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Four-Parameter Potential Function with Negative Energy Bound States

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Abstract: Using the Tridiagonal Representation Approach (A method where we work in a complete set of square integrable basis that carries a tridiagonal matrix representation for the wave operator. Consequently, the matrix wave equation becomes a three-term recursion relation for the expansion coefficients of the wavefunction. Finding a solution of this recursion relation in terms of orthogonal polynomials is equivalent to solving the original problem) we obtain solutions for a new four-parameter one-dimensional potential function. We obtained the energy spectrum and corresponding wavefunction.
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1 Introduction and Formulation

Recently, we solved a new five - parameter potential box in one dimensional [1] using TRA. We got the energy spectrum and the wavefunction of this five parameter potential function. In this article we further consider a new four parameter potential function in one dimensional. This potential function is given as:

$$V(x)=\frac{1}{e^{\lambda x}-1}\left[V_0+V_1\left(1-2e^{-\lambda x}\right)+\frac{V_R}{1-e^{-\lambda x}}\right] \qquad (1)$$

for $0\le x\le\infty$, V_i are real parameters such that V_R isgreater than or equal to zero. Fig 1 is the plot of the potential function where V_R is vary (keeping V_0 and V_1 constant) and varying V_0 and V_1 (keeping V_R constant). This potential has never been studied in the published literature. However, when deformed, this potential can be compared to a three – parameter potential in

$$V(x)=V_1\frac{e^{-\lambda x}-\gamma}{e^{\lambda x}-1} \qquad (2)$$

Where V_1 are the potential strength and the range parameter λ is positive with inverse length unit. The dimensionless parameter γ is in the open range $0<\gamma<1$. Graphically, this potential function cross the x –axis at $x_0=-\ln\gamma/\lambda$ and then reaches a local extremum value of $V(x_1)=-V_0\left(1-\sqrt{1-\gamma}\right)^2$ at $x_1=-\frac{1}{\lambda}\ln\left(1-\sqrt{1-\gamma}\right)$. We observed that (1) and (2) are short range potentials with $1/x$ singularity at the origin. Simple algebraic manipulation in (1) will easily produce (2). Note (1) is same as

$$V(x)=\frac{V_0}{e^{\lambda x}-1}+\frac{V_1\left(1-2e^{-\lambda x}\right)}{e^{\lambda x}-1}+\frac{V_Re^{\lambda x}}{\left(e^{\lambda x}-1\right)^2} \qquad (3)$$
$$=V_1\frac{\gamma-e^{-\lambda x}}{e^{\lambda x}-1}+\frac{V_Re^{\lambda x}}{\left(e^{\lambda x}-1\right)^2}$$

When $V_R=0$, such that we defined a dimensionless ratio $\gamma=\frac{V_0+V_1}{2V_1}$ for $V_1\neq0$; then we easily get (2).

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Detailed study of these potentials; show that they can be used practically as an appropriate model for the interaction of an electron with extended molecules whose electron cloud is congregated near the centre of
the molecules. Also, there is a resemblance between
this potential and attractive Coulomb potential for nonzero angular momentum at short distances hence we expect them to finite bound states. In this paper, we are more interested in the generalized potential given in (1) where none of the potential parameters is zero in order to obtain the energy spectrum and wave function.
We now formulate this problem and solve it using the Tridiagonal Representation Approach (TRA) [2-7].

We write the wavefunction as the bounded sum $\psi(E,x)=\sum_n f_n(E)\phi_n(x)$, where $\{\phi_n(x)\}$ is a complete set of square integrable basis functions and $\{f_n(E)\}$ are proper expansion coefficients in the energy. If we make the coordinate transformation $y(x)=1-2e^{-\lambda x}$, then the Schrödinger wave equation in the new configuration space becomes

$$(H-E)|\psi\rangle=-\frac{1}{2}\left[(y')^2\frac{d^2}{dy^2}+y''\frac{d}{dy}-2V(y)+2E\right]|\psi\rangle=0 \quad (4)$$

