

WILSON - QUANTUM SYSTEM WITH EXPONENTIAL HAMILTONIAN AND ENERGY SPECTRUM

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Abstract

In this paper, we obtain another new quantum system (named Wilson Quantum System) associated with the Wilson orthogonal polynomial. We derived the potential function of the quantum system using any of the four proposed formulae which was possible using the matrix elements of the potential function and the basis element of the configuration space.

Keywords: Kinetic operator matrix elements, Hamiltonian matrix element, Potential function matrix elements, Hermite polynomial, Basis elements, Wilson Orthogonal Polynomial, PACS numbers: 03.65.Ge, 03.65.Fd, 34.80.Bm, 03.65.Ca

1. Introduction

Using our recent reformulation of quantum mechanics without potential function, we get another quantum system associated with the Wilson orthogonal polynomial. In appendix B (or in [1-6]), we give precise theoretical framework for this reformulation, with all physical parameters associated with any quantum systems are defined. And the aim of this recent reformulation is to enlarge the class of solvable quantum systems. It has been observed there are quantum systems that could be described analytically but their potential function are either difficult to specify or impossible to realize analytically. For instance, the potential functions might be non-analytic, nonlocal, energy dependent, or the corresponding differential wave equation is higher than second order and so on.

In order to establish a correspondence with the conventional formulation of quantum mechanics, procedures for reconstructing the potential function numerically in this new reformulation were formulated as will be shown later. In using these formulas, once the potential matrix element of the potential function is gotten and with the basis element; the potential function can be derived using any of the four formulas. Although, each of the four formulas gives different degree of accuracy.

Here, using our reformulation, we derived a new quantum system which we called the **Wilson Quantum System**. In section 2, we show how the energy spectrum, scattering phase shift, and wavefunction are derived. In section 3, we obtained the potential matrix elements of the new Wilson quantum system; and finally, a plot of the potential function was given.

2. The Wilson Quantum System

As shown in [Appendix A8], the asymptotic ($n \rightarrow \infty$) of the Wilson orthogonal polynomial is

$$\mathcal{W}_n^{\mu, \nu}(y^2; v; a, b) \approx \frac{2}{n} \Gamma(\mu + \nu) \Gamma(a + b) |A(iy)| \cos\{2y \ln(n) - \arg[A(iy)]\} + O(n^{-1}) \quad (1)$$

where $A(iy) = \Gamma(2iy) / \Gamma(\mu + iy) \Gamma(\nu + iy) \Gamma(a + iy) \Gamma(b + iy)$, the scattering amplitude. The scattering phase shift for any associated physical system is

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$$\delta(\varepsilon) = \arg[\Gamma(2iy)/\Gamma(\mu+iy)\Gamma(\nu+iy)\Gamma(a+iy)\Gamma(b+iy)] \quad (2)$$

where $y = \varepsilon(E)$ such that $y \geq 0$. For this quantum system, we choose $\varepsilon^2 = \ln(1+k^2/\lambda^2)$, where $E = \frac{1}{2}k^2$ and λ^{-1} is the length scale of the system in atomic units $\hbar = m = 1$, then $y = \sqrt{\ln(1+k^2/\lambda^2)}$. If all the parameters of the Wilson polynomial are positive, there will be no bound states (that is continuous scattering states) while if $\mu < 0$ and $\mu + \nu$, $\mu + a$, $\mu + b$ are positive then there co-exist the continuum scattering states and N bound states, where N is the largest integer less than or equal to $-\mu$. Now from the zero of the scattering amplitude $A(\varepsilon)$ dictates that the bound states occur at energies $\{\varepsilon_m\}_{m=0}^N$ such that $iy = -(m + \mu)$; giving the bound states energy spectrum as

$$E_m = \frac{\lambda^2}{2} [e^{-(m+\mu)^2} - 1] \quad (3)$$

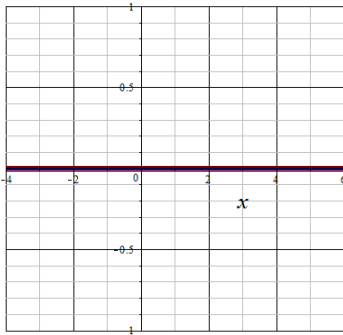


FIG.1. The bound states energy spectrum (6) for the new quantum system with physical parameters: $\lambda = 0.2$, $\mu = -0.7$, and $m = 0, 1, 2, \dots$

Here, as m increases, the gaps between the bound states energy level becomes small, and hence shows the discreteness. The happens as m goes from 4 due to exponential expression in (3)

Now, the total wavefunction for the continuous energy ε and discrete energy ε_m will also be given as

$$\psi_m(E, x) = \sqrt{\rho^\mu(\varepsilon)} \sum_{n=0}^{\infty} W_n^\mu(\varepsilon^2; \nu, a, b) \phi_n(x) + \sqrt{\rho_m^N(\varepsilon)} \sum_{n=0}^N W_n^\mu(-(m+\mu)^2; \nu, a, b) \phi_n(x) \quad (4)$$

where $\rho^\mu(\varepsilon)$ and $\rho_m^N(\varepsilon)$ are the continuous and discrete normalized weight function from the augmented continuous orthogonality relation of the Wilson polynomial (See appendix B) $W_n^\mu(\varepsilon^2; \nu, a, b)$ is the Wilson orthogonal polynomial. The basis function is chosen in one dimensional configuration space with coordinate $-\infty < x < \infty$ as $\phi_n(x) = [\pi 2^{n+m} n!]^{-1/2} e^{-x^2/2} H_n(\lambda x)$, where $H_n(z)$ is the Hermite Polynomial of degree n in z . It can be seen that Equation (4) will give a different wave function different from that of equation (7) in [2]

because the energy parameter is $\varepsilon^2 = \ln(1+k^2/\lambda^2)$ as compared to $\varepsilon = \lambda/k$ in [2]

