

## Research Article

# Approximate Solutions of Schrodinger Equation with Some Diatomic Molecular Interactions Using Nikiforov-Uvarov Method

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We used a tool of conventional Nikiforov-Uvarov method to determine bound state solutions of Schrodinger equation with quantum interaction potential called Hulthen-Yukawa inversely quadratic potential (HYIQP). We obtained the energy eigenvalues and the total normalized wave function. We employed Hellmann-Feynman Theorem (HFT) to compute expectation values  $\langle r^{-2} \rangle$ ,  $\langle r^{-1} \rangle$ ,  $\langle T \rangle$ , and  $\langle p^2 \rangle$  for four different diatomic molecules: hydrogen molecule ( $H_2$ ), lithium hydride molecule (LiH), hydrogen chloride molecule (HCl), and carbon (II) oxide molecule. The resulting energy equation reduces to three well-known potentials which are as follows: Hulthen potential, Yukawa potential, and inversely quadratic potential. The bound state energies for Hulthen and Yukawa potentials agree with the result reported in existing literature. We obtained the numerical bound state energies of the expectation values by implementing MATLAB algorithm using experimentally determined spectroscopic constant for the different diatomic molecules. We developed mathematica programming to obtain wave function and probability density plots for different orbital angular quantum number.

## 1. Introduction

The study of diatomic molecules is very significant and applicable in many areas of chemical and physical sciences. The excitation of atoms of some diatomic molecules especially the homonuclear diatomic molecules is the principle used in spectrophotometric technique. Diatomic molecules contains two atoms per molecule and can either be homonuclear if it contains two atoms of the same kind per molecule or be heteronuclear if its contains two atoms of different kind per molecule [1–5]. Bound state solutions of relativistic and nonrelativistic wave equation arouse a lot of interest for decades. Schrodinger wave equations constitute nonrelativistic wave equation while Klein-Gordon and Dirac equations constitute the relativistic wave equations [6–10]. Bound state solutions predominantly have negative energies because the energy of the particle is less than the maximum potential energy [11]. The quantum interaction potential (HYIQP)

can be used to compute the bound state energies for both homonuclear and heteronuclear diatomic molecules. Other potentials have been used in studying bound state solutions like the following: Hulthen, Poschl-Teller, Eckart, Coulomb, Hylleraas, pseudoharmonic, and scarf II potentials and many others [6, 12–19]. These potentials are studied with some specific methods and techniques like the following: asymptotic iteration method, Nikiforov-Uvarov method, supersymmetric quantum mechanics approach, formular method, exact quantisation, and many more [19–29]. This article is divided into seven sections. Section 1 is the introduction; Section 2 is the brief introduction of conventional Nikiforov-Uvarov method. In Section 3, we presented the radial solution to Schrodinger wave equation using the proposed potential and obtained both the energy eigenvalue and their corresponding normalized wave function. In Section 4, we have deductions of three well-known potentials from the proposed potential. The numerical results of two of the potentials are compared

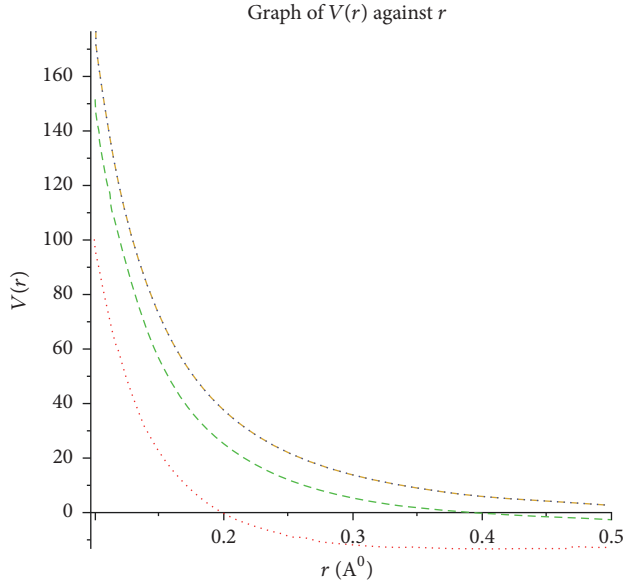


FIGURE 1: The graph of the quantum interaction potential (HYIQP) for various value of  $\alpha$ .

to that of existing literature. In Section 5, we applied HFT to compute the expectation values for different diatomic molecules. In Section 6, we present numerical results of the expectation values by implementing MATLAB algorithm. Section 7 gives the analytical solutions of finding the normalization constant using confluent hypergeometric function while Section 8 gives the general conclusion of the article.

The proposed quantum interaction potential is given by

$$V(r) = -\frac{V_0 e^{-2\alpha r}}{(1 - e^{-2\alpha r})} - \frac{Ae^{-\alpha r}}{r} + \frac{B}{r^2} + C, \quad (1)$$

where  $V_0$  is the potential depth,  $\alpha$  is the adjustable parameter known as the screening parameter.  $A$ ,  $B$ , and  $C$  are all spectroscopic constants which are molecular bond length, molecular constant, and potential range, respectively.

Figure 1 shows the graph of quantum interaction potential for various values of the screening parameter  $\alpha$  which decays exponentially. Meanwhile, Figure 2 shows the graph of individual potentials plotted in the same scale with the quantum interaction potential (HYIQP). From this MATLAB plot, it can be seen that HYIQP is best suitable in describing bound state energies of diatomic molecules. In elementary quantum mechanics, the wave function implicitly described the behaviour of quantum mechanical systems. The developed potential model is used to study the behaviour of four diatomic molecules, namely, hydrogen, carbon (II) oxide, lithium hydride, and hydrogen chloride molecules. The wave function and probability density plots, gotten from mathematica programming as seen in Figures 3–8 for wave function plots and Figure 9 for probability density plots for orbital angular quantum numbers  $l = 0, 1, 2, 3, 4$ , and 5, respectively, is very significant in investigating the behaviour of diatomic molecules. This plot shows that carbon (II) oxide with maximum peak is very flammable and a