where the prime stands for the derivative with respect to x and we adopted the atomic units $\hbar=m=1$. With $y\in[-1,+1]$, we can choose the following square integrable functions in the new configuration space with coordinate y as basic elements for the expansion of the wavefunction

$$\phi_n(y)=A_n(1-y)^{\alpha}(1+y)^{\beta}P_n^{(\mu,\nu)}(y) \quad (5)$$

Where $P_n^{(\mu,\nu)}(x)$ is the Jacobi polynomial of degree $n=0,1,2,..$ in y, the parameters μ and ν are larger than -1 and $A_n=\sqrt{\frac{2n+\mu+\nu+1}{2^{\mu+\nu+1}}\frac{\Gamma(n+1)\Gamma(n+\mu+\nu+1)}{\Gamma(n+\nu+1)\Gamma(n+\mu+1)}}$. For simplicity, we rewrite (4) as

$$(H-E)|\psi\rangle=-\frac{1}{2}\frac{(y')^2}{(1-y^2)}\begin{pmatrix}(1-y^2)\frac{d^2}{dy^2}+\frac{y''}{(y')^2}(1-y^2)\frac{d}{dy}+\\ 2\frac{(1-y^2)}{(y')^2}[E-V]\end{pmatrix}|\psi\rangle=0 \quad (6)$$

We applied the wave operator on the basis element to get

$$(H-E)|\phi_n\rangle=J|\phi_n\rangle=-\frac{\lambda^2}{2}\frac{(1-y)}{(1+y)}\begin{pmatrix}(1-y^2)\frac{d^2}{dy^2}-(1+y)\frac{d}{dy}+\\ \frac{2(1+y)E}{\lambda^2(1-y)}-\frac{2V_0}{\lambda^2}-\frac{2V_1y}{\lambda^2}-\frac{4V_R}{\lambda^2(1+y)}\end{pmatrix}|\phi_n\rangle=0 \quad (7)$$

where we had used $y'=\lambda(1-y)$, $\frac{y''}{(y')^2}=-1/(1-y)$, and the potential function in new configuration space as $V(y)=\frac{(1-y)}{(1+y)}\left[V_0+V_1y+\frac{2V_R}{(1+y)}\right]$. Using $u_i=\left(2/\lambda^2\right)V_i$ and $\varepsilon=\left(2/\lambda^2\right)E$ in (7) we have

$$\frac{2}{\lambda^2}J|\phi_n\rangle=-\frac{(1-y)}{(1+y)}\begin{pmatrix}(1-y^2)\frac{d^2}{dy^2}-(1+y)\frac{d}{dy}\\ -(\varepsilon+u_0)-u_1y+\frac{2\varepsilon}{(1-y)}-\frac{2u_R}{(1+y)}\end{pmatrix}|\phi_n\rangle=0 \quad (8)$$

Now, the boundary conditions and square integrability (with respect to the integral measure dx) dictate that the matrix wave operator becomes

$$\langle\phi_n|F[y]|\phi_m\rangle=-A_nA_m\int_{-1}^{+1}(1-y)^{2\alpha}(1+y)^{2\beta}\frac{(1-y)}{(1+y)}[F(y)]P_n^{(\mu,\nu)}(y)P_m^{(\mu,\nu)}(y)\frac{dy}{\lambda(1-y)}$$

$$=\frac{-A_nA_m}{\lambda}\int_{-1}^{+1}(1-y)^{2\alpha}(1+y)^{2\beta-1}[F(y)]P_n^{(\mu,\nu)}(y)P_m^{(\mu,\nu)}(y)dy \quad (9)$$

where

$$F(y)=(1-y^2)\frac{d^2}{dy^2}-(1+y)\frac{d}{dy}-(\varepsilon+u_0)-u_1y+\frac{2\varepsilon}{(1-y)}-\frac{2u_R}{(1+y)}$$