3. Potential Function of Wilson Quantum System

Since the Hamiltonian, $H = T + V$, is sum of the kinetic energy operator T and the potential function V . Therefore, we have $V = H - T$. Now to get the potential matrix elements in the basis $\{\phi_n(x)\}$, we need first to get the matrix elements of the Hamiltonian operator H and kinetic energy operator both in this basis. Since $T = -\frac{1}{2} \frac{d^2}{dx^2}$, in one dimension coordinate x , and also given as $T = -\frac{1}{2} \frac{d^2}{dr^2} + \frac{1(1+1)}{2r^2}$, in three dimensions with spherical symmetry and radial coordinate r (l is the angular momentum quantum number), its matrix representation could be easily derived by operating T , the kinetic operator, on the basis elements $\{\phi_n(x)\}$.

Since the total wave function of the system is $\Psi(t, x) = e^{-iEt/\hbar} \psi(E, x)$; so we have $H\Psi = i\hbar \frac{\partial}{\partial t} \Psi = E\Psi$. Hence, we can therefore write the wave operation as

$$H|\psi\rangle = E|\psi\rangle \quad (5)$$

H is the Hamiltonian operator and E is the energy of the quantum system. Easily (5) is same as

$$\hat{H}|P\rangle = E\Omega|P\rangle \quad (6)$$

where \hat{H} is the matrix representation of the Hamiltonian operator in the basis $\{\phi_n(x)\}$ and Ω is the overlap matrix of the basis elements, $\Omega_{n,m} = \langle \phi_n | \phi_m \rangle$ (i.e., matrix representation of the identity). Also, the energy polynomial satisfies the three term recursion relation which can be written in matrix form as $\Sigma|P\rangle = \varepsilon|P\rangle$, where $\Sigma_{n,m} = a_n^\mu \delta_{n,m} + b_{n-1}^\mu \delta_{n,m+1} + b_n^\mu \delta_{n,m-1}$, a tridiagonal symmetric matrix. Therefore, the wave equation (6) is equivalent to three term recursion relation of the energy polynomials $\{P_n^\mu(\varepsilon)\}$ and implies that the wave operator matrix $J = \hat{H} - E\Omega$ will be tridiagonal and symmetric. By this, the matrix representation of Hamiltonian operator can be easily gotten from the three term recursion relation of the energy polynomial and the potential matrix elements of the potential function are easily obtained too.

Since, we always require the matrix wave operator $J = V + T - E\Omega$ be tridiagonal; but if Ω is non-tridiagonal (i.e., the basis elements are neither orthogonal nor tri-thogonal), then the kinetic energy matrix T will have corresponding energy – dependent components to cancel out the non tridiagonal components. After this, if there still exist further non-tridiagonal components then they will be eliminated by the counter components in V . From the potential function matrix elements $\{V_{mm}\}_{n,m=0}^{N-1}$, which is a $N \times N$ matrix elements of the potential function $V(x)$ in a given a basis set $\{\phi_n(x)\}$ such that $\langle \phi_n^\circ | \phi_m \rangle = \langle \phi_n | \phi_m^\circ \rangle = \Omega_{nm}$, where $\{\phi_n^\circ(x)\}$ is the conjugate basis set, and $V_{mm} = \langle \phi_n | V | \phi_m \rangle$ the potential function $V(x)$ can be calculated using any of the following methods:

3.1.1 First Method

Using the Dirac notation,

$$\langle x | V | x' \rangle = V(x) \delta(x - x') \quad (7)$$

where $\delta(x - x') = \langle x | x' \rangle$, x is the configuration space coordinate, V is the Hermitian operator of the real potential energy, and $V(x)$ is the potential function. Also, we demand $\langle x | \phi_n^\circ \rangle = \phi_n^\circ(x)$ and $\langle x | \phi_n \rangle = \phi_n(x)$. By the completeness of the basis set

$\sum_n |\phi_n^\circ\rangle \langle \phi_n| = \sum_n |\phi_n\rangle \langle \phi_n^\circ| = I$, the left hand side of (7) can be written as

$$\begin{aligned} \sum_{n,m=0}^{\infty} \langle x | \phi_n^\circ \rangle \langle \phi_n | V | \phi_m \rangle \langle \phi_m^\circ | x' \rangle &= \sum_{n,m=0}^{\infty} \phi_n^\circ(x) V_{nm} \phi_m^\circ(x') \\ &= \frac{1}{2} \sum_{n,m=0}^{\infty} V_{nm} [\phi_n^\circ(x) \phi_m^\circ(x') + \phi_m^\circ(x) \phi_n^\circ(x')] \end{aligned} \quad (8)$$

and the right hand side becomes

$$V(x) \sum_{n=0}^{\infty} \langle x | \frac{|\phi_n\rangle \langle \phi_n^\circ| + |\phi_n^\circ\rangle \langle \phi_n|}{2} | x' \rangle = \frac{1}{2} V(x) \sum_{n=0}^{\infty} [\phi_n(x) \phi_n^\circ(x') + \phi_n^\circ(x) \phi_n(x')] \quad (9)$$

so approximately, we can write

$$V(x) \sum_{n=0}^{N-1} [\phi_n(x) \phi_n^\circ(x') + \phi_n^\circ(x) \phi_n(x')] \cong \sum_{n,m=0}^{N-1} V_{nm} [\phi_n^\circ(x) \phi_m^\circ(x') + \phi_m^\circ(x) \phi_n^\circ(x')] \quad (10)$$

where N is some large enough natural integer number. Taking $x = x'$, gives

$$V(x) \cong \frac{\sum_{n,m=0}^{N-1} V_{nm} \phi_n^\circ(x) \phi_m^\circ(x)}{\sum_{n=0}^{N-1} \phi_n(x) \phi_n^\circ(x)} \quad (11)$$