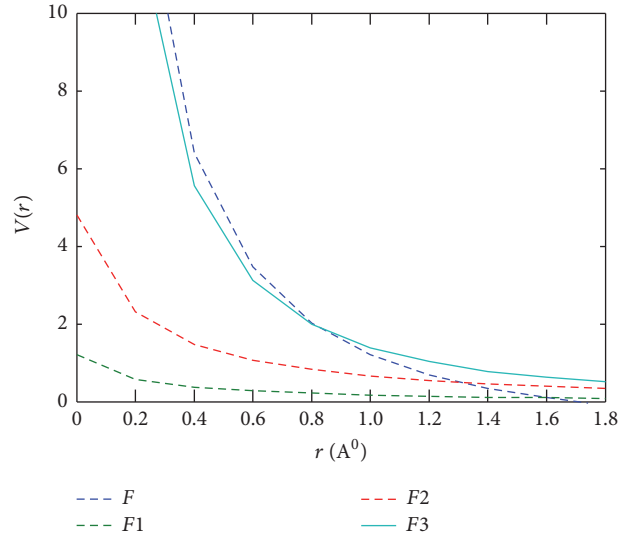


FIGURE 2: The graph of the HYIQP as compared to that of individual potentials.  $F$  = HYIQP potential,  $F1$  = Hulthen potential,  $F2$  = Yukawa potential, and  $F3$  = inversely quadratic potential.

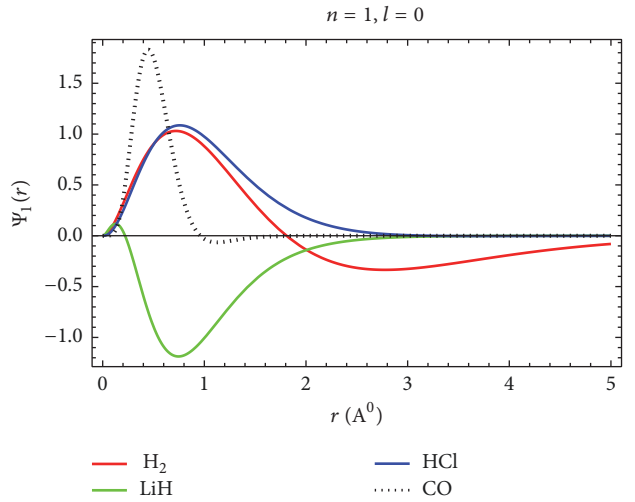


FIGURE 3: Wave function plot for the interaction potential with orbital angular quantum number  $l = 0$ .

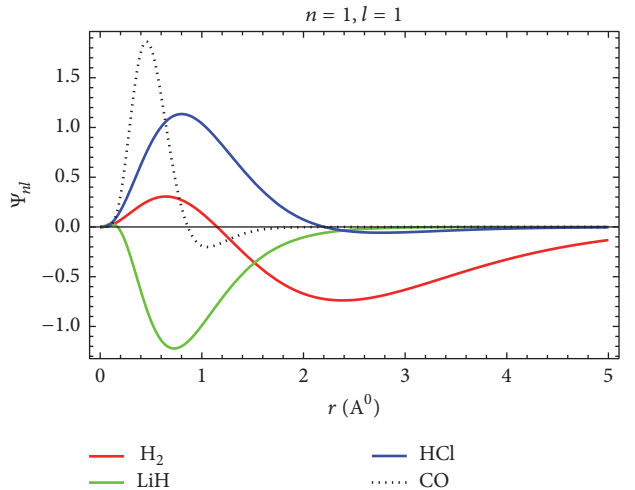


FIGURE 4: Wave function plot for the interaction potential with orbital angular quantum number  $l = 1$ .

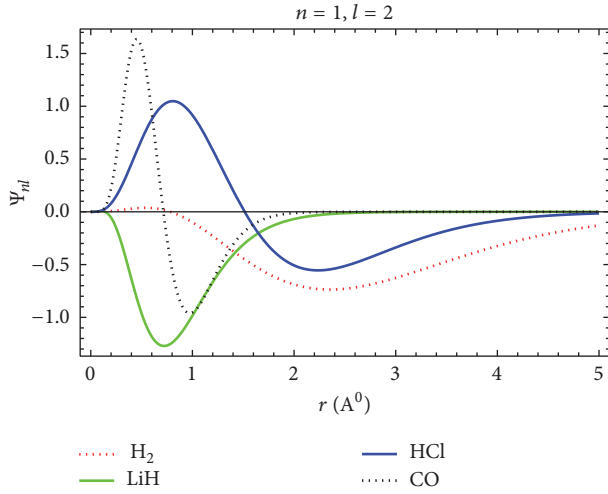


FIGURE 5: Wave function plot for the interaction potential with orbital angular quantum number  $l = 2$ .

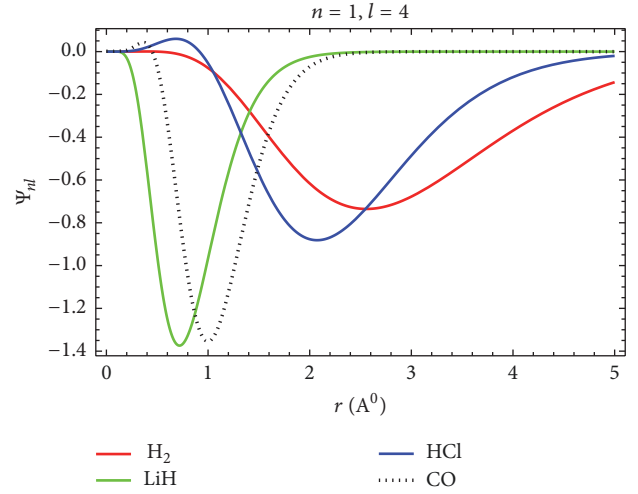


FIGURE 7: Wave function plot for the interaction potential with orbital angular quantum number  $l = 4$ .