Hence we have $2\alpha=\mu$ and $2\beta=\nu+1$. As a result of these conditions with the fact that $y'=\lambda(1-y)$, the normalization constant will be $A_n=\sqrt{\frac{2n+\mu+\nu+1}{2^{\mu+\nu+1}}\frac{\Gamma(n+1)\Gamma(n+\mu+\nu+1)}{\Gamma(n+\nu+1)\Gamma(n+\mu+1)}}$. Using the first and second derivatives of the basis element with respect to y in (8) gives

$$\frac{2}{\lambda^2}J|\phi_n\rangle=-A_n(1-y)^{\alpha}(1+y)^{\beta}\begin{pmatrix}(1-y^2)\frac{d^2}{dy^2}+[2\beta(1-y)-(2\alpha+1)(1+y)]\frac{d}{dy}\\ +\frac{1}{(1+y)}(2\beta(\beta-1)-2u_R)\\ -\frac{1}{(1-y)}(2\alpha^2+2\varepsilon)-(\alpha^2+\beta^2)-(\varepsilon+u_0)-u_1y\end{pmatrix}P_n^{(\mu,\nu)}(y)=0 \quad (10)$$

The second order differential equation of the Jacobi Polynomial $P_n^{(\mu,\nu)}(y)$ is

$$(1-y^2)\frac{d^2}{dy^2}P_n^{(\mu,\nu)}(y)=\left\{\begin{matrix}[(\mu+\nu+2)y+\mu-\nu]\frac{d}{dy}\\ -n(n+\mu+\nu+1)\end{matrix}\right\}\frac{d}{dy} \quad (11)$$

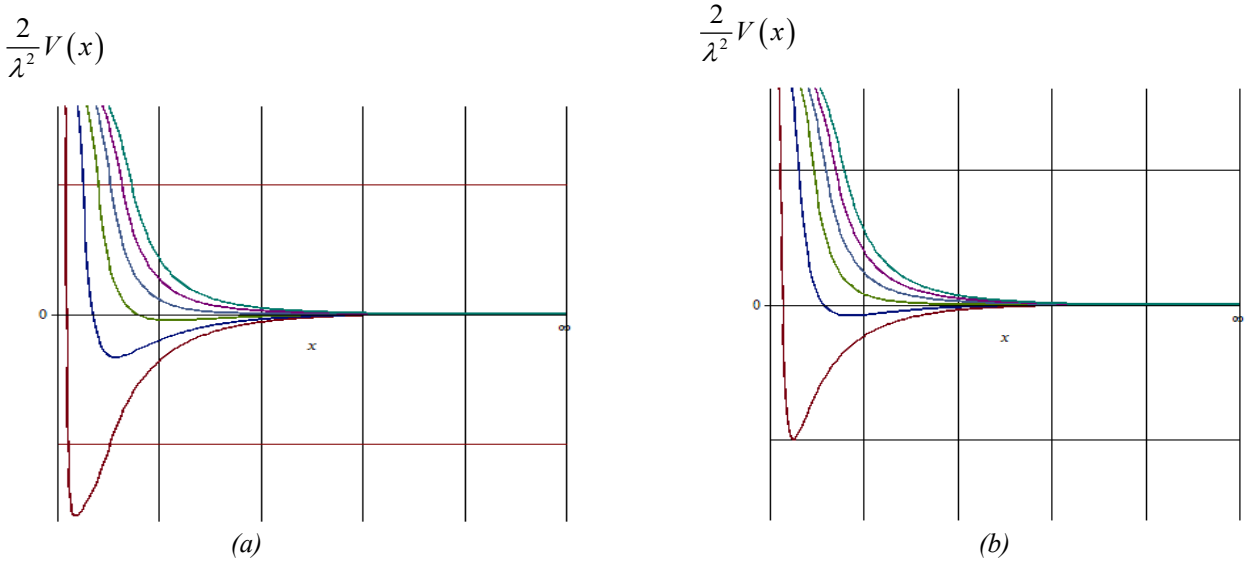

Fig 1. Plot of the potential function given by (1) with $\lambda = 1$. (a) is obtained by vary $u_r = 1,..,11$(in step of 2) while keeping $u_1 = -5$ and $u_0 = -2$. (b) is obtained by $u_1 = -3$ and $u_0 = -2$ while $u_r = 1,..,11$(in steps of 2). It is observed that further variations in u_1 and u_0 will result in an upper shift of the potential function in positive *xy* plane.

