x-1+d)(2x+d)} & :\mathrm{R} \\ -\tilde{d}\,\dfrac{(1-a^{-1}dq^x)(1-b^{-1}dq^x)(1-c^{-1}dq^x)(1-q^x)}{(1-dq^{2x-1})(1-dq^{2x})} & :q\mathrm{R}, \end{cases} \tag{8.4}$$

in which a new parameter $\tilde{d}$ is defined by

$$\tilde{d}\stackrel{\text{def}}{=}\begin{cases} a+b+c-d-1 & :\mathrm{R} \\ abcd^{-1}q^{-1} & :q\mathrm{R} \end{cases}. \tag{8.5}$$

We adopt the following choice of the parameter ranges:

$$\mathrm{R}:\quad a=-N,\quad 0<d<a+b,\quad 0<c<1+d, \tag{8.6}$$

$$q\mathrm{R}:\quad a=q^{-N},\quad 0<ab<d<1,\quad qd<c<1. \tag{8.7}$$

The eigenvalue problem and its factorised eigenvectors are:

$$\mathcal{H}(\boldsymbol{\lambda})\phi_n(x;\boldsymbol{\lambda})=\mathcal{E}(n;\boldsymbol{\lambda})\phi_n(x;\boldsymbol{\lambda})\quad (x=0,1,\ldots,N;n=0,1,\ldots,N), \tag{8.8}$$

$$\phi_n(x;\boldsymbol{\lambda})=\phi_0(x;\boldsymbol{\lambda})\check{P}_n(x;\boldsymbol{\lambda}), \tag{8.9}$$

$$\mathcal{E}(n;\boldsymbol{\lambda})=\begin{cases} n(n+\tilde{d}) & :\mathrm{R} \\ (q^{-n}-1)(1-\tilde{d}q^n) & :q\mathrm{R} \end{cases}\quad \eta(x;\boldsymbol{\lambda})=\begin{cases} x(x+d) & :\mathrm{R} \\ (q^{-x}-1)(1-dq^x) & :q\mathrm{R} \end{cases} \tag{8.10}$$

$$\check{P}_n(x;\boldsymbol{\lambda})=P_n\big(\eta(x;\boldsymbol{\lambda});\boldsymbol{\lambda}\big)=\begin{cases} {}_4F_3\Big(\begin{matrix}-n,\,n+\tilde{d},\,-x,\,x+d\\ a,\,b,\,c\end{matrix}\Big|\,1\Big) & :\mathrm{R} \\ {}_4\phi_3\Big(\begin{matrix}q^{-n},\,\tilde{d}q^n,\,q^{-x},\,dq^x\\ a,\,b,\,c\end{matrix}\Big|\,q\,;q\Big) & :q\mathrm{R} \end{cases} \tag{8.11}$$

$$\phi_0(x;\boldsymbol{\lambda})^2=\begin{cases} \dfrac{(a,b,c,d)_x}{(1+d-a,1+d-b,1+d-c,1)_x}\,\dfrac{2x+d}{d} & :\mathrm{R} \\ \dfrac{(a,b,c,d\,;q)_x}{(a^{-1}dq,b^{-1}dq,c^{-1}dq,q\,;q)_x\,\tilde{d}^x}\,\dfrac{1-dq^{2x}}{1-d} & :q\mathrm{R} \end{cases}, \tag{8.12}$$

$$d_n(\boldsymbol{\lambda})^2=\begin{cases} \dfrac{(a,b,c,\tilde{d})_n}{(1+\tilde{d}-a,1+\tilde{d}-b,1+\tilde{d}-c,1)_n}\,\dfrac{2n+\tilde{d}}{\tilde{d}} \\ \quad\times\dfrac{(-1)^N(1+d-a,1+d-b,1+d-c)_N}{(\tilde{d}+1)_N(d+1)_{2N}} & :\mathrm{R} \\ \dfrac{(a,b,c,\tilde{d}\,;q)_n}{(a^{-1}\tilde{d}q,b^{-1}\tilde{d}q,c^{-1}\tilde{d}q,q\,;q)_n\,d^n}\,\dfrac{1-\tilde{d}q^{2n}}{1-\tilde{d}} \\ \quad\times\dfrac{(-1)^N(a^{-1}dq,b^{-1}dq,c^{-1}dq\,;q)_N\,\tilde{d}^Nq^{\frac12N(N+1)}}{(\tilde{d}q\,;q)_N(dq\,;q)_{2N}} & :q\mathrm{R} \end{cases}. \tag{8.13}$$

Here $(a)_n$ ($(a;q)_n$) is the (q-)shifted factorial ((q-)Pochhammer symbol), see (A.1), (A.2).

The (q-)Racah polynomials are expressed by truncated (basic)-hypergeometric series (8.11) and they are polynomials in the sinusoidal coordinates $\eta(x;\boldsymbol{\lambda})$ (8.10). In fact, if a (Laurent) polynomial $\check{f}$ in x (q^x) is invariant under the involution $\mathcal{I}$

$$\mathcal{I}(x) = -x - d \quad : \mathrm{R}, \qquad \mathcal{I}(q^x) = q^{-x}d^{-1} \quad : q\mathrm{R}, \quad \mathcal{I}^2 = \mathrm{id}, \tag{8.14}$$

$$\mathcal{I}\bigl(\check{f}(x)\bigr) = \check{f}(x) \;\Leftrightarrow\; \check{f}(x) = f\bigl(\eta(x;\boldsymbol{\lambda})\bigr), \tag{8.15}$$

it is a polynomial in the sinusoidal coordinate $\eta(x;\boldsymbol{\lambda})$. The parameter dependence of $\eta(x;\boldsymbol{\lambda})$ is important, since parameters are shifted by the multi-indexed deformation.

By similarity transforming $\mathcal{H}$ in terms of the ground state eigenfunction $\phi_0(x)$, we obtain the second order difference operator $\widetilde{\mathcal{H}}$ governing the classical polynomial $\check{P}_n(x)$:

$$\begin{aligned}
&\widetilde{\mathcal{H}} \stackrel{\text{def}}{=} \phi_0(x)\circ\mathcal{H}\circ\phi_0(x) = B(x)(1-e^{\partial}) + D(x)(1-e^{-\partial}),\\
&B(x)\bigl(\check{P}_n(x) - \check{P}_n(x+1)\bigr) + D(x)\bigl(\check{P}_n(x) - \check{P}_n(x-1)\bigr) = \mathcal{E}(n)\check{P}_n(x).
\end{aligned}$$

8.2 Discrete symmetry and virtual state vectors

Here we introduce discrete symmetry and virtual state vectors of the (q-)Racah system. In ordinary QM, the virtual state solutions are square non-integrable solutions of the Schrödinger equation. In the (q-)Racah case, the Hamiltonians are finite-dimensional real symmetric tri-diagonal matrices. The eigenvalue equation for a given Hamiltonian matrix cannot have any extra solution other than the genuine eigenvectors. Thus we will use the term *virtual state vectors*. As will be shown shortly, virtual state vectors are the 'solutions' of the eigenvalue problem for a *virtual* Hamiltonian $\mathcal{H}'$, except for one of the boundaries, $x = x_{\max}$ (8.30). For the polynomials corresponding to infinite dimensional matrix eigenvalue problems, another type of virtual state vectors is possible [37].