This is a valid approximation for finite N . Note as $N \rightarrow \infty$, (11) blows up because

$$\sum_{n=0}^{\infty} \phi_n(x) \phi_n^\circ(x') = \sum_{n=0}^{\infty} \phi_n^\circ(x) \phi_n(x') = \delta(x - x')$$

3.1.2 Second Method

Using the completeness of (or identity in) configuration space $\int |x'\rangle \langle x'| dx' = 1$, the left hand side of equation (7), can be written as

$$\langle x | V | \phi_n \rangle = \int \langle x | V | x' \rangle \langle x' | \phi_n \rangle dx' = V(x) \phi_n(x') \quad (12)$$

Also by the completeness of the basis set, we can still have

$$\langle x|V|\phi_n\rangle = \sum_{m=0}^{\infty} \langle x|\phi_m^0\rangle \langle \phi_m|V|\phi_n\rangle = \sum_{m=0}^{\infty} \phi_m^0(x) V_{nm} \cong \sum_{m=0}^{N-1} \phi_m^0(x) V_{nm} \quad (13)$$

equating both sides ($x = x'$),

$$V(x) \cong \sum_{m=0}^{N-1} \frac{\phi_m^0(x)}{\phi_n(x)} V_{nm}, \quad n = 0, 1, \dots, N-1 \quad (14)$$

Here only information in one column of the potential matrix (or row, since its symmetric) to determine the potential function. Specifically, one can have $n = 0$, then

$$V(x) \cong \sum_{m=0}^{N-1} \frac{\phi_m^0(x)}{\phi_0(x)} V_{m,0} \quad (15)$$

3.6.3 Third Method

by completeness of the basis enables us to integrate (3.66) over x' , Then

$$\begin{aligned} V(x) &= \int \langle x|V|x'\rangle dx' = \sum_{n,m=0}^{\infty} \int \langle x|\phi_n^0\rangle \langle \phi_n|V|\phi_m\rangle \langle \phi_m^0|x'\rangle dx' = \sum_{n,m=0}^{\infty} \int \phi_n^0(x) V_{nm} \phi_m^0(x') dx' \\ &\cong \sum_{n,m=0}^{N-1} V_{nm} \phi_n^0(x) \int \phi_m^0(x') dx' \end{aligned} \quad (16)$$

To evaluate the integral in (16), we use the **Gauss quadrature** compatible with the L^2 space spanned by $\{\phi_m^0(x)\}$, which gives

$$\int \phi_m^0(x') dx' = \int \rho(x') \frac{\phi_m^0(x')}{\rho(x')} dx' = \sum_{k=0}^{K-1} \omega_k \frac{\phi_m^0(\tau_k)}{\rho(\tau_k)} = \sum_{k=0}^{K-1} \omega_k^d \phi_m^0(\tau_k) \quad (17)$$

where $\omega_k^d = \frac{\omega_k}{\rho(\tau_k)}$ are element of the weight derivative $\{\omega_k^d\}_{k=0}^{K-1}$. $K \geq N$ is a some

large integer and $\{\tau_k, \omega_k\}_{k=0}^{K-1}$ are the abscissa and numerical weights of the quadrature. Therefore (16) becomes

$$V(x) \cong \sum_{n,m=0}^{N-1} \left[\sum_{k=0}^{K-1} V_{nm} \omega_k^d \phi_m^0(\tau_k) \right] \phi_n^0(x) \cong \sum_{n=0}^{N-1} U_n \phi_n^0(x) \quad (18)$$

where $U_n = \sum_{m=0}^{N-1} \sum_{k=0}^{K-1} V_{nm} \omega_k^d \phi_m^0(\tau_k)$.

3.6.4 Fourth Method

Here, we give an idea of how **Gauss Quadrature (also applicable in the fourth method and an outline of it)** is used. Specifically, when the element of the basis set is Hermite function which we used in calculating the potential function of the Wilson quantum system

Let $\{p_n(x)\}_{n=0}^{\infty}$ be a complete set of orthonormal polynomials over some interval in configuration space $[x_-, x_+]$ with $\rho(x)$ being the normalized weight function. Then the polynomials satisfy the orthogonality

$$\int_{x_-}^{x_+} \rho(x) p_n(x) p_m(x) dx = \delta_{nm} \quad (19)$$

and the symmetric three term recursion relation

$$xp_n(x) = a_n p_n(x) + b_{n-1} p_{n-1}(x) + b_n p_{n+1}(x) \quad n = 1, 2, 3, \dots, \quad (20)$$

with $b_n \neq 0$, $p_0(x) = 1$, and $p_1(x) = \alpha x + \beta$. If $\alpha = b_0^{-1}$ and $\beta = -a_0 b_0^{-1}$, then we call this the ‘‘polynomials of the first kind.