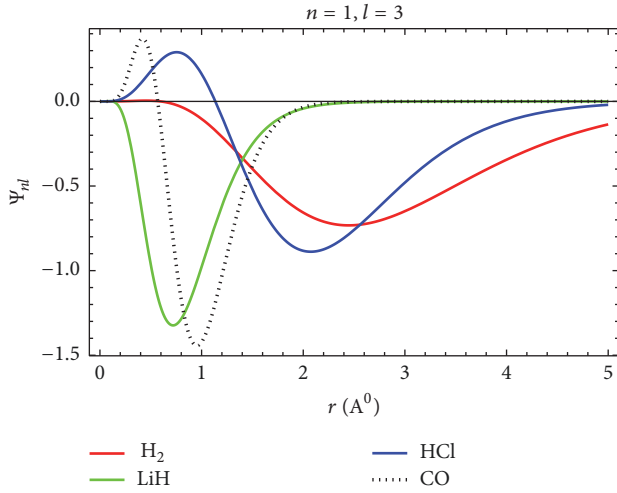


FIGURE 6: Wave function plot for the interaction potential with orbital angular quantum number  $l = 3$ .

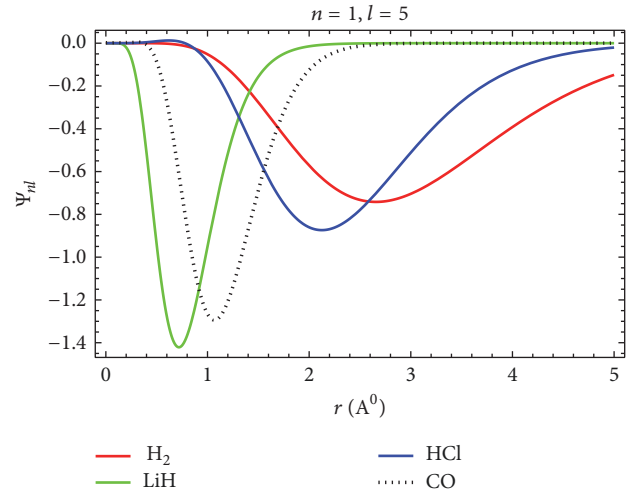


FIGURE 8: Wave function plot for the interaction potential with orbital angular quantum number  $l = 5$ .

highly toxic gas though industrially it is a good reducing agent. Lithium hydride possesses similar characteristic being a toxic and poisonous gas. However, the various plot shows that hydrogen chloride and hydrogen molecules are less reactive as compared to lithium hydride and carbon (II) oxide molecules.

## 2. Conventional Nikiforov-Uvarov Method

The NU method is based on reducing second-order linear differential equation to a generalized equation of hypergeometric type [30, 31]. This method provides exact solutions in terms of special orthogonal functions as well as corresponding energy eigenvalues. The NU method is applicable to both relativistic and nonrelativistic equations. With appropriate

coordinate transformation  $S = S(x)$  the equation can be written as

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0. \quad (2)$$

$\tilde{\tau}(s)$  is a polynomial of degree one while  $\sigma(s)$  and  $\tilde{\sigma}(s)$  are polynomials of at most degree two.

In order to find the exact solution to (2), we set the wave function as

$$\Psi(s) = \phi(s)\chi(s) \quad (3)$$

and substituting (3) into (2) reduces (2) into hypergeometric type.