Therefore equation (10) becomes

$$\frac{2}{\lambda^2}J|\phi_n\rangle = -A_n(1-y)^{\alpha}(1+y)^{\beta}\left\{\begin{array}{l}\left[\mu-v+y(\mu+v+2)\right]\frac{d}{dy}+\left[2\beta(1-y)-(2\alpha+1)(1+y)\right]\frac{d}{dy}+\frac{1}{(1+y)}\left(2\beta(\beta-1)-2u_R\right)\\ +\frac{1}{(1-y)}\left(2\alpha^2+2\varepsilon\right)-\left(\alpha^2+\beta^2\right)-\left(\varepsilon+u_0\right)-u_1y-n(n+\mu+v+1)\end{array}\right\}P_n^{(\mu,v)}(y) \qquad (12)$$

$$= -A_n(1-y)^{\mu/2}(1+y)^{v+1/2}\left(\frac{1}{2(1+y)}\left(v^2-1-4u_R\right)+\frac{1}{2(1-y)}\left(\mu^2+4\varepsilon\right)-\left(\varepsilon+u_0\right)-u_1y-\left(n+\frac{\mu+v+1}{2}\right)^2\right)P_n^{(\mu,v)}(y)$$

Since the matrix representation of the wave operator is required to be tridiagonal and symmetric, in line with the recursion relation of the Jacobi polynomial and its orthogonality; we eliminate the two non -linear terms in (12). Hence the basis parameters must be chosen as follows:

$$v^2 = 1+4u_R \text{ and } \mu^2 = -4\varepsilon \qquad (13)$$

It is explicit here that the solution of this problem will give negative energy $\mu^2 = -8E/\lambda^2$ and the potential parameter V_R ($u_R \geq -1/4$) should be greater than or equal to zero. Now equation (12) becomes

$$\frac{2}{\lambda^2}J|\phi_n\rangle = -A_n(1-y)^{\mu/2}(1+y)^{v+1/2}\left(-\left(\varepsilon+u_0\right)-u_1y-\left(n+\frac{\mu+v+1}{2}\right)^2\right)P_n^{(\mu,v)}(y) \qquad (14)$$

Using the three term recursion relation of the Jacobi polynomial and their orthogonality property,

$A_nA_m\int_{-1}^{+1}(1-y)^{\mu}(1+y)^{v}P_n^{(\mu,v)}(y)P_m^{(\mu,v)}(y)dy = \delta_{nm}$ in (14) after operating $\langle\phi_m|$ on the L.H.S of it; we have the tridiagonal and symmetric representation of the wave operator as

$$\frac{2}{\lambda^2}J_{nm}=\left[\left(n+\frac{\mu+v+1}{2}\right)^2+\left(\varepsilon+u_0\right)+u_1C_n\right]\delta_{nm}+u_1\left(D_{n-1}\delta_{n,m+1}+D_n\delta_{n,m-1}\right) \quad (15)$$

where $C_n=\dfrac{v^2-\mu^2}{(2n+\mu+v)(2n+\mu+v+2)}$ and $D_n=\dfrac{2}{2n+\mu+v+2}\sqrt{\dfrac{(n+1)(n+\mu+1)(n+v+1)(n+\mu+v+1)}{(2n+\mu+v+1)(2n+\mu+v+3)}}$

Hence, we can now write the matrix wave equation as $\langle\phi_n|J|\psi\rangle=\sum_m\langle\phi_n|J|\phi_m\rangle f_m=\sum_m J_{nm}f_m=0$ which give the three –term recursion relation for the expansion coefficient of the wave function as

$$-\left(\varepsilon+u_0\right)f_n=\left[\left(n+\frac{\mu+v+1}{2}\right)^2+u_1C_n\right]f_n+u_1\left(D_{n-1}f_{n-1}+D_nf_{n+1}\right) \quad (16)$$

writing $G_n(E)=G_0(E)f_0(\varepsilon)$, will make $f_0=1$ and $f_1=\dfrac{(z-a_0)f_0}{b_0}$ where $z=-(\varepsilon+u_0)$, $a_0=\left(\dfrac{\mu+v+1}{2}\right)^2+u_1C_0$, and $b_0=u_1D_0$. This relation is valid for $n=1,2,3,\ldots$.