By the twist operation $\mathfrak{t}$ of the parameters:

$$\mathfrak{t}(\boldsymbol{\lambda}) \stackrel{\text{def}}{=} (\lambda_4 - \lambda_1 + 1, \lambda_4 - \lambda_2 + 1, \lambda_3, \lambda_4), \quad \mathfrak{t}^2 = \mathrm{id}, \tag{8.16}$$

we introduce two functions $B'(x)$ and $D'(x)$ by

$$B'(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} B\bigl(x;\mathfrak{t}(\boldsymbol{\lambda})\bigr), \quad D'(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} D\bigl(x;\mathfrak{t}(\boldsymbol{\lambda})\bigr), \tag{8.17}$$

namely,

$$B'(x;\boldsymbol{\lambda}) = \begin{cases} -\dfrac{(x+d-a+1)(x+d-b+1)(x+c)(x+d)}{(2x+d)(2x+1+d)} & : \mathrm{R} \\[2ex] -\dfrac{(1-a^{-1}dq^{x+1})(1-b^{-1}dq^{x+1})(1-cq^x)(1-dq^x)}{(1-dq^{2x})(1-dq^{2x+1})} & : q\mathrm{R} \end{cases}, \tag{8.18}$$

$$D'(x;\boldsymbol{\lambda}) = \begin{cases} -\dfrac{(x+a-1)(x+b-1)(x+d-c)x}{(2x-1+d)(2x+d)} & : \mathrm{R} \\[2ex] -\dfrac{cdq}{ab}\,\dfrac{(1-aq^{x-1})(1-bq^{x-1})(1-c^{-1}dq^x)(1-q^x)}{(1-dq^{2x-1})(1-dq^{2x})} & : q\mathrm{R} \end{cases}. \tag{8.19}$$

We restrict the parameter range to

$$\mathrm{R}: \quad d+M<a+b, \qquad q\mathrm{R}: \quad ab<dq^M, \tag{8.20}$$

in which M is a positive integer and later it will be identified with the possible maximal number of repeated Darboux transformations. It is easy to verify

$$B(x;\boldsymbol{\lambda})D(x+1;\boldsymbol{\lambda})=\alpha(\boldsymbol{\lambda})^2B'(x;\boldsymbol{\lambda})D'(x+1;\boldsymbol{\lambda}), \tag{8.21}$$
$$B(x;\boldsymbol{\lambda})+D(x;\boldsymbol{\lambda})=\alpha(\boldsymbol{\lambda})\big(B'(x;\boldsymbol{\lambda})+D'(x;\boldsymbol{\lambda})\big)+\alpha'(\boldsymbol{\lambda}), \tag{8.22}$$
$$B'(x;\boldsymbol{\lambda})>0 \ \ (x=0,1,\ldots,x_{\max}+M-1), \tag{8.23}$$
$$D'(x;\boldsymbol{\lambda})>0 \ \ (x=1,2,\ldots,x_{\max}), \ \ D'(0;\boldsymbol{\lambda})=D'(x_{\max}+1;\boldsymbol{\lambda})=0. \tag{8.24}$$

Here the constant $\alpha(\boldsymbol{\lambda})$ is positive and $\alpha'(\boldsymbol{\lambda})$ is negative:

$$0<\alpha(\boldsymbol{\lambda})=\left\{\begin{array}{ll}1 & :\mathrm{R}\\ abd^{-1}q^{-1} & :q\mathrm{R},\end{array}\right. \quad 0>\alpha'(\boldsymbol{\lambda})=\left\{\begin{array}{ll}-c(a+b-d-1) & :\mathrm{R}\\ -(1-c)(1-abd^{-1}q^{-1}) & :q\mathrm{R}.\end{array}\right. \tag{8.25}$$

The above relations (8.21)–(8.24) imply a linear relation between the original Hamiltonian $\mathcal{H}$ and virtual Hamiltonian $\mathcal{H}'$

$$\mathcal{H}(\boldsymbol{\lambda})=\alpha(\boldsymbol{\lambda})\mathcal{H}'+\alpha'(\boldsymbol{\lambda}), \quad \mathcal{H}'\stackrel{\text{def}}{=}\mathcal{H}\big(\mathfrak{t}(\boldsymbol{\lambda})\big), \tag{8.26}$$

which is defined by the twisted parameters (the $\boldsymbol{\lambda}$ dependence is suppressed for simplicity):

$$\mathcal{H}\big(\mathfrak{t}(\boldsymbol{\lambda})\big)=-\sqrt{B'(x)}\,e^{\partial}\sqrt{D'(x)}-\sqrt{D'(x)}\,e^{-\partial}\sqrt{B'(x)}+B'(x)+D'(x). \tag{8.27}$$

This means that $\mathcal{H}(\mathfrak{t}(\boldsymbol{\lambda}))$ is *positive definite* and it has *no zero-mode*. In other words, the two term recurrence relation determining the 'zero-mode' of $\mathcal{H}(\mathfrak{t}(\boldsymbol{\lambda}))$

$$\begin{aligned}&\mathcal{A}\big(\mathfrak{t}(\boldsymbol{\lambda})\big)=\sqrt{B'(x;\boldsymbol{\lambda})}-e^{\partial}\sqrt{D'(x;\boldsymbol{\lambda})},\\ &\mathcal{A}\big(\mathfrak{t}(\boldsymbol{\lambda})\big)\tilde{\phi}_0(x;\boldsymbol{\lambda})=0 \quad (x=0,1,\ldots,x_{\max}-1),\end{aligned} \tag{8.28}$$

can be 'solved' from $x=0$ to $x=x_{\max}-1$ to determine all the components

$$\tilde{\phi}_0(x;\boldsymbol{\lambda})\stackrel{\text{def}}{=}\sqrt{\prod_{y=0}^{x-1}\frac{B'(y;\boldsymbol{\lambda})}{D'(y+1;\boldsymbol{\lambda})}} \qquad (x=0,1,\ldots,x_{\max}). \tag{8.29}$$