From (20), we have the $N \times N$ tridiagonal symmetric matrix

$$J = \begin{pmatrix} a_0 & b_0 & 0 & \dots & 0 \\ b_0 & a_1 & b_1 & \dots & 0 \\ 0 & b_1 & a_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & b_{N,N-1} & a_{N,N-1} \end{pmatrix} \quad (21)$$

and let $\{\tau_n\}_{n=0}^{N-1}$ be its distinct eigenvalues with corresponding normalized eigenvectors $\{\Lambda_{nm}\}_{m=0}^{N-1}$ and of the zero of the polynomial of the first kind $p_N(x)$. Its can be easily shown that

$$p_m(\tau_n) = \Lambda_{mm} / \Lambda_{0n} \quad n = 0, 1, \dots, m-1$$

$$m = 1, 2, \dots, N-1. \quad (22)$$

Gauss Quadrature Integral Approximation

If $f(x)$ is integrable in the interval $x \in [x_-, x_+]$ with respect to the measure $\rho(x)dx$ then,

$$\int_{x_-}^{x_+} \rho(x) f(x) dx \cong \sum_{n=0}^{N-1} \omega_n f(\tau_n) \quad (23)$$

where $\{\omega_n\}_{n=0}^{N-1}$ are referred to as the “numerical weights” associated with the quadrature, which could be computed by

$$\omega_n = \Lambda_{0n}^2 \quad \text{or}$$

$$\omega_n = \frac{\prod_{m=0}^{N-2} \tau_n - \theta_m^0}{\prod_{\substack{k=0 \\ k \neq n}}^{N-1} \tau_n - \tau_k} \quad (24)$$

where $\{\theta_m^0\}_{m=0}^{N-2}$ is the set of eigenvalues of the sub-matrix J obtained from (21) by deleting the top (zeroth) row and left (zeroth) column. As an example, to evaluate the integral in (17), where the Hermite basis is used. Let the polynomial variable x be related to the configuration space coordinate r by $x = x(\lambda r)$ where λ is a length scale parameter.

Since the basis element are orthonormal in the configuration space, so we write as $\phi_n(r) = \sqrt{\gamma(x)\rho(x)} p_n(x)$, where $\gamma(x)$ is some proper function. Using the integral measure $\lambda \int \dots dr = \int \dots (x')^{-1} dx$ where $x' = \lambda^{-1} (dx/dr)$ and the orthogonality (19), we have

$$\phi_n^0(r) = [x'(x)/\gamma(x)] \phi_n(r) = x'(x) \sqrt{\gamma(x)/\rho(x)} p_n(x) \quad (25)$$

For the Hermite basis element $\phi_n(x) = [\sqrt{\pi} 2^n n!]^{-1/2} e^{-\lambda^2 x^2/2} H_n(\lambda x)$ in 1D: $x' = 1$, $p_n(x) = [2^n n!]^{-1/2} H_n(x)$,

$$\rho(x) = \pi^{-1/2} e^{-x^2}, \quad \text{and} \quad \gamma(x) = 1$$

So (17) can be written as

$$\lambda \int \phi_n^0 dr = \int \rho(x) \frac{p_m(x)}{\sqrt{\gamma(x)\rho(x)}} dx \cong \sum_{n=0}^{N-1} \omega_n \frac{p_m(\tau_n)}{\sqrt{\gamma(\tau_n)\rho(\tau_n)}} = \sum_{n=0}^{N-1} \frac{\Lambda_{mm}\Lambda_{0n}}{\sqrt{\gamma(\tau_n)\rho(\tau_n)}} = (\Lambda W \Lambda^T)_{m0} \quad (26)$$

where W is $N \times N$ diagonal matrix with elements $w_{mm} = 1/\sqrt{\gamma(\tau_n)\rho(\tau_n)}$.

So (26) can be written as

$$V(r) \cong \sum_{n,m=0}^{N-1} \phi_n^0(r) V_{nm} (\Lambda W \Lambda^T)_{m0} = \sum_{n=0}^{N-1} U_n \phi_n^0(r) \quad (27)$$

where $U_n = (V \Lambda W \Lambda^T)_{n0}$. With these formulas, one can get the potential function numerically of quantum systems in our reformulation of quantum mechanics without potential function. However, there are cases where the potential functions can be gotten analytically.

So, now operating the kinetic operator T on the basis element gives

$$T_{n,m} = -\frac{1}{2} \langle \phi_n | \frac{d^2}{dx^2} | \phi_m \rangle = \lambda^2 \left(n + \frac{1}{2} \right) \delta_{n,m} - \frac{1}{2} \lambda^2 \langle n | (\lambda x)^2 | m \rangle \quad (28)$$

where $\langle n | f(z) | m \rangle = [\pi 2^{n+m} n! m!]^{-1/2} \int_{-\infty}^{+\infty} e^{-z^2} f(z) H_n(z) H_m(z) dz$. Since (28) will not be tridiagonal due to the last expression in R.H.S, then it will be eliminated by a counter - term in the sought after potential function. So, it is eliminated by the term $+\frac{1}{2} \lambda^4 x^2$, which is a harmonic oscillator potential term. Hence, the potential function we are looking for is

$$V(x) = \frac{1}{2} \lambda^4 x^2 + \mathcal{V}^0(x) \quad (29)$$

The unknown potential function $\mathcal{V}^0(x)$ associated with first term in (28) will be resolved numerically. Using the recursion relation of the Hermite polynomial in (28) without the last term we have