This is a new polynomial that we discovered recently and is not found in any mathematics literature. Hence, its analytic properties, that is, weight function, generating function, orthogonality, zero, etc. are yet to be known. Therefore we resolved to a numerical techniques to calculate the energy spectrum of the potential given in (1) for a given set of parameters.

2. Energy spectrum and wavefunction

To calculate the energy spectrum, we obtain first the Hamiltonian matrix from the wave operator matrix (15) as $H=J|_{E=0}$. Then, the energy spectrum is calculated from the wave equation $H|\psi\rangle=E|\psi\rangle$ as the generalized eigenvalues $\{E\}$ of the matrix equation $\sum_m H_{n,m}f_m=E\sum_m\Omega_{n,m}f_m$; where Ω_{nm} is the overlap basis element given as

$$\Omega_{n,m}=\langle\phi_n|\phi_m\rangle=A_nA_m\int_{-1}^{1}(1-y)^{\mu}(1+y)^{v}P_n^{(\mu,v)}(y)P_m^{(\mu,v)}(y)\times\left[(1-y)^{2\alpha-\mu-a}(1+y)^{2\beta-v-b}\right]dy$$

$$\equiv\langle n|(1-y)^{2\alpha-\mu-a}(1+y)^{2\beta-v-b}|m\rangle \quad (17)$$

Using the conditions for the parameters of the basis element $2\alpha=\mu$ and $2\beta=v+1$ with $a=1$ and $b=0$; the overlap basis element becomes

$$\Omega_{nm}=\langle n|\frac{(1+y)}{(1-y)}|m\rangle=\frac{(1+C_n)\delta_{nm}+D_{n-1}\delta_{n,m+1}+D_n\delta_{n,m-1}}{(1-C_n)\delta_{nm}-D_{n-1}\delta_{n,m+1}-D_n\delta_{n,m-1}} \quad (18)$$

Table 1 is a list of the energy spectrum for a given set of values of the potential parameters and for basis size of $N=20$ .We show only significant decimal digits that do not change with any substantial increase in the basis size (e.g. from size 10 to 50).Also, variation (increase) in N ; we observed a rapid convergence of these values with the size of the basis size

In Figure 2, we plot the bound state wavefunction corresponding to the physical configuration and energy spectrum of Table 1. We calculate the m^{th} bound state using the sum $\psi(E_m,x)\sim\sum_{n=0}^{N-1}P_n(\varepsilon_m)\phi_n(x)$, for some eigenvalues, where N is some large enough integer An energy resonance (scattering phase shift) phenomenon is observed with this potential function, which will observed when plotting the wavefunction using some of the eigenvalues in table 1. However, this can be further study using **complex rotation method** [15-17]

3. Conclusion

In this paper, in effort to enlarge the class of solvable potentials, we solve a new potential function that has not been solved in the physics literature to the best of our knowledge. This potential is of greater importance and we will encourage readers to put this into applications. The problem was formulated using the **Tridiagonal Representation Approach**. This method (algebraic in nature) is more encompassing then the conventional methods in solving the Schrödinger equation and allows for more realization of unknown potential functions which are yet to be associated with any physical systems. It has been shown that this approach has contributed greatly to the class of solvable quantum mechanical systems [8]

Table 1: The finite energy spectrum for the potential function (1) with $u_0 = -6$, $u_1 = 10$, and $u_R = 2.5$. It was obtained by diagonalizing the Hamiltonian matrix for different basis size.