But at the end point $x=x_{\max}$, the 'zero-mode' equation (8.28) is not satisfied. The eigenvalue problem for the virtual Hamiltonian

$$\mathcal{H}'(\boldsymbol{\lambda})\tilde{\varphi}_{\mathrm{v}}(x;\boldsymbol{\lambda})=\mathcal{E}'_{\mathrm{v}}(\boldsymbol{\lambda})\tilde{\varphi}_{\mathrm{v}}(x;\boldsymbol{\lambda}), \tag{8.30}$$

can be *solved except for the end point* $x=x_{\max}$ by the factorisation ansatz

$$\tilde{\varphi}_{\mathrm{v}}(x;\boldsymbol{\lambda})\stackrel{\text{def}}{=}\tilde{\phi}_0(x;\boldsymbol{\lambda})\check{\xi}_{\mathrm{v}}(x;\boldsymbol{\lambda}),$$

as in the original (q-)Racah system. By using the explicit form of $\tilde{\phi}_0(x;\boldsymbol{\lambda})$ (8.29), the new Schrödinger equation for $x = 0, \ldots, x_{\max} - 1$ is rewritten as

$$B'(x;\boldsymbol{\lambda})\big(\check{\xi}_{\rm v}(x;\boldsymbol{\lambda}) - \check{\xi}_{\rm v}(x+1;\boldsymbol{\lambda})\big) + D'(x;\boldsymbol{\lambda})\big(\check{\xi}_{\rm v}(x;\boldsymbol{\lambda}) - \check{\xi}_{\rm v}(x-1;\boldsymbol{\lambda})\big) = \mathcal{E}'_{\rm v}(\boldsymbol{\lambda})\check{\xi}_{\rm v}(x;\boldsymbol{\lambda}). \tag{8.31}$$

This is the same form of equation as that for the (q-)Racah polynomials. So its solution for $x \in \mathbb{C}$ is given by the (q-)Racah polynomial (8.11) with the twisted parameters:

$$\check{\xi}_{\rm v}(x;\boldsymbol{\lambda}) = \check{P}_{\rm v}\big(x;\mathfrak{t}(\boldsymbol{\lambda})\big), \qquad \mathcal{E}'_{\rm v}(\boldsymbol{\lambda}) = \mathcal{E}_{\rm v}\big(\mathfrak{t}(\boldsymbol{\lambda})\big). \tag{8.32}$$

Among such 'solutions' of (8.30), those with the negative energy and having definite sign

$$\check{\xi}_{\rm v}(x;\boldsymbol{\lambda}) > 0 \quad (x = 0, 1, \ldots, x_{\max}, x_{\max}+1; {\rm v} \in \mathcal{V}), \tag{8.33}$$
$$\tilde{\mathcal{E}}_{\rm v}(\boldsymbol{\lambda}) < 0 \quad ({\rm v} \in \mathcal{V}), \tag{8.34}$$

are called the *virtual state vectors*: $\{\tilde{\varphi}_{\rm v}(x)\}$, ${\rm v} \in \mathcal{V}$. The index set of the virtual state vectors is

$$\mathcal{V} = \{1, 2, \ldots, {\rm v}_{\max}\}, \quad {\rm v}_{\max} = \min\big\{[\lambda_1 + \lambda_2 - \lambda_4 - 1]', [\tfrac{1}{2}(\lambda_1 + \lambda_2 - \lambda_3 - \lambda_4)]\big\}, \tag{8.35}$$

where $[x]$ denotes the greatest integer not exceeding x and $[x]'$ denotes the greatest integer not equal or exceeding x. The negative virtual state energy conditions (8.34) is met by ${\rm v}_{\max} \leq [\lambda_1 + \lambda_2 - \lambda_4 - 1]'$. For the positivity of $\check{\xi}_{\rm v}(x;\boldsymbol{\lambda})$ (8.33), we write them down explicitly:

$$\check{\xi}_{\rm v}(x;\boldsymbol{\lambda}) = \begin{cases} {}_4F_3\Big(\begin{matrix} -{\rm v},\ {\rm v} - a - b + c + d + 1,\ -x,\ x + d \\ d - a + 1,\ d - b + 1,\ c \end{matrix} \Big|\, 1\Big) & : \mathrm{R} \\ {}_4\phi_3\Big(\begin{matrix} q^{-{\rm v}},\ a^{-1}b^{-1}cdq^{{\rm v}+1},\ q^{-x},\ dq^x \\ a^{-1}dq,\ b^{-1}dq,\ c \end{matrix} \Big|\, q\,;q\Big) & : q\mathrm{R} \end{cases} \tag{8.36}$$

$$= \begin{cases} \displaystyle\sum_{k=0}^{\rm v} \frac{(-{\rm v}, {\rm v} - a - b + c + d + 1, -x, x + d)_k}{(d - a + 1, d - b + 1, c)_k} \frac{1}{k!} & : \mathrm{R} \\ \displaystyle\sum_{k=0}^{\rm v} \frac{(q^{-{\rm v}}, a^{-1}b^{-1}cdq^{{\rm v}+1}, q^{-x}, dq^x; q)_k}{(a^{-1}dq, b^{-1}dq, c; q)_k} \frac{q^k}{(q;q)_k} & : q\mathrm{R} \end{cases}. \tag{8.37}$$

Each k-th term in the sum is non-negative for $2{\rm v}_{\max} \leq \lambda_1 + \lambda_2 - \lambda_3 - \lambda_4$. As shown shortly (8.47), it is the virtual state polynomial $\check{\xi}_{\rm v}(x)$ rather than the full virtual state vector $\tilde{\varphi}_{\rm v}(x)$ that plays an important role in the Darboux transformations.

For later use, we summarise the properties of the virtual state vectors:

$$\tilde{\phi}_0(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \phi_0\bigl(x;\mathfrak{t}(\boldsymbol{\lambda})\bigr),\quad \tilde{\varphi}_{\rm v}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \phi_{\rm v}\bigl(x;\mathfrak{t}(\boldsymbol{\lambda})\bigr) = \tilde{\phi}_0(x;\boldsymbol{\lambda})\check{\xi}_{\rm v}(x;\boldsymbol{\lambda}), \tag{8.38}$$

$$\check{\xi}_{\rm v}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \check{P}_{\rm v}\bigl(x;\mathfrak{t}(\boldsymbol{\lambda})\bigr) = P_{\rm v}\bigl(\eta(x;\mathfrak{t}(\boldsymbol{\lambda}));\mathfrak{t}(\boldsymbol{\lambda})\bigr), \tag{8.39}$$

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

$$\mathcal{H}(\boldsymbol{\lambda})\tilde{\varphi}_{\rm v}(x_{\max};\boldsymbol{\lambda}) \neq \tilde{\mathcal{E}}_{\rm v}(\boldsymbol{\lambda})\tilde{\varphi}_{\rm v}(x_{\max};\boldsymbol{\lambda}),\qquad \mathcal{E}'_{\rm v}(\boldsymbol{\lambda}) = \mathcal{E}_{\rm v}\bigl(\mathfrak{t}(\boldsymbol{\lambda})\bigr), \tag{8.40}$$

$$\tilde{\mathcal{E}}_{\rm v}(\boldsymbol{\lambda}) = \alpha(\boldsymbol{\lambda})\mathcal{E}'_{\rm v}(\boldsymbol{\lambda}) + \alpha'(\boldsymbol{\lambda}) = \left\{\begin{array}{ll} -(c+{\rm v})(a+b-d-1-{\rm v}) & :{\rm R}\\ -(1-cq^{\rm v})(1-abd^{-1}q^{-1-{\rm v}}) & :q{\rm R}\end{array}\right., \tag{8.41}$$

$$\nu(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{\phi_0(x;\boldsymbol{\lambda})}{\tilde{\phi}_0(x;\boldsymbol{\lambda})} = \left\{\begin{array}{ll} \dfrac{\Gamma(1-a)\Gamma(x+b)\Gamma(d-a+1)\Gamma(b-d-x)}{\Gamma(1-a-x)\Gamma(b)\Gamma(x+d-a+1)\Gamma(b-d)} & :{\rm R}\\ \dfrac{(a^{-1}q^{1-x},b,a^{-1}dq^{x+1},bd^{-1};q)_\infty}{(a^{-1}q,bq^x,a^{-1}dq,bd^{-1}q^{-x};q)_\infty} & :q{\rm R}\end{array}\right.. \tag{8.42}$$