$$\sigma(s)\chi''(s) + \tau(s)\chi'(s) + \lambda\chi(s) = 0, \quad (4)$$

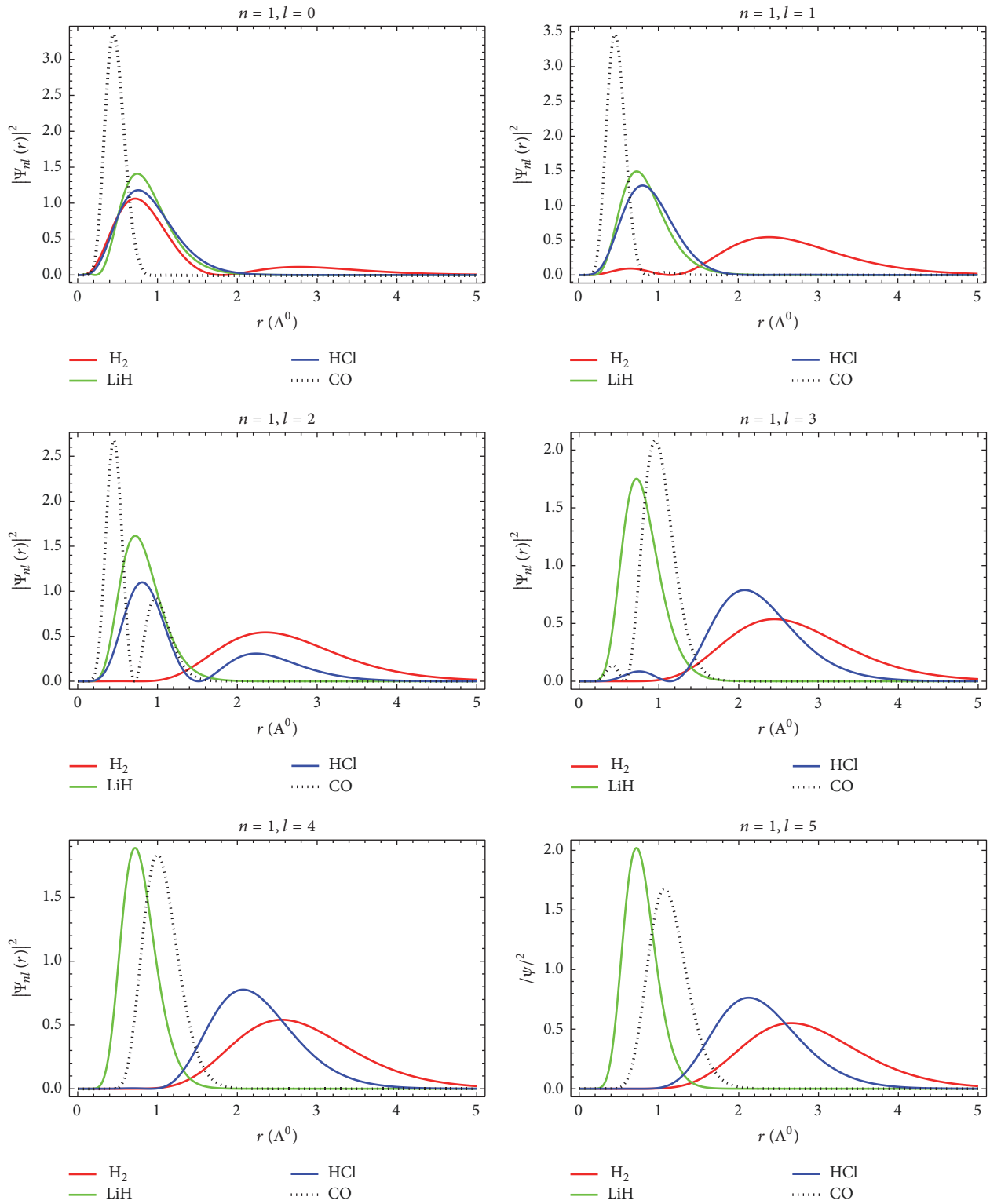


FIGURE 9: Probability density plots for the interaction potential with orbital angular quantum number  $l = 0, 1, 2, 3, 4,$  and  $5$ .

where the wave function  $\psi(s)$  is defined as the logarithmic derivative

$$\frac{\phi^1(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}, \quad (5)$$

where  $\pi(s)$  is at most polynomial of degree one.

Likewise, the hypergeometric type function  $\chi(s)$  in (4) for a fixed  $n$  is given by the Rodrigue relation

$$\chi_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma''(s) \rho(s)]. \quad (6)$$

$B_n$  is the normalization constant and the weight function  $\rho(s)$  satisfies the condition

$$\frac{d}{ds} (\sigma(s) \rho(s)) = \tau(s) \rho(s) \quad (7)$$

such that

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s). \quad (8)$$

In order to accomplish the conditions imposed on the weight function  $\rho(s)$ , it is necessary that the classical orthogonal polynomials  $\tau(s)$  be equal to zero and its derivative be less than zero; that is,

$$\frac{d\tau(s)}{ds} < 0. \quad (9)$$

Therefore, the function  $\pi(s)$  and the parameter  $\lambda$  required for the NU method are defined as follows:

$$\pi(s) = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma}, \quad (10)$$

$$\lambda = k + \pi'(s). \quad (11)$$

The  $k$ -values in (10) are possible to evaluate if the expression under the square root must be square of polynomials. This is possible, if and only if its discriminant is zero. With this, a new eigenvalue equation becomes

$$\lambda = \lambda_n = \frac{nd\tau}{ds} - \frac{n(n-1)}{2} \frac{d^2\sigma}{ds^2}, \quad n = 0, 1, 2, \dots, \quad (12)$$

where  $\tau(s)$  is as defined in (8) and, on comparing (11) and (12), we obtain the energy eigenvalues.

### 3. Radial Solution of Schrodinger Equation

The Schrodinger wave equation is given by

$$\frac{d^2\psi(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[ E - V(r) - \frac{\hbar^2 l(l+1)}{2\mu r^2} \right] \psi(r) = 0. \quad (13)$$

Substituting (1) into (13) gives

$$\frac{d^2\psi(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[ E + \frac{V_0 e^{-2\alpha r}}{(1 - e^{-2\alpha r})} + \frac{Ae^{-\alpha r}}{r} - \frac{B}{r^2} - C - \frac{\hbar^2 l(l+1)}{2\mu r^2} \right] \psi(r) = 0. \quad (14)$$

Equation (14) can only be solved analytically to obtain exact solution if the angular orbital momentum number  $l = 0$ . However, for  $l > 0$  (14) can only be solve by using some approximations to the centrifugal term. Greene Aldrich approximation is best suitable for (14).

Let us define Greene Aldrich approximation as

$$\begin{aligned} \frac{1}{r^2} &= \frac{4\alpha^2 e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} \implies \\ \frac{1}{r} &= \frac{2\alpha e^{-\alpha r}}{(1 - e^{-2\alpha r})}. \end{aligned} \quad (15)$$

Substituting (15) into (14) with the transformation  $s = e^{-2\alpha r}$  gives

$$\begin{aligned} \frac{d^2\psi(s)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{d\psi(s)}{ds} + \frac{1}{s^2(1-s)^2} [-\epsilon^2(1-s)^2 \\ + \delta^2 s(1-s) + \sigma_1 s(1-s) - \sigma_2 s - \sigma_3(1-s)^2 \\ - sl(l+1)] \psi(s) = 0, \end{aligned} \quad (16)$$

where

$$\begin{aligned} \epsilon^2 &= -\frac{\mu E}{2\hbar^2 \alpha^2}, \\ \delta^2 &= \frac{\mu V_0}{2\hbar^2 \alpha^2}, \\ \sigma_1 &= \frac{\mu A}{\hbar^2 \alpha}, \\ \sigma_2 &= \frac{2\mu B}{\hbar^2}, \\ \sigma_3 &= \frac{\mu C}{2\hbar^2 \alpha^2}. \end{aligned} \quad (17)$$

Simplifying (16) further reduced to

$$\begin{aligned} \frac{d^2\psi(s)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{d\psi(s)}{ds} \\ + \frac{1}{s^2(1-s)^2} [- (\epsilon^2 + \delta^2 + \sigma_1 + \sigma_3) s^2 \\ + (2\epsilon^2 + \delta^2 + \sigma_1 - \sigma_2 + 2\sigma_3 - l(l+1)) s \\ - (\epsilon^2 + \sigma_3)] \psi(s) = 0. \end{aligned} \quad (18)$$

Comparing (18) to (2) we obtained the following:

$$\begin{aligned} \sigma(s) &= s(1-s), \\ \tilde{\sigma}(s) &= -(\epsilon^2 + \delta^2 + \sigma_1 + \sigma_3) s^2 \\ &\quad + (2\epsilon^2 + \delta^2 + \sigma_1 - \sigma_2 + 2\sigma_3 - l(l+1)) s \\ &\quad - (\epsilon^2 + \sigma_3), \\ \tilde{\tau}(s) &= (1-s). \end{aligned} \quad (19)$$