n	ε_n	n	ε_n
0	4126.9891447498	10	32.4394977694
1	1542.8903686294	11	22.4398560240
2	787.2186135745	12	15.2463797234
3	462.6214937613	13	10.1007245429
4	294.0660278716	14	6.4695140302
5	195.9554935304	15	3.9657920559
6	134.3972745542	16	2.2930653158
7	93.7323498172	17	0.0664830132
8	65.8910440926	18	0.4757637553
9	46.3583338365	19	1.1960489428

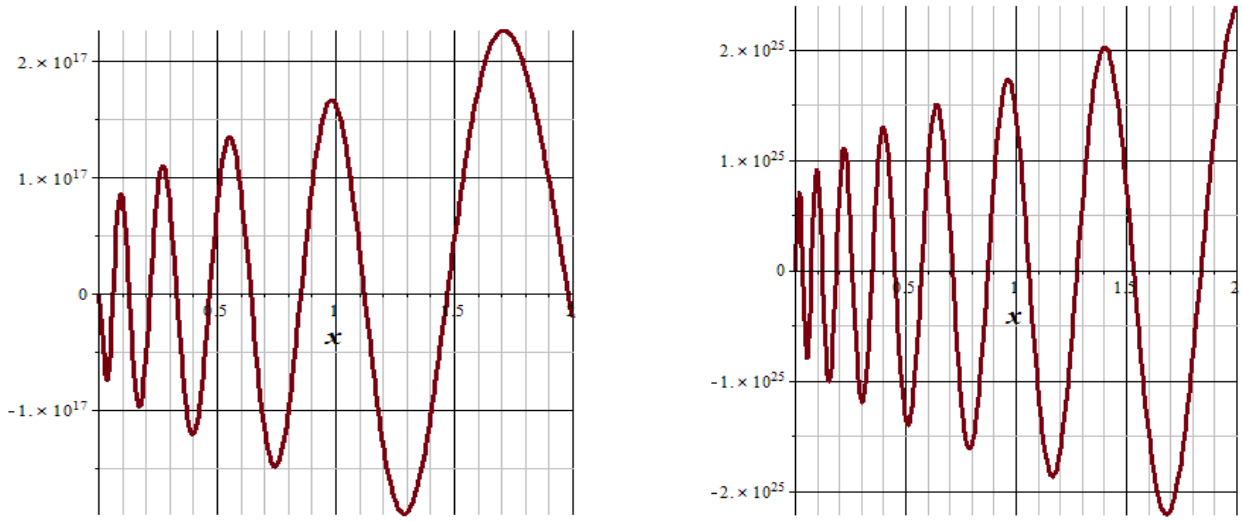

Fig.2. The graph of the wavefunction as we move down (however there coexist bound states and resonance) the table 1 with physical parameters: $\lambda = 1$, $u_0 = -6$, $u_1 = 10$, and $u_R = 2.5$.

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Appendix: The Jacobi Polynomials and Manipulations of the Basis Elements

Below are the useful properties of the Jacobi polynomial and the effects of the relevant differential operators on the basis element (5). These are identities are available in textbooks and monographs on orthogonal polynomials [10]

The Jacobi polynomials $P_n^{(\mu,\nu)}(y)$, where $y\in[-1,+1]$ and $\mu>-1$, $\nu>-1$:

$$yP_n^{(\mu,\nu)}(y)=\frac{\nu^2-\mu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}P_n^{(\mu,\nu)}(y)+\frac{2(n+\mu)(n+\nu)}{(2n+\mu+\nu)(2n+\mu+\nu+1)}P_{n-1}^{(\mu,\nu)}(y)$$
$$+\frac{2(n+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+2)}P_{n+1}^{(\mu,\nu)}(y) \tag{A1}$$

$$P_n^{(\mu,\nu)}(y)=\frac{\Gamma(n+\mu+1)}{\Gamma(n+1)\Gamma(\mu+1)}\,{}_2F_1\left(-n,n+\mu+\nu+1;\mu+1;\frac{1-y}{2}\right)=(-1)^n\,P_n^{(\mu,\nu)}(-y) \tag{A2}$$