Note that $\alpha'(\boldsymbol{\lambda}) = \tilde{\mathcal{E}}_0(\boldsymbol{\lambda}) < 0$. The function $\nu(x;\boldsymbol{\lambda})$ can be analytically continued into a meromorphic function of x or q^x through the functional relations:

$$\nu(x+1;\boldsymbol{\lambda}) = \frac{B(x;\boldsymbol{\lambda})}{\alpha B'(x;\boldsymbol{\lambda})}\nu(x;\boldsymbol{\lambda}),\quad \nu(x-1;\boldsymbol{\lambda}) = \frac{D(x;\boldsymbol{\lambda})}{\alpha D'(x;\boldsymbol{\lambda})}\nu(x;\boldsymbol{\lambda}). \tag{8.43}$$

By $B(x_{\max};\boldsymbol{\lambda}) = 0$, it vanishes for integer $x_{\max}+1 \leq x \leq x_{\max}+M$, $\nu(x;\boldsymbol{\lambda}) = 0$, and at negative integer points it takes nonzero finite values in general.

8.3 Darboux transformations

Darboux transformations for the simplest QM have been introduced in [20], in which Wronskian's roles are played by Casoratians. The Casorati determinant of a set of n functions $\{f_j(x)\}$ is defined by

$$\mathrm{W}_C[f_1,\ldots,f_n](x) \stackrel{\text{def}}{=} \det\Bigl(f_k(x+j-1)\Bigr)_{1\leq j,k\leq n}, \tag{8.44}$$

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

$$\mathrm{W}_C[gf_1,gf_2,\ldots,gf_n](x) = \prod_{k=0}^{n-1} g(x+k)\cdot \mathrm{W}_C[f_1,f_2,\ldots,f_n](x), \tag{8.45}$$

$$\begin{aligned}&\mathrm{W}_C\bigl[\mathrm{W}_C[f_1,f_2,\ldots,f_n,g],\mathrm{W}_C[f_1,f_2,\ldots,f_n,h]\,\bigr](x)\\ &\ = \mathrm{W}_C[f_1,f_2,\ldots,f_n](x+1)\,\mathrm{W}_C[f_1,f_2,\ldots,f_n,g,h](x)\quad (n\geq 0).\end{aligned} \tag{8.46}$$

For simplicity of presentation the parameter ($\boldsymbol{\lambda}$) dependence of various quantities is suppressed in this subsection. Let us deform the (q-)Racah system by a Darboux transformation with a seed 'solution' which is one of the virtual state vectors $\tilde{\varphi}_{d_1}(x)$ $(1 \leq d_1 \in \mathcal{V})$ (8.38).

We rewrite the original Hamiltonian in such a factorisation in which the virtual state vectors $\tilde{\varphi}_{d_1}(x)$ are almost annihilated except for the upper end point:

$$
\begin{aligned}
&\mathcal{H} = \hat{\mathcal{A}}_{d_1}^{\dagger}\hat{\mathcal{A}}_{d_1} + \tilde{\mathcal{E}}_{d_1},\\
&\hat{\mathcal{A}}_{d_1} \stackrel{\text{def}}{=} \sqrt{\hat{B}_{d_1}(x)} - e^{\partial}\sqrt{\hat{D}_{d_1}(x)},\quad \hat{\mathcal{A}}_{d_1}^{\dagger} = \sqrt{\hat{B}_{d_1}(x)} - \sqrt{\hat{D}_{d_1}(x)}\,e^{-\partial},\\
&\hat{\mathcal{A}}_{d_1}\tilde{\varphi}_{d_1}(x) = 0 \ \ (x = 0, 1, \ldots, x_{\max} - 1),\quad \hat{\mathcal{A}}_{d_1}\tilde{\varphi}_{d_1}(x_{\max}) \neq 0.
\end{aligned}
$$

This is achieved by introducing potential functions $\hat{B}_{d_1}(x)$ and $\hat{D}_{d_1}(x)$ determined by the virtual state polynomial $\check{\xi}_{d_1}(x)$:

$$
\hat{B}_{d_1}(x) \stackrel{\text{def}}{=} \alpha B'(x)\frac{\check{\xi}_{d_1}(x+1)}{\check{\xi}_{d_1}(x)},\quad \hat{D}_{d_1}(x) \stackrel{\text{def}}{=} \alpha D'(x)\frac{\check{\xi}_{d_1}(x-1)}{\check{\xi}_{d_1}(x)}. \tag{8.47}
$$

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

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

where use is made of (8.31) in the second equation.

A new deformed Hamiltonian system with $\mathcal{H}_{d_1}$, $\phi_{d_1 n}(x)$, $\tilde{\varphi}_{d_1\mathrm{v}}(x)$, is obtained by changing the order of the two matrices $\hat{\mathcal{A}}_{d_1}^{\dagger}$ and $\hat{\mathcal{A}}_{d_1}$:

$$
\mathcal{H}_{d_1} \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1}\hat{\mathcal{A}}_{d_1}^{\dagger} + \tilde{\mathcal{E}}_{d_1}, \tag{8.48}
$$

$$
\phi_{d_1 n}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1}\phi_n(x) \ \ (x = 0, 1, \ldots, x_{\max}; n = 0, 1, \ldots, n_{\max}), \tag{8.49}
$$

$$
\tilde{\varphi}_{d_1\mathrm{v}}(x) \stackrel{\text{def}}{=} \hat{\mathcal{A}}_{d_1}\tilde{\varphi}_{\mathrm{v}}(x) + \delta_{x,x_{\max}}\rho_{d_1\mathrm{v}} \ \ (x = 0, 1, \ldots, x_{\max}; \mathrm{v} \in \mathcal{V}\backslash\{d_1\}), \tag{8.50}
$$

$$
\rho_{d_1\mathrm{v}} \stackrel{\text{def}}{=} -\frac{\sqrt{\alpha B'(x_{\max})}\,\tilde{\phi}_0(x_{\max})}{\sqrt{\check{\xi}_{d_1}(x_{\max})\check{\xi}_{d_1}(x_{\max}+1)}}\,\check{\xi}_{d_1}(x_{\max})\check{\xi}_{\mathrm{v}}(x_{\max}+1), \tag{8.51}
$$

$$
\mathcal{H}_{d_1}\phi_{d_1 n}(x) = \mathcal{E}(n)\phi_{d_1 n}(x) \ \ (x = 0, 1, \ldots, x_{\max}; n = 0, 1, \ldots, n_{\max}), \tag{8.52}
$$