$$T_{n,m} = -\frac{1}{2} \langle \phi_n | \frac{d^2}{dx^2} | \phi_m \rangle = \frac{\lambda^2}{4} \left[(2n+1) \delta_{n,m} - \sqrt{n(n-1)} \delta_{n,m+2} - \sqrt{(n+1)(n+2)} \delta_{n,m-2} \right] \quad (30)$$

which is tridiagonal in function space with only odd and or only even indices. Since our physical parameters are different we will have interesting Hamiltonian matrix elements. Now we use $y = \sqrt{\ln(1+k^2/\lambda^2)}$, $\mu = \nu$, and $a = b$ in the three term recursion relation of the Wilson orthogonal polynomial (A7)

$$H_{nm} = \frac{\lambda^2}{2} (e^\Sigma - 1) \quad (31)$$

where

$$\Sigma = \frac{1}{2} \left[\left(n + \mu + a - \frac{1}{2} \right)^2 - \left(\mu - \frac{1}{2} \right)^2 - \left(a - \frac{1}{2} \right)^2 + \frac{1}{4} \right] \delta_{n,m} \quad (32)$$

$$-\frac{1}{4} \left\{ (n + \mu + a - 1) \sqrt{\frac{n(n+2\mu-1)(n+2a-1)(n+2\mu+2a-2)}{(n+\mu+a-1)^2 - \frac{1}{4}}} \delta_{n,m+1} + (n + \mu + a) \sqrt{\frac{(n+1)(n+2\mu)(n+2a)(n+2\mu+2a-1)}{(n+\mu+a)^2 - \frac{1}{4}}} \delta_{n,m-1} \right\}$$

The Hamiltonian matrix is not tridiagonal symmetric matrix but full matrix. The reason for this is due to the matrix exponential in (31). Now, the matrix elements of the potential function $V(x)$ is $V_{nm} = H_{nm} - T_{nm}$. As before, below is the full plot of the potential function. We obtained a more accurate and stable result when the order of matrix elements increase from $N = 10$ to $N = 20$.

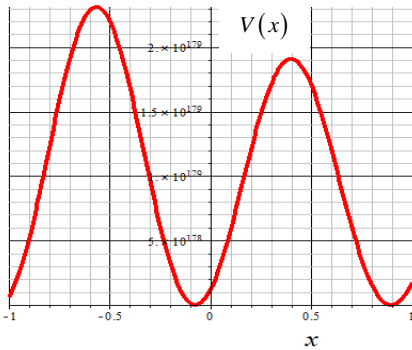


FIG.2. The potential function (29) computed by equation (14) and (15) with physical parameters: $\lambda = 0.5$, $a = 0.6$, $b = 0.5$, $\mu = 0.8$, $\nu = 0.3$ and both gave stable result.

4. Conclusion

In this paper, we derived analytically another new quantum system associated with the Wilson orthogonal polynomial and called the **Wilson Quantum system**. The energy spectrum, scattering phase shift, and wavefunction of the system were shown. In an effort to establish the correspondence between recent reformulation of quantum mechanics without potential function and the convention method; we were able to graphically get the potential function of the new quantum system using two of the formulas given in section 3

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Appendix A: The Wilson Orthogonal Polynomial

The Wilson polynomial, $W_n^{\theta}(y^2; \nu; a, b)$ can be defined

$$W_n^{\theta}(y^2; \nu; a, b) = \frac{(\mu+a)_n (\mu+b)_n}{(a+b)_n n!} {}_4F_3 \left(\begin{matrix} -n, n+\mu+\nu+a+b-1, \mu+iy, \mu-iy \\ \mu+\nu, \mu+a, \mu+b \end{matrix} \middle| 1 \right) \quad (A1)$$

where ${}_4F_3 \left(\begin{matrix} a, b, c, d \\ e, f, g \end{matrix} \middle| z \right) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n (c)_n (d)_n}{(e)_n (f)_n (g)_n} \frac{z^n}{n!}$ is the Hypergeometric function and $(a)_n = a(a+1)(a+2)\dots(a+n-1) = \frac{\Gamma(n+a)}{\Gamma(a)}$. The generating function of these polynomials is

$$\sum_{n=0}^{\infty} \mathcal{W}_n^{\mu} (y^2; v; a, b) t^n = {}_2F_1 \left(\begin{matrix} \mu + iy, v + iy \\ \mu + v \end{matrix} \middle| t \right) {}_2F_1 \left(\begin{matrix} a - iy, b - iy \\ a + b \end{matrix} \middle| t \right) \quad (\text{A2})$$

Their three term recursion relation ($n = 1, 2, 3, \dots$) is

$$y^2 \mathcal{W}_n^{\mu} = \left[\frac{(n + \mu + v)(n + \mu + a)(n + \mu + b)(n + \mu + v + a + b - 1)}{(2n + \mu + v + a + b)(2n + \mu + v + a + b - 1)} + \frac{n(n + v + a - 1)(n + v + b - 1)(n + a + b - 1)}{(2n + \mu + v + a + b - 1)(2n + \mu + v + a + b - 2)} - \mu^2 \right] \mathcal{W}_n^{\mu} \\ - \frac{(n + \mu + a - 1)(n + \mu + b - 1)(n + v + a - 1)(n + v + b - 1)}{(2n + \mu + v + a + b - 1)(2n + \mu + v + a + b - 2)} \mathcal{W}_{n-1}^{\mu} - \frac{(n + 1)(n + \mu + v)(n + a + b)(n + \mu + v + a + b - 1)}{(2n + \mu + v + a + b)(2n + \mu + v + a + b - 1)} \mathcal{W}_{n+1}^{\mu} \quad (\text{A3})$$

The initial seeds ($n = 0$) for this recursion are $\mathcal{W}_0^{\mu} = 1$ and $\mathcal{W}_1^{\mu} = \frac{(\mu + a)(\mu + b)}{(a + b)} - \frac{\mu + v + a + b}{(\mu + v)(a + b)} (y^2 + \mu^2)$.