Then, using (10), the polynomial equation  $\pi(s)$  then becomes

$$\pi(s) = \frac{-s}{2} \pm \sqrt{\left(\frac{1}{4} + \varepsilon^2 + \delta^2 + \sigma_1 + \sigma_3 - k\right) s^2 - (2\varepsilon^2 + \delta^2 + \sigma_1 - \sigma_2 + 2\sigma_3 - l(l+1) - k) s - (\varepsilon^2 + \sigma_3)} \quad (20)$$

To find the value of  $k$  we consider the discriminant such that  $b^2 - 4ac = 0$

$$\begin{aligned} a &= \left(\frac{1}{4} + \varepsilon^2 + \delta^2 + \sigma_1 + \sigma_3 - k\right), \\ b &= -(2\varepsilon^2 + \delta^2 + \sigma_1 - \sigma_2 + 2\sigma_3 - l(l+1) - k), \\ c &= -(\varepsilon^2 + \sigma_3). \end{aligned} \quad (21)$$

Hence,

$$\begin{aligned} k_1 &= -(\sigma_2 - \sigma_1 - \delta^2 + l(l+1)) \\ &\quad + \sqrt{(\varepsilon^2 + \sigma_3)(4\sigma_2 + 4l(l+1) + 1)}, \\ k_2 &= -(\sigma_2 - \sigma_1 - \delta^2 + l(l+1)) \\ &\quad - \sqrt{(\varepsilon^2 + \sigma_3)(4\sigma_2 + 4l(l+1) + 1)}. \end{aligned} \quad (22)$$

Substituting the values of  $k_1$  and  $k_2$  into (20), then the four values of  $\pi(s)$  are given below.

$$\begin{aligned} \pi(s) &= \frac{-s}{2} \\ &\pm \left\{ \left(\frac{1}{2} \sqrt{4\sigma_2 + 4l(l+1) + 1} + \sqrt{(\varepsilon^2 + \sigma_3)}\right) s - \sqrt{(\varepsilon^2 + \sigma_3)}, \quad k_1 = -(\sigma_2 - \sigma_1 - \delta^2 + l(l+1)) + \sqrt{(\varepsilon^2 + \sigma_3)(4\sigma_2 + 4l(l+1) + 1)} \right. \\ &\quad \left. \pm \left(\frac{1}{2} \sqrt{4\sigma_2 + 4l(l+1) + 1} - \sqrt{(\varepsilon^2 + \sigma_3)}\right) s - \sqrt{(\varepsilon^2 + \sigma_3)}, \quad k_2 = -(\sigma_2 - \sigma_1 - \delta^2 + l(l+1)) - \sqrt{(\varepsilon^2 + \sigma_3)(4\sigma_2 + 4l(l+1) + 1)} \right. \end{aligned} \quad (22a)$$

$\pi(s)$  has four solutions and one of the solutions satisfied bound state condition which is

$$\begin{aligned} \pi(s) &= -\frac{s}{2} \\ &- \left[ \left(\frac{1}{2} \sqrt{4\sigma_2 + 4l(l+1) + 1} - \sqrt{(\varepsilon^2 + \sigma_3)}\right) s \right. \\ &\quad \left. - \sqrt{(\varepsilon^2 + \sigma_3)} \right]. \end{aligned} \quad (22b)$$

$d\tau(s)/ds < 0$  is the condition for bound state solution. Using (8) we have it that

$$\begin{aligned} \tau(s) &= 1 - 2s \\ &- 2 \left[ \left(\frac{1}{2} \sqrt{4\sigma_2 + 4l(l+1) + 1} - \sqrt{(\varepsilon^2 + \sigma_3)}\right) s \right. \\ &\quad \left. - \sqrt{(\varepsilon^2 + \sigma_3)} \right] \end{aligned} \quad (23)$$

such that

$$\begin{aligned} \tau'(s) &= -2 - 2 \left[ \left(\frac{1}{2} \sqrt{4\sigma_2 + 4l(l+1) + 1} - \sqrt{(\varepsilon^2 + \sigma_3)}\right) \right] \\ &< 0 \end{aligned} \quad (24)$$

which satisfies the bound state condition. However using (11)

$$\begin{aligned} \lambda &= k + \pi'(s) \\ &= -\frac{1}{2} - \left(\frac{1}{2} \sqrt{4\sigma_2 + 4l(l+1) + 1} - \sqrt{(\varepsilon^2 + \sigma_3)}\right) \\ &\quad + \sqrt{(\varepsilon^2 + \sigma_3)(4\sigma_2 + 4l(l+1) + 1)} \\ &\quad - (\sigma_2 - \sigma_1 - \delta^2 + l(l+1)). \end{aligned} \quad (25)$$

Using (12)

$$\begin{aligned} \lambda_n &= n^2 + n + n \sqrt{4\sigma_2 + 4l(l+1) + 1} \\ &\quad - 2n \sqrt{(\varepsilon^2 + \sigma_3)}. \end{aligned} \quad (26)$$

Equating (25) and (26) gives the result

$$\varepsilon^2 = \left[ \frac{(n^2 + n + 1/2) + (n + 1/2) \sqrt{4\sigma_2 + 4l(l+1) + 1} + (\sigma_2 - \sigma_1 - \delta^2 + l(l+1))}{(2n + 1 + \sqrt{4\sigma_2 + 4l(l+1) + 1})} \right]^2 - \sigma_3. \quad (27)$$

Substituting parameters of (17) into (27) gives

$$E_{nl} = -\frac{2\hbar^2\alpha^2}{\mu} \left[ \frac{(2\mu B/\hbar^2 - \mu A/\hbar^2\alpha - \mu V_0/2\hbar^2\alpha^2 + l(l+1)) + (n^2 + n + 1/2) + (n+1/2)\sqrt{(8\mu B/\hbar^2 + 4l(l+1) + 1)}}{(1 + 2n + \sqrt{(8\mu B/\hbar^2 + 4l(l+1) + 1)})} \right]^2 + c \quad (28)$$

Equation (28) is the energy for the combined potential.