$$
\begin{aligned}
&\mathcal{H}_{d_1}\tilde{\varphi}_{d_1\mathrm{v}}(x) = \tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\varphi}_{d_1\mathrm{v}}(x) \ \ (x = 0, 1, \ldots, x_{\max} - 1; \mathrm{v} \in \mathcal{V}\backslash\{d_1\}),\\
&\qquad\qquad \mathcal{H}_{d_1}\tilde{\varphi}_{d_1\mathrm{v}}(x_{\max}) \neq \tilde{\mathcal{E}}_{\mathrm{v}}\tilde{\varphi}_{d_1\mathrm{v}}(x_{\max}),
\end{aligned} \tag{8.53}
$$

$$
\phi_{d_1 n}(x) = \frac{-\sqrt{\alpha B'(x)}\,\tilde{\phi}_0(x)}{\sqrt{\check{\xi}_{d_1}(x)\check{\xi}_{d_1}(x+1)}}\,\mathrm{W}_C\big[\check{\xi}_{d_1}, \nu\check{P}_n\big](x), \tag{8.54}
$$

$$
\tilde{\varphi}_{d_1\mathrm{v}}(x) = \frac{-\sqrt{\alpha B'(x)}\,\tilde{\phi}_0(x)}{\sqrt{\check{\xi}_{d_1}(x)\check{\xi}_{d_1}(x+1)}}\,\mathrm{W}_C[\check{\xi}_{d_1}, \check{\xi}_{\mathrm{v}}](x). \tag{8.55}
$$

The $\rho_{d_1\mathrm{v}}$ term is necessary for the Casoratian expression for $\tilde{\varphi}_{d_1\mathrm{v}}(x)$ in (8.55) to hold at $x = x_{\max}$.

The non-classical orthogonal polynomial is extracted from the above Casoratian $\mathrm{W}_C\big[\check{\xi}_{d_1}, \nu\check{P}_n\big](x)$ by separating certain kinematical factors as will be shown in the next subsection, see (8.65). As in ordinary QM, the positivity of each virtual state vector is inherited by the next generation $\tilde{\varphi}_{d_1\mathrm{v}}$.

8.4 Multi-indexed (q-)Racah polynomials

Let us prepare a set of distinct positive integers which specify the degrees of virtual state vectors:

$$\mathcal{D} = \{d_1, d_2, \ldots, d_M\} \subseteq \mathcal{V}. \tag{8.56}$$

After M-step Darboux transformations, we arrive at the deformed Hamiltonian $\mathcal{H}_{\mathcal{D}}$, $\mathcal{A}_{\mathcal{D}}^{\dagger}$, $\mathcal{A}_{\mathcal{D}}$, and its eigenvectors $\{\phi_{\mathcal{D},n}(x)\}$:

$$\mathcal{H}_{\mathcal{D}} = \mathcal{A}_{\mathcal{D}}^{\dagger}\mathcal{A}_{\mathcal{D}}, \quad \mathcal{H}_{\mathcal{D}}\phi_{\mathcal{D}\,n}(x) = \mathcal{E}(n)\phi_{\mathcal{D}\,n}(x), \tag{8.57}$$

$$\phi_{\mathcal{D}\,n}(x) = \frac{(-1)^M\sqrt{\prod_{j=1}^{M}\alpha B'(x+j-1)}\,\tilde{\phi}_0(x)\,\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}, \nu\check{P}_n](x)}{\sqrt{\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}](x)\,\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}](x+1)}}, \tag{8.58}$$

$$\mathcal{A}_{\mathcal{D}} \stackrel{\text{def}}{=} \sqrt{B_{\mathcal{D}}(x)} - e^{\partial}\sqrt{D_{\mathcal{D}}(x)}, \quad \mathcal{A}_{\mathcal{D}}^{\dagger} = \sqrt{B_{\mathcal{D}}(x)} - \sqrt{D_{\mathcal{D}}(x)}\,e^{-\partial}, \tag{8.59}$$

with

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

The potential functions $B_{\mathcal{D}}(x)$ and $D_{\mathcal{D}}(x)$ are:

$$B_{\mathcal{D}}(x) \stackrel{\text{def}}{=} \alpha B'(x+M)\frac{\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}](x)}{\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}](x+1)}\,\frac{\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}, \nu](x+1)}{\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}, \nu](x)}, \tag{8.60}$$

$$D_{\mathcal{D}}(x) \stackrel{\text{def}}{=} \alpha D'(x)\frac{\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}](x+1)}{\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}](x)}\,\frac{\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}, \nu](x-1)}{\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}, \nu](x)}. \tag{8.61}$$

In order to extract the multi-indexed (q-)Racah polynomials, we need some auxiliary functions $\varphi(x;\boldsymbol{\lambda})$ and $\varphi_M(x;\boldsymbol{\lambda})$, $M \in \mathbb{Z}_{\geq 0}$:

$$\varphi(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \frac{\eta(x+1;\boldsymbol{\lambda}) - \eta(x;\boldsymbol{\lambda})}{\eta(1;\boldsymbol{\lambda})}, \tag{8.62}$$

$$\begin{aligned}\varphi_M(x;\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \prod_{1\leq j<k\leq M}\frac{\eta(x+k-1;\boldsymbol{\lambda}) - \eta(x+j-1;\boldsymbol{\lambda})}{\eta(k-j;\boldsymbol{\lambda})}\\ &= \prod_{1\leq j<k\leq M}\varphi\bigl(x+j-1;\boldsymbol{\lambda}+(k-j-1)\boldsymbol{\delta}\bigr),\end{aligned} \tag{8.63}$$

and $\varphi_0(x;\boldsymbol{\lambda}) = \varphi_1(x;\boldsymbol{\lambda}) = 1$. Two polynomials $\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})$ and $\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})$, to be called the *denominator polynomial* and the *multi-indexed orthogonal polynomial*, respectively, are extracted from the Casoratians as follows:

$$\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}](x;\boldsymbol{\lambda}) = \mathcal{C}_{\mathcal{D}}(\boldsymbol{\lambda})\varphi_M(x;\boldsymbol{\lambda})\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}), \tag{8.64}$$

$$\mathrm{W}_C[\check{\xi}_{d_1}, \ldots, \check{\xi}_{d_M}, \nu\check{P}_n](x;\boldsymbol{\lambda}) = \mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})\varphi_{M+1}(x;\boldsymbol{\lambda})\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})\nu(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}}), \tag{8.65}$$

$$\tilde{\boldsymbol{\delta}} \stackrel{\text{def}}{=} (0,0,1,1), \qquad \mathfrak{t}(\boldsymbol{\lambda}) + \beta\boldsymbol{\delta} = \mathfrak{t}(\boldsymbol{\lambda}+\beta\tilde{\boldsymbol{\delta}}) \quad (\forall\beta \in \mathbb{R}). \tag{8.66}$$