The orthogonality relation of the polynomial is

$$\frac{1}{2\pi} \int_0^{\infty} \frac{\Gamma(\mu + v + a + b) \Gamma(\mu + iy) \Gamma(v + iy) \Gamma(a + iy) \Gamma(b + iy)}{\Gamma(\mu + v) \Gamma(a + b) \Gamma(\mu + a) \Gamma(\mu + b) \Gamma(v + a) \Gamma(v + b) \Gamma(2iy)^2} \mathcal{W}_n^{\mu} (y^2; v; a, b) \mathcal{W}_m^{\mu} (y^2; v; a, b) dy \\ = \left(\frac{n + \mu + v + a + b - 1}{2n + \mu + v + a + b - 1} \right) \frac{(\mu + a)_n (\mu + b)_n (v + a)_n (v + b)_n}{(\mu + v)_n (a + b)_n (\mu + v + a + b)_n n!} \delta_{nm} \quad (\text{A4})$$

The normalized weight function is

$$\rho^{\mu} (y; v; a, b) = \frac{1}{2\pi} \frac{\Gamma(\mu + v + a + b) \Gamma(\mu + iy) \Gamma(v + iy) \Gamma(a + iy) \Gamma(b + iy) / \Gamma(2iy)^2}{\Gamma(\mu + v) \Gamma(a + b) \Gamma(\mu + a) \Gamma(\mu + b) \Gamma(v + a) \Gamma(v + b)} \quad (\text{A5})$$

Finally, the orthonormal version of this polynomial is

$$W_n^{\mu} (y^2; v; a, b) = \sqrt{\frac{(2n + \mu + v + a + b - 1)}{n + \mu + v + a + b - 1}} \frac{(\mu + v)_n (a + b)_n (\mu + v + a + b)_n n!}{(\mu + a)_n (\mu + b)_n (v + a)_n (v + b)_n} \mathcal{W}_n^{\mu} (y^2; v; a, b) \\ = \sqrt{\frac{(2n + \mu + v + a + b - 1)}{n + \mu + v + a + b - 1}} \frac{(\mu + v)_n (\mu + a)_n (\mu + b)_n (\mu + v + a + b)_n}{(a + b)_n (v + a)_n (v + b)_n n!} {}_4F_3 \left(\begin{matrix} -n, n + \mu + v + a + b - 1, \mu + iy, \mu - iy \\ \mu + v, \mu + a, \mu + b \end{matrix} \middle| 1 \right) \quad (\text{A6})$$

The three – term recursion relation for the orthonormal version is

$$y^2 W_n^{\mu} = \left[\frac{(n + \mu + v)(n + \mu + a)(n + \mu + b)(n + \mu + v + a + b - 1)}{(2n + \mu + v + a + b)(2n + \mu + v + a + b - 1)} + \frac{n(n + v + a - 1)(n + v + b - 1)(n + a + b - 1)}{(2n + \mu + v + a + b - 1)(2n + \mu + v + a + b - 2)} - \mu^2 \right] W_n^{\mu} \\ - \frac{1}{2n + \mu + v + a + b - 2} \sqrt{\frac{n(n + \mu + v - 1)(n + a + b - 1)(n + \mu + a)(n + \mu + b - 1)(n + v + a - 1)(n + v + b - 1)(n + \mu + v + a + b - 2)}{(2n + \mu + v + a + b - 3)(2n + \mu + v + a + b - 1)}} W_{n-1}^{\mu} \\ - \frac{1}{2n + \mu + v + a + b} \sqrt{\frac{(n + 1)(n + \mu + v)(n + a + b)(n + \mu + a)(n + \mu + b)(n + v + a)(n + v + b)(n + \mu + v + a + b - 1)}{(2n + \mu + v + a + b - 1)(2n + \mu + v + a + b - 1)}} W_{n+1}^{\mu} \quad (\text{A7})$$

Using Darboux method, the asymptotic of this polynomial is

$$\mathcal{W}_n^{\mu} (y^2; v; a, b) \approx \frac{2}{n} \Gamma(\mu + v) \Gamma(a + b) |A(iy)| \cos \{ 2y \ln(n) + \arg [A(iy)] \} + O(n^{-1}) \quad (\text{A8})$$

where $A(iy) = \Gamma(2iy) / \Gamma(\mu + iy) \Gamma(v + iy) \Gamma(a + iy) \Gamma(b + iy)$ is the scattering amplitude. Hence the asymptotics of the orthonormal version of the polynomial will be

$$\mathcal{W}_n^{\mu} (y^2; v; a, b) \approx B(\mu, v, a, b) \sqrt{\frac{2}{n}} \Gamma(\mu + v) \Gamma(a + b) \{ 2|A(iy)| \cos [2y \ln(n) + \arg A(iy)] \} + O(n^{-1}) \quad (\text{A9})$$

where $B(\mu, v, a, b) = \sqrt{\frac{\Gamma(\mu + v) \Gamma(a + b) \Gamma(\mu + a) \Gamma(\mu + b) \Gamma(v + a) \Gamma(v + b)}{\Gamma(\mu + v + a + b)}}$, this is same as (A8).