3.1. *Calculation of the Wave Function.* By using (5), but

$$\begin{aligned} \sigma(s) &= s - s^2, \\ \pi(s) &= -\frac{s}{2} \\ &- \left[ \left( \frac{1}{2} \sqrt{(4\sigma_2 + 4l(l+1) + 1)} + \sqrt{(\varepsilon^2 + \sigma_3)} \right) s \right. \\ &\left. - \sqrt{(\varepsilon^2 + \sigma_3)} \right], \end{aligned} \quad (29)$$

then

$$\begin{aligned} \frac{\pi(s)}{\sigma(s)} &= -\frac{1}{2(1-s)} \\ &- \frac{1}{s(1-s)} \left[ \left( \frac{1}{2} \sqrt{(4\sigma_2 + 4l(l+1) + 1)} \right. \right. \\ &\left. \left. + \sqrt{(\varepsilon^2 + \sigma_3)} \right) s - \sqrt{(\varepsilon^2 + \sigma_3)} \right], \end{aligned} \quad (30)$$

$$\begin{aligned} \frac{\phi^1(s)}{\phi(s)} &= \frac{\pi(s)}{\sigma(s)} = -\frac{1}{2(1-s)} \\ &- \frac{1}{s(1-s)} \left[ \left( \frac{1}{2} \sqrt{(4\sigma_2 + 4l(l+1) + 1)} \right. \right. \\ &\left. \left. + \sqrt{(\varepsilon^2 + \sigma_3)} \right) s - \sqrt{(\varepsilon^2 + \sigma_3)} \right], \end{aligned} \quad (31)$$

$$\begin{aligned} \frac{\phi^1(s)}{\phi(s)} &= -\frac{1}{2(1-s)} \\ &- \frac{1}{s(1-s)} \left[ \left( \frac{1}{2} \sqrt{(4\sigma_2 + 4l(l+1) + 1)} \right. \right. \\ &\left. \left. + \sqrt{(\varepsilon^2 + \sigma_3)} \right) s - \sqrt{(\varepsilon^2 + \sigma_3)} \right]. \end{aligned} \quad (32)$$

Taking integral of (32) gives

$$\begin{aligned} \int \frac{\phi^1(s)}{\phi(s)} ds &= -\frac{1}{2} \int \frac{1}{(1-s)} ds \\ &- \frac{1}{2} \sqrt{(4\sigma_2 + 4l(l+1) + 1)} \int \frac{1}{(1-s)} ds \end{aligned}$$

$$\begin{aligned} &- \sqrt{(\varepsilon^2 + \sigma_3)} \int \frac{1}{(1-s)} ds \\ &+ \sqrt{(\varepsilon^2 + \sigma_3)} \int \left[ \frac{1}{s} + \frac{1}{(1-s)} \right] ds \end{aligned} \quad (33)$$

which then leads to

$$\begin{aligned} \ln \phi(s) &= \ln [1-s]^{1/2} + \ln [1-s]^{(1/2)\sqrt{(4\sigma_2 + 4l(l+1) + 1)}} \\ &+ \ln [1-s]^{\sqrt{(\varepsilon^2 + \sigma_3)}} + \ln [s]^{\sqrt{(\varepsilon^2 + \sigma_3)}} \\ &- \ln [1-s]^{\sqrt{(\varepsilon^2 + \sigma_3)}}. \end{aligned} \quad (34)$$

Equation (34) can further be reduced to

$$\begin{aligned} \ln \phi(s) &= \ln \left\{ [1-s]^{(1/2 + (1/2)\sqrt{(4\sigma_2 + 4l(l+1) + 1)})} \cdot [s]^{\sqrt{(\varepsilon^2 + \sigma_3)}} \right\}. \end{aligned} \quad (35)$$

The integration constant is ignored since the final equation is to be expressed in terms of Rodrique relation with normalization constant. Taking exponent of (35) gives

$$\phi(s) = [1-s]^{(1/2 + (1/2)\sqrt{(4\sigma_2 + 4l(l+1) + 1)})} s^{\sqrt{(\varepsilon^2 + \sigma_3)}}. \quad (36)$$

Equation (36) gives the first part of the wave function. To determine the second part of the wave function, we first of all calculate the weight function.

3.2. *Calculation of Weight Function.* Using (7)

$$\begin{aligned} \frac{d}{ds} (\sigma(s) \rho(s)) &= \tau(s) \rho(s) \implies \\ \int \frac{\rho'(s)}{\rho(s)} ds &= \int \frac{\tau(s) - \sigma'(s)}{\sigma(s)} ds. \end{aligned} \quad (37)$$

Substituting the parameters gives

$$\ln \rho(s) = \int \frac{1-2s-2 \left[ \left( (1/2) \sqrt{(4\sigma_2+4l(l+1)+1)} + \sqrt{(\epsilon^2+\sigma_3)} \right) s \right] + 2\sqrt{(\epsilon^2+\sigma_3)} - 1 + 2s}{s(1-s)} ds. \quad (38)$$

Integrating (38) gives

$$\rho(s) = [1-s]^{(-2\sqrt{(\epsilon^2+\sigma_3)}-\sqrt{(4\sigma_2+4l(l+1)+1)})} s^{4\sqrt{(\epsilon^2+\sigma_3)}}. \quad (39)$$

Rewriting (39) in its Rodrigue form by making use of (6) gives

$$\begin{aligned} Y_n(s) &= B_n(s) s^{-4\sqrt{(\epsilon^2+\sigma_3)}} [1 \\ &\quad - s]^{-(2\sqrt{(\epsilon^2+\sigma_3)}-\sqrt{(4\sigma_2+4l(l+1)+1)})} \\ &\quad \times \frac{d^n}{ds^n} \left[ s^{n+4\sqrt{(\epsilon^2+\sigma_3)}} [1 \right. \\ &\quad \left. - s]^{n+(-2\sqrt{(\epsilon^2+\sigma_3)}-\sqrt{(4\sigma_2+4l(l+1)+1)})} \right]. \end{aligned} \quad (40)$$