The constants $\mathcal{C}_\mathcal{D}(\boldsymbol{\lambda})$ and $\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})$ are specified later. The eigenvector (8.58) is rewritten as

$$\phi^{\text{gen}}_{\mathcal{D}\,n}(x;\boldsymbol{\lambda})=(-1)^M\kappa^{\frac14 M(M-1)}\frac{\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})}{\mathcal{C}_\mathcal{D}(\boldsymbol{\lambda})}\sqrt{\prod_{j=1}^{M}\alpha(\boldsymbol{\lambda})B'\bigl(0;\boldsymbol{\lambda}+(j-1)\tilde{\boldsymbol{\delta}}\bigr)}$$
$$\times\frac{\phi_0(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})}{\sqrt{\check{\Xi}_\mathcal{D}(x;\boldsymbol{\lambda})\check{\Xi}_\mathcal{D}(x+1;\boldsymbol{\lambda})}}\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}). \tag{8.67}$$

The multi-indexed orthogonal polynomial $\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})$ (8.65) has an expression

$$\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})=\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})^{-1}\varphi_{M+1}(x;\boldsymbol{\lambda})^{-1}$$
$$\times\begin{vmatrix}\check{\xi}_{d_1}(x_1)&\cdots&\check{\xi}_{d_M}(x_1)&r_1(x_1)\check{P}_n(x_1)\\ \check{\xi}_{d_1}(x_2)&\cdots&\check{\xi}_{d_M}(x_2)&r_2(x_2)\check{P}_n(x_2)\\ \vdots&\cdots&\vdots&\vdots\\ \check{\xi}_{d_1}(x_{M+1})&\cdots&\check{\xi}_{d_M}(x_{M+1})&r_{M+1}(x_{M+1})\check{P}_n(x_{M+1})\end{vmatrix}, \tag{8.68}$$

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

$$r_j\bigl(x+j-1;\boldsymbol{\lambda},M\bigr)$$
$$\stackrel{\text{def}}{=}\begin{cases}\dfrac{(x+a,x+b)_{j-1}(x+d-a+j,x+d-b+j)_{M+1-j}}{(d-a+1,d-b+1)_M} & :\text{R}\\ \dfrac{(aq^x,bq^x;q)_{j-1}(a^{-1}dq^{x+j},b^{-1}dq^{x+j};q)_{M+1-j}}{(abd^{-1}q^{-1})^{j-1}q^{Mx}(a^{-1}dq,b^{-1}dq;q)_M} & :q\text{R}\end{cases}. \tag{8.69}$$

One can show that $\check{\Xi}_\mathcal{D}$ (8.64) and $\check{P}_{\mathcal{D},n}$ (8.68) are indeed polynomials in η:

$$\check{\Xi}_\mathcal{D}(x;\boldsymbol{\lambda})\stackrel{\text{def}}{=}\Xi_\mathcal{D}\bigl(\eta(x;\boldsymbol{\lambda}+(M-1)\tilde{\boldsymbol{\delta}});\boldsymbol{\lambda}\bigr),\quad \check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})\stackrel{\text{def}}{=}P_{\mathcal{D},n}\bigl(\eta(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}});\boldsymbol{\lambda}\bigr), \tag{8.70}$$

and their degrees are generically $\ell_\mathcal{D}$ and $\ell_\mathcal{D}+n$, respectively, with (see (2.66)):

$$\ell_\mathcal{D}\stackrel{\text{def}}{=}\sum_{j=1}^{M}d_j-\tfrac12 M(M-1). \tag{8.71}$$

The involution properties (8.15) of these polynomials are the consequence of those of the basic polynomials $\check{P}_n(x)$ and $\check{\xi}_{d_j}(x)$. We adopt the standard normalisation for $\check{\Xi}_\mathcal{D}$ and $\check{P}_{\mathcal{D},n}$: $\check{\Xi}_\mathcal{D}(0;\boldsymbol{\lambda})=1$, $\check{P}_{\mathcal{D},n}(0;\boldsymbol{\lambda})=1$, which determine the constants $\mathcal{C}_\mathcal{D}(\boldsymbol{\lambda})$ and $\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})$,

$$\mathcal{C}_\mathcal{D}(\boldsymbol{\lambda})\stackrel{\text{def}}{=}\frac{1}{\varphi_M(0;\boldsymbol{\lambda})}\prod_{1\le j<k\le M}\frac{\tilde{\mathcal{E}}_{d_j}(\boldsymbol{\lambda})-\tilde{\mathcal{E}}_{d_k}(\boldsymbol{\lambda})}{\alpha(\boldsymbol{\lambda})B'(j-1;\boldsymbol{\lambda})}, \tag{8.72}$$

$$\mathcal{C}_{\mathcal{D},n}(\boldsymbol{\lambda})\stackrel{\text{def}}{=}(-1)^M\mathcal{C}_\mathcal{D}(\boldsymbol{\lambda})\tilde{d}_{\mathcal{D},n}(\boldsymbol{\lambda})^2,\ \tilde{d}_{\mathcal{D},n}(\boldsymbol{\lambda})^2\stackrel{\text{def}}{=}\frac{\varphi_M(0;\boldsymbol{\lambda})}{\varphi_{M+1}(0;\boldsymbol{\lambda})}\prod_{j=1}^{M}\frac{\mathcal{E}(n;\boldsymbol{\lambda})-\tilde{\mathcal{E}}_{d_j}(\boldsymbol{\lambda})}{\alpha(\boldsymbol{\lambda})B'(j-1;\boldsymbol{\lambda})}. \tag{8.73}$$

The expression for $\tilde{d}^2_{\mathcal{D},n}$ shows the necessity of the negative virtual state energies $\{\tilde{\mathcal{E}}_{d_j} < 0\}$. The lowest degree multi-indexed orthogonal polynomial $\check{P}_{\mathcal{D},0}(x;\boldsymbol{\lambda})$ is related to $\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})$ by the parameter shift $\boldsymbol{\lambda} \to \boldsymbol{\lambda} + \boldsymbol{\delta}$:

$$\check{P}_{\mathcal{D},0}(x;\boldsymbol{\lambda}) = \check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta}). \tag{8.74}$$

The potential functions $B_{\mathcal{D}}$ and $D_{\mathcal{D}}$ (8.60)–(8.61) can be expressed neatly in terms of the denominator polynomial:

$$B_{\mathcal{D}}(x;\boldsymbol{\lambda}) = B(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\,\frac{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}\frac{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})}, \tag{8.75}$$

$$D_{\mathcal{D}}(x;\boldsymbol{\lambda}) = D(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\,\frac{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})}\frac{\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})}. \tag{8.76}$$