$$\left\{(1-y^2)\frac{d^2}{dy^2}-\left[(\mu+\nu+2)y+\mu-\nu\right]\frac{d}{dy}+n(n+\mu+\nu+1)\right\}P_n^{(\mu,\nu)}(y)=0 \tag{A3}$$

$$(1-y^2)\frac{d}{dy}P_n^{(\mu,\nu)}(y)=-n\left(y+\frac{\nu-\mu}{2n+\mu+\nu}\right)P_n^{(\mu,\nu)}(y)+2\frac{(n+\mu)(n+\nu)}{2n+\mu+\nu}P_{n-1}^{(\mu,\nu)}(y) \tag{A4}$$

$$\int_{-1}^{+1}(1-y)^{\mu}(1+y)^{\nu}P_n^{(\mu,\nu)}(y)P_m^{(\mu,\nu)}(y)dy=\frac{2^{\mu+\nu+1}}{2n+\mu+\nu+1}\frac{\Gamma(n+\mu+1)\Gamma(n+\nu+1)}{\Gamma(n+1)\Gamma(n+\mu+\nu+1)}\delta_{nm} \tag{A5}$$

Using the above, with some algebraic manipulations, the effect of differential operators on the basis elements give:

$$(1-y^2)\frac{d^2\phi_n}{dy^2}=\left[-2\alpha\beta-n(n+\mu+\nu+1)-n\left(y+\frac{\nu-\mu}{2n+\mu+\nu}\right)\left(\frac{2\alpha-\nu-1}{1+y}+\frac{1+\mu-2\beta}{1-y}\right)+\beta(\beta-1)\frac{1+y}{1-y}+\alpha(\alpha-1)\frac{1-y}{1+y}\right]\phi_n$$
$$+2\frac{(n+\mu)(n+\nu)}{2n+\mu+\nu}\left(\frac{2\alpha-\nu-1}{1+y}+\frac{1+\mu-2\beta}{1-y}\right)\frac{A_n}{A_{n-1}}\phi_{n-1} \tag{A6}$$

$$\frac{d\phi_n}{dy}=\left[\frac{\alpha}{1+y}-\frac{\beta}{1-y}-\frac{n}{1-y^2}\left(y+\frac{\nu-\mu}{2n+\mu+\nu}\right)\right]\phi_n+\frac{2}{1-y^2}\frac{(n+\mu)(n+\nu)}{2n+\mu+\nu}\frac{A_n}{A_{n-1}}\phi_{n-1} \tag{A7}$$

The matrix elements of an integrable function $F(y)$ is defined as

$$\langle n|F(y)|m\rangle=A_nA_m\int_{-1}^{+1}(1-y)^{\mu}(1+y)^{\nu}F(y)P_n^{(\mu,\nu)}(y)P_m^{(\mu,\nu)}(y)dy \tag{A8}$$

then we obtain

$$\langle n|y|m\rangle=\frac{\nu^2-\mu^2}{(2n+\mu+\nu)(2n+\mu+\nu+2)}\delta_{nm}+\frac{2}{(2n+\mu+\nu)}\sqrt{\frac{n(n+\mu)(n+\nu)(n+\mu+\nu)}{(2n+\mu+\nu-1)(2n+\mu+\nu+1)}}\delta_{n,m+1}$$
$$+\frac{2}{(2n+\mu+\nu+2)}\sqrt{\frac{(n+1)(n+\mu+1)(n+\nu+1)(n+\mu+\nu+1)}{(2n+\mu+\nu+1)(2n+\mu+\nu+3)}}\delta_{n,m-1} \tag{A9}$$

as a special case

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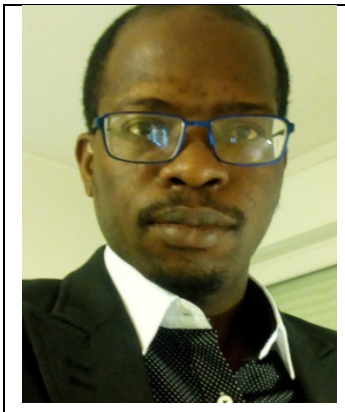

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