Let us define standard associated Laguerre polynomial as

$$\begin{aligned} \chi_n(s) &= B_n(s) s^{-v} (1-s)^{-\mu} \frac{d^n}{ds^n} [s^{n+v} (1-s)^{n+\mu}] \\ &= P_n^{[\mu+v, \mu]}(1-s). \end{aligned} \quad (41)$$

$$\Psi_n(s) = \phi(s) Y_n(s)$$

$$\begin{aligned} &= B_n(s) P_n^{[(2\sqrt{(\mu c/2\hbar^2\alpha^2-\mu E/2\hbar^2\alpha^2)-4\sqrt{(8\mu B/\hbar^2+4l(l+1)+1)}), (-2\sqrt{(\mu c/2\hbar^2\alpha^2-\mu E/2\hbar^2\alpha^2)-4\sqrt{(8\mu B/\hbar^2+4l(l+1)+1)})}] (1-e^{-2\alpha r}) \\ &\quad \times [1-e^{-2\alpha r}]^{(1/2+(1/2)\sqrt{(8\mu B/\hbar^2+4l(l+1)+1)})} (e^{-2\alpha r})^{\sqrt{((\mu c/2\hbar^2\alpha^2-\mu E/2\hbar^2\alpha^2))}}. \end{aligned} \quad (44a)$$

Equation (44) is the total wave function for the proposed potential. Equation (44) can further be reduced to

$$\begin{aligned} \Psi_n(s) &= \phi(s) Y_n(s) \\ &= B_n(s) P_n^{[(2\sqrt{(\mu c/2\hbar^2\alpha^2-\mu E/2\hbar^2\alpha^2)-4\sqrt{(8\mu B/\hbar^2+4l(l+1)+1)}), (-2\sqrt{(\mu c/2\hbar^2\alpha^2-\mu E/2\hbar^2\alpha^2)-4\sqrt{(8\mu B/\hbar^2+4l(l+1)+1)})}] (1-s) \\ &\quad \times [1-s]^{(1/2+(1/2)\sqrt{(8\mu B/\hbar^2+4l(l+1)+1)})} (s)^{\sqrt{((\mu c/2\hbar^2\alpha^2-\mu E/2\hbar^2\alpha^2))}}. \end{aligned} \quad (44b)$$

The normalized wave function of (44b) is given as

$$\begin{aligned} \Psi_n(s) &= \frac{1}{\sqrt{S_1}} (s) P_n^{[(2\sqrt{(\mu c/2\hbar^2\alpha^2-\mu E/2\hbar^2\alpha^2)-4\sqrt{(8\mu B/\hbar^2+4l(l+1)+1)}), (-2\sqrt{(\mu c/2\hbar^2\alpha^2-\mu E/2\hbar^2\alpha^2)-4\sqrt{(8\mu B/\hbar^2+4l(l+1)+1)})}] (1-s) \\ &\quad \times [1-s]^{(1/2+(1/2)\sqrt{(8\mu B/\hbar^2+4l(l+1)+1)})} (s)^{\sqrt{((\mu c/2\hbar^2\alpha^2-\mu E/2\hbar^2\alpha^2))}}, \end{aligned} \quad (44c)$$

Then rewriting (40) in terms of (41) gives the second part of the wave function as

$$\begin{aligned} Y_n(s) &= B_n(s) \\ &\quad \cdot P_n^{[(2\sqrt{(\epsilon^2+\sigma_3)-4\sqrt{(4\sigma_2+4l(l+1)+1)}), (-2\sqrt{(\epsilon^2+\sigma_3)-4\sqrt{(4\sigma_2+4l(l+1)+1)})}] (1-s). \end{aligned} \quad (42)$$

Hence the total wave function is given by

$$\begin{aligned} \Psi_n(s) &= \phi(s) Y_n(s) = B_n(s) \\ &\quad \cdot P_n^{[(2\sqrt{(\epsilon^2+\sigma_3)-4\sqrt{(4\sigma_2+4l(l+1)+1)}), (-2\sqrt{(\epsilon^2+\sigma_3)-4\sqrt{(4\sigma_2+4l(l+1)+1)})}] (1-s) \\ &\quad \times [1-s]^{(1/2+(1/2)\sqrt{(4\sigma_2+4l(l+1)+1)})} s^{\sqrt{(\epsilon^2+\sigma_3)}}. \end{aligned} \quad (43)$$

Substituting (17) into (43) reduced it to



where the normalization constant is given as

$$B_n = 1/\sqrt{s_1}, \text{ where}$$

$$s_1 = -(-1)^n \frac{\Gamma(n - 2\xi_1 - 4\Lambda + 1)^2 \Gamma(n + 2\xi_1 - 4\Lambda + 1)^2}{2\alpha\Gamma(n + 1)\Gamma(1 - 2\xi_1 - 4\Lambda)} \times \frac{\Gamma(n + r + 1 - 8\Lambda)}{\Gamma(n + 1 - 8\Lambda)} \cdot \sum_{p=0}^n \sum_{r=0}^n (-1)^{p+r} \frac{2^{-n-r} (2-s)^p}{p!(n-p)!r!(n-r)!\Gamma(n + 2\xi_1 - 4\Lambda - p + 1)\Gamma(p - 2\xi_1 - 4\Lambda + 1)\Gamma(r + 2\xi_1 - 4\Lambda + 1)} \times \frac{\Gamma(\alpha_0 + 1)\Gamma(\Lambda + 2)}{\alpha_0\Gamma(\alpha_0 + \Lambda + 2)}. \quad (44d)$$

The detail of the analytical solution to the normalization constant is given in Section 7.