The groundstate eigenvector $\phi_{\mathcal{D}\,0}$ is expressed by $\phi_0(x)$ and $\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})$:

$$\begin{aligned}
\phi_{\mathcal{D}\,0}(x;\boldsymbol{\lambda}) &= \sqrt{\prod_{y=0}^{x-1}\frac{B_{\mathcal{D}}(y)}{D_{\mathcal{D}}(y+1)}}\\
&= \phi_0(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\sqrt{\frac{\check{\Xi}_{\mathcal{D}}(1;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}}\,\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})\\
&= \psi_{\mathcal{D}}(x;\boldsymbol{\lambda})\check{P}_{\mathcal{D},0}(x;\boldsymbol{\lambda}) \propto \phi^{\text{gen}}_{\mathcal{D}\,0}(x;\boldsymbol{\lambda}),
\end{aligned} \tag{8.77}$$

$$\psi_{\mathcal{D}}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \sqrt{\check{\Xi}_{\mathcal{D}}(1;\boldsymbol{\lambda})}\,\frac{\phi_0(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})}{\sqrt{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})\,\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}}, \quad \psi_{\mathcal{D}}(0;\boldsymbol{\lambda}) = 1. \tag{8.78}$$

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

$$\phi_{\mathcal{D}\,n}(x;\boldsymbol{\lambda}) \stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x;\boldsymbol{\lambda})\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}) \propto \phi^{\text{gen}}_{\mathcal{D}\,n}(x;\boldsymbol{\lambda}), \quad \phi_{\mathcal{D}\,n}(0;\boldsymbol{\lambda}) = 1, \tag{8.79}$$

$$\sum_{x=0}^{x_{\max}}\frac{\psi_{\mathcal{D}}(x;\boldsymbol{\lambda})^2}{\check{\Xi}_{\mathcal{D}}(1;\boldsymbol{\lambda})}\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda})\check{P}_{\mathcal{D},m}(x;\boldsymbol{\lambda}) = \frac{\delta_{nm}}{d_n(\boldsymbol{\lambda})^2\tilde{d}_{\mathcal{D},n}(\boldsymbol{\lambda})^2} \quad (n,m = 0,\ldots,n_{\max}). \tag{8.80}$$

The similarity transformed Hamiltonian is

$$\begin{aligned}
\widetilde{\mathcal{H}}_{\mathcal{D}}(\boldsymbol{\lambda}) &\stackrel{\text{def}}{=} \psi_{\mathcal{D}}(x;\boldsymbol{\lambda})^{-1}\circ\mathcal{H}_{\mathcal{D}}(\boldsymbol{\lambda})\circ\psi_{\mathcal{D}}(x;\boldsymbol{\lambda})\\
&= B(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\,\frac{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}\biggl(\frac{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})} - e^{\partial}\biggr)\\
&\quad + D(x;\boldsymbol{\lambda}+M\tilde{\boldsymbol{\delta}})\,\frac{\check{\Xi}_{\mathcal{D}}(x+1;\boldsymbol{\lambda})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda})}\biggl(\frac{\check{\Xi}_{\mathcal{D}}(x-1;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\Xi}_{\mathcal{D}}(x;\boldsymbol{\lambda}+\boldsymbol{\delta})} - e^{-\partial}\biggr),
\end{aligned} \tag{8.81}$$

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

$$\widetilde{\mathcal{H}}_{\mathcal{D}}(\boldsymbol{\lambda})\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}) = \mathcal{E}(n;\boldsymbol{\lambda})\check{P}_{\mathcal{D},n}(x;\boldsymbol{\lambda}). \tag{8.82}$$

It should be stressed that these multi-indexed orthogonal polynomials in simple QM provide infinitely many examples of exactly solvable birth and death processes [4, 16, 15].

8.4.1 Explicit examples of multi-indexed (q-)Racah polynomials

We present a simple and explicit example of multi-indexed orthogonal polynomials of the Racah and q-Racah systems corresponding to $\mathcal{D} = \{\ell\}$, ($\ell \geq 1$, $M = 1$). In this case $\check{\Xi}_\ell(x;\boldsymbol{\lambda}) \equiv \check{\xi}_\ell(x;\boldsymbol{\lambda})$ (8.36). The 1-indexed (q-)Racah polynomials are obtained by evaluating (8.68) at $M = 1$. They are a degree $\ell + n$ polynomial in $\eta = x(x+d+1)$ (R) and $\eta = (q^{-x}-1)(1-dq^{x+1})$ (qR):

$$
\begin{aligned}
\text{R: } \check{P}_{\ell,n}(x;\boldsymbol{\lambda}) &= \frac{c}{(2x+d+1)\big(\mathcal{E}(n;\boldsymbol{\lambda}) - \tilde{\mathcal{E}}_\ell(\boldsymbol{\lambda})\big)} \\
&\quad\times \Big(\check{\xi}_\ell(x;\boldsymbol{\lambda})(x+a)(x+b)\check{P}_n(x+1;\boldsymbol{\lambda}) \\
&\qquad - \check{\xi}_\ell(x+1;\boldsymbol{\lambda})(x+d-a+1)(x+d-b+1)\check{P}_n(x;\boldsymbol{\lambda})\Big), \\
q\text{R: } \check{P}_{\ell,n}(x;\boldsymbol{\lambda}) &= \frac{1-c}{(1-dq^{2x+1})\big(\mathcal{E}(n;\boldsymbol{\lambda}) - \tilde{\mathcal{E}}_\ell(\boldsymbol{\lambda})\big)} \\
&\quad\times \Big(\check{\xi}_\ell(x;\boldsymbol{\lambda})(aq^x, bq^x;q)\check{P}_n(x+1;\boldsymbol{\lambda}) \\
&\qquad - \check{\xi}_\ell(x+1;\boldsymbol{\lambda})abd^{-1}q^{-1}(a^{-1}dq^{x+1}, b^{-1}dq^{x+1};q)\check{P}_n(x;\boldsymbol{\lambda})\Big).
\end{aligned}
$$

They satisfy a second order difference equation:

$$
\begin{aligned}
&\widetilde{\mathcal{H}}_\ell(\boldsymbol{\lambda})\check{P}_{\ell,n}(x;\boldsymbol{\lambda}) = \mathcal{E}(n;\boldsymbol{\lambda})\check{P}_{\ell,n}(x;\boldsymbol{\lambda}), \\
&\widetilde{\mathcal{H}}_\ell(\boldsymbol{\lambda}) = B(x;\boldsymbol{\lambda}+\tilde{\boldsymbol{\delta}})\,\frac{\check{\xi}_\ell(x;\boldsymbol{\lambda})}{\check{\xi}_\ell(x+1;\boldsymbol{\lambda})}\bigg(\frac{\check{\xi}_\ell(x+1;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\xi}_\ell(x;\boldsymbol{\lambda}+\boldsymbol{\delta})} - e^{\partial}\bigg) \\
&\qquad + D(x;\boldsymbol{\lambda}+\tilde{\boldsymbol{\delta}})\,\frac{\check{\xi}_\ell(x+1;\boldsymbol{\lambda})}{\check{\xi}_\ell(x;\boldsymbol{\lambda})}\bigg(\frac{\check{\xi}_\ell(x-1;\boldsymbol{\lambda}+\boldsymbol{\delta})}{\check{\xi}_\ell(x;\boldsymbol{\lambda}+\boldsymbol{\delta})} - e^{-\partial}\bigg), \\
&\mathcal{E}(n;\boldsymbol{\lambda}) = \begin{cases} n(n+\tilde{d}), & \text{R}, \\ (q^{-n}-1)(1-\tilde{d}q^n), & q\text{R}. \end{cases}
\end{aligned}
$$

8.5 Krein-Adler polynomials

The Krein-Adler polynomials for the systems in simplest QM or discrete QM with real shifts have been presented in [8]. Most formulas look quite similar to those of the multi-indexed polynomials in §8.4, (8.56)–(8.61), (8.67)–(8.82). Now $\mathcal{D}$ (8.56) denotes the degrees of eigenpolynomials to be used as seed solutions and it has to satisfy the same conditions as (2.49). The virtual state polynomial $\check{\xi}_{d_j}(x)$ is replaced by the eigenpolynomial $\check{P}_{d_j}(x)$.