As said earlier in this reformulation, the existence of bound states dictates that the scattering amplitude $|A(iy)|$ vanishes i.e. $\mu + iy = -m$, as $m = 0, 1, 2, \dots, N$. Hence this implies that $\mu < 0$ and $0 < N \leq -\mu$. Using this in the Wilson polynomial changes it to become the **discrete Racah Polynomial** defined as

$$R_n^{\delta} (m; \alpha, \beta, \gamma) = \frac{(\alpha + 1)_n (\gamma + 1)_n}{(\alpha + \beta + N + 2)_n n!} {}_4F_3 \left(\begin{matrix} -n, -m, n + \alpha + \beta + 1, m - \beta + \gamma - N \\ \alpha + 1, \gamma + 1, -N \end{matrix} \middle| 1 \right) \quad (\text{A10})$$

where $\alpha = \mu + a - 1 (\alpha > -1)$, $\gamma = \mu + b - 1 (\gamma > -1)$, $\beta = v + b - 1 (\beta > N - 1)$, and $\delta = -(N + \beta + 1) = \mu - b$.

However using the inverse parameter map $\mu = \frac{1}{2}(\gamma + \delta + 1)$, $\nu = \beta + \frac{1}{2}(\delta - \gamma + 1)$, $a = \alpha - \frac{1}{2}(\gamma + \delta - 1)$ and $b = \frac{1}{2}(\gamma - \delta + 1)$ takes the Racah polynomial back to the Wilson Polynomial. Also, the generating function of the Racah polynomial is

$$\sum_{n=0}^N \mathcal{R}_n^{\theta}(m; \alpha; \beta, \gamma) t^n = {}_2F_1 \left(\begin{matrix} -m, -m + \beta - \gamma \\ -N \end{matrix} \middle| t \right) {}_2F_1 \left(\begin{matrix} m + \alpha + 1, m + \gamma + 1 \\ \alpha + \beta + N + 2 \end{matrix} \middle| t \right) \quad (\text{A11})$$

and the three - term recursion relation is

$$\begin{aligned} & \frac{1}{4}(N + \beta - \gamma - 2m)^2 \mathcal{R}_n^{\theta} = \\ & \left[\frac{1}{4}(N + \beta - \gamma)^2 - \frac{(n-N)(n+\alpha+1)(n+\gamma+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)} - \frac{n(n+\beta)(n+\alpha+\beta-\gamma)(n+N+\alpha+\beta+1)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)} \right] \mathcal{R}_n^{\theta} \\ & + \frac{(n+\alpha)(n+\beta)(n+\gamma)(n+\alpha+\beta-\gamma)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)} \mathcal{R}_{n-1}^{\theta} + \frac{(n+1)(n-N)(n+\alpha+\beta+1)(n+N+\alpha+\beta+2)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)} \mathcal{R}_{n+1}^{\theta} \end{aligned} \quad (\text{A12})$$

The discrete orthogonality relation for the Racah polynomial is

$$\begin{aligned} & \sum_{m=0}^N \frac{2m + \gamma - \beta - N}{m + \gamma - \beta - N} \frac{(-N)_m (\alpha + 1)_m (\gamma + 1)_m (\gamma - \beta - N + 1)_m}{(-\beta - N)_m (\gamma - \beta + 1)_m (\gamma - \alpha - \beta - N)_m m!} \bar{R}_n^N(m; \alpha, \beta, \gamma) \bar{R}_n^N(m; \alpha, \beta, \gamma) \\ & = \frac{n + \alpha + \beta + 1}{2n + \alpha + \beta + 1} \frac{(-\alpha - \beta - N - 1)_N (\gamma - \beta - N + 1)_N (\beta + 1)_n (\alpha + \beta - \gamma + 1)_n (\alpha + \beta + N + 2)_n n!}{(-\beta - N)_N (\gamma - \alpha - \beta - N)_N (-N)_n (\alpha + 1)_n (\gamma + 1)_n (\alpha + \beta + 2)_n} \delta_{n,n'} \end{aligned} \quad (\text{A13})$$

where $\bar{R}_n^N(m; \alpha, \beta, \gamma) = {}_4F_3 \left(\begin{matrix} -n, -m, n + \alpha + \beta + 1, m - \beta + \gamma - N \\ \alpha + 1, \gamma + 1, -N \end{matrix} \middle| 1 \right)$ and

$$\rho^N(m; \alpha, \beta, \gamma) = \frac{2m + \gamma - \beta - N}{m + \gamma - \beta - N} \frac{(-N)_m (\alpha + 1)_m (\gamma + 1)_m (\gamma - \beta - N + 1)_m}{(-\beta - N)_m (\gamma - \beta + 1)_m (\gamma - \alpha - \beta - N)_m m!} \times \frac{(-\beta - N)_N (\gamma - \alpha - \beta - N)_N}{(-\alpha - \beta - N - 1)_N (\gamma - \beta - N + 1)_N}$$

Similarly like the Wilson polynomial, the discrete Racah polynomial has an orthonormal version defined as

$$\begin{aligned} & R_n^N(m; \alpha, \beta, \gamma) = \sqrt{\frac{2n + \alpha + \beta + 1}{n + \alpha + \beta + 1} \frac{(-N)_n (\alpha + 1)_n (\gamma + 1)_n (\alpha + \beta + 2)_n}{(\beta + 1)_n (\alpha + \beta - \gamma + 1)_n (\alpha + \beta + N + 2)_n n!}} \\ & \times {}_4F_3 \left(\begin{matrix} -n, -m, n + \alpha + \beta + 1, m - \beta + \gamma - N \\ \alpha + 1, \gamma + 1, -N \end{matrix} \middle| 1 \right) \end{aligned} \quad (\text{A14})$$

with orthogonality

$$\sum_{m=0}^N \rho^N(m; \alpha, \beta, \gamma) R_n^N(m; \alpha, \beta, \gamma) R_{n'}^N(m; \alpha, \beta, \gamma) = \delta_{n,n'} \quad (\text{A15})$$