9 Summary and comments

Amongst many achievements of the quantum mechanical reformulation of the theory of classical orthogonal polynomials, we have reported on the subject of non-classical orthogonal polynomials, which satisfy second order differential or difference equations. They form a complete set of orthogonal vectors in a certain Hilbert space in spite of a 'hole' in their degrees. For more details of the multi-indexed Laguerre and Jacobi polynomials, see [27] and [35] for (q-) Racah systems.

A Symbols, Definitions & Formulas

∘ shifted factorial (Pochhammer symbol) $(a)_n$:

$$(a)_n \stackrel{\text{def}}{=} \prod_{k=1}^{n}(a+k-1) = a(a+1)\cdots(a+n-1) = \frac{\Gamma(a+n)}{\Gamma(a)}. \tag{A.1}$$

∘ q-shifted factorial (q-Pochhammer symbol) $(a\,;q)_n$:

$$(a\,;q)_n \stackrel{\text{def}}{=} \prod_{k=1}^{n}(1-aq^{k-1}) = (1-a)(1-aq)\cdots(1-aq^{n-1}) = \frac{(a\,;q)_\infty}{(aq^n\,;q)_\infty}. \tag{A.2}$$

∘ hypergeometric function ${}_rF_s$:

$${}_rF_s\Bigl(\begin{matrix}a_1,\,\cdots,a_r\\ b_1,\,\cdots,b_s\end{matrix}\Bigm| z\Bigr) \stackrel{\text{def}}{=} \sum_{n=0}^{\infty}\frac{(a_1,\,\cdots,a_r)_n}{(b_1,\,\cdots,b_s)_n}\frac{z^n}{n!}\,, \tag{A.3}$$

where $(a_1,\,\cdots,a_r)_n \stackrel{\text{def}}{=} \prod_{j=1}^{r}(a_j)_n = (a_1)_n\cdots(a_r)_n$.
∘ q-hypergeometric series (the basic hypergeometric series) ${}_r\phi_s$:

$${}_r\phi_s\Bigl(\begin{matrix}a_1,\,\cdots,a_r\\ b_1,\,\cdots,b_s\end{matrix}\Bigm| q\,;z\Bigr) \stackrel{\text{def}}{=} \sum_{n=0}^{\infty}\frac{(a_1,\,\cdots,a_r\,;q)_n}{(b_1,\,\cdots,b_s\,;q)_n}(-1)^{(1+s-r)n}q^{(1+s-r)n(n-1)/2}\frac{z^n}{(q\,;q)_n}\,, \tag{A.4}$$

where $(a_1,\,\cdots,a_r\,;q)_n \stackrel{\text{def}}{=} \prod_{j=1}^{r}(a_j\,;q)_n = (a_1\,;q)_n\cdots(a_r\,;q)_n$.
∘ differential equations

$$\text{H, Hermite}:\quad \partial_x^2H_n(x) - 2x\partial_xH_n(x) + 2nH_n(x) = 0, \tag{A.5}$$

$$\text{L, Laguerre}:\quad x\partial_x^2L_n^{(\alpha)}(x) + (\alpha+1-x)\partial_xL_n^{(\alpha)}(x) + nL_n^{(\alpha)}(x) = 0, \tag{A.6}$$

$$\begin{aligned}\text{J, Jacobi}:\quad &(1-x^2)\partial_x^2P_n^{(\alpha,\beta)}(x) + \bigl(\beta-\alpha-(\alpha+\beta+2)x\bigr)\partial_xP_n^{(\alpha,\beta)}(x)\\ &\qquad + n(n+\alpha+\beta+1)P_n^{(\alpha,\beta)}(x) = 0.\end{aligned} \tag{A.7}$$

∘ Rodrigues formulas

$$\text{H}:\quad H_n(x) = (-1)^ne^{x^2}\Bigl(\frac{d}{dx}\Bigr)^ne^{-x^2}, \tag{A.8}$$

$$\text{L}:\quad L_n^{(\alpha)}(x) = \frac{1}{n!}\frac{1}{e^{-x}x^\alpha}\Bigl(\frac{d}{dx}\Bigr)^n\bigl(e^{-x}x^{n+\alpha}\bigr), \tag{A.9}$$

$$\text{J}:\quad P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^nn!}\frac{1}{(1-x)^\alpha(1+x)^\beta}\Bigl(\frac{d}{dx}\Bigr)^n\bigl((1-x)^{n+\alpha}(1+x)^{n+\beta}\bigr). \tag{A.10}$$

B Three Term Recurrence Relations

Any orthogonal polynomial starting from degree 0 constant satisfies *three term recurrence relations*

$$\begin{aligned}\eta Q_n(\eta) &= A_n Q_{n+1}(\eta) + B_n Q_n(\eta) + C_n Q_{n-1}(\eta), \\ Q_0(\eta) &= \text{constant}, \quad Q_{-1}(\eta) = 0.\end{aligned} \tag{B.1}$$

Here real constants A_n, B_n and C_n depend on the normalisation of the polynomial. Three term recurrence relations are a simple consequence of the orthogonality.

$$(\!(Q_n, Q_m)\!) \stackrel{\text{def}}{=} \int W(\eta) Q_n(\eta) Q_m(\eta) d\eta = 0, \quad n \neq m,$$

in which $W(\eta)$ is the orthogonality weight function. For its positive definiteness $A_{n-1}C_n > 0$ is necessary. Since $\eta Q_n(\eta)$ is a degree $n+1$ polynomial, it is expressed as

$$\eta Q_n(\eta) = A_n Q_{n+1}(\eta) + B_n Q_n(\eta) + C_n Q_{n-1}(\eta) + D_n(\eta),$$

in which $D_n(\eta)$ is a degree k $(0 \leq k < n-1)$ polynomial, if it is not vanishing. This means $(\!(Q_k, D_n)\!) \neq 0$ but this leads to a contradiction as $(\!(Q_k, \eta Q_n)\!) = (\!(\eta Q_k, Q_n)\!) = 0$ and $(\!(Q_k, Q_{n+1})\!) = (\!(Q_k, Q_n)\!) = (\!(Q_k, Q_{n-1})\!) = 0$ require $D_n(\eta) \equiv 0$. Conversely, any polynomial starting from degree 0 and satisfying three term recurrence relations is an orthogonal polynomial (Favard).

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