Note we made use of the following identities in our calculations: $\frac{(a+1)_n}{(a)_n} = \frac{n+a}{a}$, $\frac{(a)_{n+1}}{(a)_n} = n+a$, $(n+a)_n = \frac{\Gamma(2n+a)}{\Gamma(n+a)}$,

$$\frac{(n+a)_n}{(a+1)_{2n}} = \frac{a!(a)_n}{2n+a}, \text{ and } (a-n)_n = \frac{\Gamma(a)}{\Gamma(a-n)}.$$

APPENDIX B: The reformulation Methodology

In this reformulation, the total wavefunction of a quantum system is written as $\Psi(t, x) = e^{-iEt/\hbar} \psi(E, x)$, giving the associated Hamiltonian as $H\Psi = i\hbar \frac{\partial}{\partial t} \Psi = E\Psi$. The radial component of the wavefunction is written as

$$\psi(E, x) = \sqrt{\rho^\mu(\varepsilon)} \sum_n P_n^\mu(\varepsilon) \phi_n^\lambda(x). \quad (\text{B1})$$

This is assumed to be a bounded sum. $\{\phi_n^\lambda(x)\}$ is the complete set of square- integrable basis functions in configuration space with coordinate x and $P_n^\mu(\varepsilon)$ is the expansion coefficient which are orthogonal polynomials of order n in the variable ε which is some proper function of the energy. Also, μ represents a set of real parameters associated with the physical

system and $\rho^\mu(\varepsilon)$ is the normalized weight function associated with the energy polynomials. Also, the basis set $\{\phi_n^\lambda(x)\}$ satisfies the boundary conditions and contains the kinematical information such as the angular momentum and the length scale. However, the detailed physical information about the system is contained in the energy polynomials $\{P_n^\mu(\varepsilon)\}$ and the corresponding weight function $\rho^\mu(\varepsilon)$. It is required the relevant energy polynomials to have the following asymptotic ($n \rightarrow \infty$)

$$P_n^\mu(\varepsilon) \approx n^{-\tau} A^\mu(\varepsilon) \times \cos[n^\xi \theta(\varepsilon) + \delta^\mu(\varepsilon)] \quad (\text{B2})$$

where τ and ξ are real positive constants that depend on the particular polynomial. $A^\mu(\varepsilon)$ is the scattering amplitude and $\delta^\mu(\varepsilon)$ is the phase shift. Bound states, if they exist, occur at (infinite or finite) energies that make the scattering amplitude vanish. That is, the m^{th} bound state occurs at an energy E_m such that $A^\mu(\varepsilon) = 0$ and the corresponding bound state is written as

$$\psi(E_m, x) = \sqrt{\omega^\mu(\varepsilon_m)} \sum_n Q_n^\mu(\varepsilon_m) \phi_n^\lambda(x) \quad (\text{B3})$$

where $\{Q_n^\mu(\varepsilon)\}$ are the discrete version of the polynomials $\{P_n^\mu(\varepsilon)\}$ and $\omega^\mu(\varepsilon_m)$ is the associated discrete weight function. On the other hand, if $A^\mu(\varepsilon) = 0$ at complex energies $\{\varepsilon_m\}$ with negative imaginary parts, then these are the resonance energies, and the imaginary part forces the wavefunction to vanish with time due to the factor $e^{-iE_m t/\hbar}$, the number of bound states and resonances could be finite or infinite. So there are three possibilities that could result for a full description of physical systems:

- *Only Continuous scattering states:* the wavefunction at energy ε is written as $\psi(\varepsilon, x) = \sqrt{\omega^\mu(\varepsilon)} \sum_n P_n^\mu(\varepsilon) \phi_n^\lambda(x)$
- *Only discrete bound states:* the m^{th} bound state wavefunction (with energy ε_m) is written as $\psi(\varepsilon_m, x) = \sqrt{\omega^\mu(\varepsilon)} \sum_n R_n^\mu(\varepsilon_m) \phi_n^\lambda(x)$, where $\{R_n^\mu(\varepsilon_m)\}$ are polynomials with discrete orthogonality relation $\sum_{n=0}^N \omega_n^\mu R_n^\mu(\varepsilon_m) R_n^\mu(\varepsilon_m) = \delta_{n,n'}$ and N is either finite or infinite.
- *Both continuum as well as discrete states:* the total wavefunction is $\psi(\varepsilon, x) = \sqrt{\omega^\mu(\varepsilon)} \sum_{n=0}^\infty P_n^\mu(\varepsilon) \phi_n^\lambda(x) + \sqrt{\omega^\mu(\varepsilon)} \sum_{n=0}^N R_n^\mu(\varepsilon) \phi_n^\lambda(x)$, where the orthogonality relation becomes $\int_\Omega \omega^\mu(\varepsilon) P_n^\mu(\varepsilon) P_n^\mu(\varepsilon) d\varepsilon + \sum_{m=0}^N \omega_m^\mu R_n^\mu(\varepsilon_m) R_n^\mu(\varepsilon_m) = \delta_{n,n'}$.

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