#### 4. Deductions from the Proposed Potential

4.1. *Hulthen Potential.* Setting  $A = B = C = 0$  in (1) results in Hulthen potential given as

$$V(r) = \frac{-V_0 e^{-2\alpha r}}{(1 - e^{-2\alpha r})}. \quad (45)$$

The energy of this potential is given as

$$E_{nl} = -\frac{2\hbar^2\alpha^2}{\mu} \left[ \frac{(-\mu V_0/2\hbar^2\alpha^2 + l(l+1)) + (n^2 + n + 1/2) + (n + 1/2)\sqrt{4l(l+1) + 1}}{(1 + 2n + \sqrt{4l(l+1) + 1})} \right]^2. \quad (46)$$

However  $\sqrt{4l(l+1) + 1} = 2l + 1$ , and then (46) becomes

$$E_{nl} = -\frac{2\hbar^2\alpha^2}{\mu} \left[ \frac{(-\mu V_0/2\hbar^2\alpha^2) + (n+l)(n+l+2) + 1}{2(n+l+1)} \right]^2. \quad (47a)$$

According to Arda and Sever, 2012, the standard Hulthen potential is given by

$$E_{nl} = -\frac{\beta^2\hbar^2}{2m} \left[ \frac{(n+l)(n+l+2) + 1 - 2mV_0/\beta^2\alpha^2}{2(n+l+1)} \right]^2. \quad (47b)$$

Setting  $\alpha = \beta/2$  and  $\mu = m$  in (47a) results in (47b). Equation (47b) is computed from parameters taken from Arda and Sever, 2012 [32], for comparison. However, the adopted parameters are  $V_0 = \beta = \delta$  and  $\mu = 1.0$ . Table 18 shows the bound state solution of Hulthen potential of the present work in comparison to other works reported in existing literature.

4.2. *Yukawa Potential.* Setting  $V_0 = B = C = 0$  in (1) then the potential reduced to Yukawa potential.

$$V(r) = -\frac{Ae^{-\alpha r}}{r}. \quad (48)$$

The corresponding energy equation for this potential is given as

$$E_{nl} = -\frac{2\hbar^2\alpha^2}{\mu} \left[ \frac{(-\mu A/\hbar^2\alpha + l(l+1)) + (n^2 + n + 1/2) + (n + 1/2)\sqrt{4l(l+1) + 1}}{(1 + 2n + \sqrt{4l(l+1) + 1})} \right]^2. \quad (49a)$$

Equation (49a) can further be simplified as

$$E_{nl} = -\frac{\hbar^2 \alpha^2}{\mu} \left[ \frac{(\mu A / \hbar^2 \alpha) - (n+1)^2 - l(2n+l+2)}{(n+l+1)} \right]^2. \quad (49b)$$

Hamzavi et al. [33] present the eigenenergy equation for Yukawa potential as

$$E_{nl} = -\frac{a^2}{2m} \left[ \frac{(mV_0/a) - (n+1)^2 - l(2n+l+2)}{(n+l+1)} \right]^2. \quad (49c)$$

Equations (49b) and (49c) are the same with just variation in parameter where

$$\begin{aligned} E_{nl} &= a = \alpha, \\ 2m &= \mu, \\ A &= V_0, \\ \hbar &= 1. \end{aligned} \quad (50)$$

4.3. *Inversely Quadratic Potential.* Setting  $V_0 = A = C = 0$  in (1) then the potential reduced to inversely quadratic potential.

$$V(r) = \frac{B}{r^2}. \quad (51)$$

The corresponding energy for this potential is given as

$$E_{nl} = -\frac{2\hbar^2 \alpha^2}{\mu} \left[ \frac{(2\mu B / \hbar^2 + l(l+1)) + (n^2 + n + 1/2) + (n+1/2) \sqrt{(8\mu B / \hbar^2 + 4l(l+1) + 1)}}{(1 + 2n + \sqrt{(8\mu B / \hbar^2 + 4l(l+1) + 1)})} \right]^2. \quad (52)$$

## 5. Hellmann-Feynman Theorem

Hellmann-Feynman theorem (HFT) is commonly used in the calculation of intermolecular forces in molecules [34]. However, in order to engage HFT in calculating the expectation values, one then needs to promote the fixed parameters which appear in the Hamiltonian to be continuous variable in order to ease the mathematical purpose of taking the derivatives. This theorem states that if Hamiltonian  $H$  for a particular quantum mechanical system is given as a function of some parameters  $q$ , then let  $E(q)$  and  $\Psi(q)$  be the eigenvalues and the eigenfunctions of Hamiltonian  $H(q)$ , respectively; then

$$\frac{\partial E_n(q)}{\partial q} = \left\langle \Psi(q) \left| \frac{\partial H(q)}{\partial q} \right| \Psi(q) \right\rangle. \quad (53)$$

However, the Hamiltonian which contains the effective potential can be expressed as

$$\begin{aligned} H &= -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{v_0 e^{-2\alpha r}}{(1 - e^{-2\alpha r})} - \frac{Ae^{-\alpha r}}{r} \\ &+ \frac{B}{r^2} + C. \end{aligned} \quad (54)$$

Let us recall the energy equation as given in (28).

5.1. *Expectation Value of  $\langle r^{-2} \rangle$ .* Substituting  $q = l$  into (53) then

$$\frac{\partial E_n(l)}{\partial l} = \left\langle \Psi(l) \left| \frac{\partial H(l)}{\partial l} \right| \Psi(l) \right\rangle. \quad (55)$$

Taking the partial derivative of (28) with respect to  $l$  gives

$$\begin{aligned} \frac{\partial E_n(l)}{\partial l} &= \frac{-4\hbar^2 \alpha^2}{\mu} \left\{ \left( \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right] [(2l+1) + (4n+2)(2l+1)] \right. \right. \\ &- \left. \left[ \frac{(2\mu B / \hbar^2 - \mu A / \hbar^2 \alpha - \mu V_0 / 2\hbar^2 \alpha^2 + l(l+1))(4l+2)}{\sqrt{8\mu B / \hbar^2 + 4l(l+1) + 1}} + \frac{(n^2 + n + 1/2)(4l+2)}{\sqrt{8\mu B / \hbar^2 + 4l(l+1) + 1}} + \left(n + \frac{1}{2}\right)(4l+2) \right] \right) \\ &\times \left( \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right]^2 \right)^{-1} \left. \right\} \\ &\times \left\{ \frac{(2\mu B / \hbar^2 - \mu A / \hbar^2 \alpha - \mu V_0 / 2\hbar^2 \alpha^2 + l(l+1)) + (n^2 + n + 1/2) + (n+1/2) \sqrt{8\mu B / \hbar^2 + 4l(l+1) + 1}}{\left[ 1 + 2n + \sqrt{8\mu B / \hbar^2 + 4l(l+1) + 1} \right]} \right\}. \end{aligned} \quad (56)$$

Taking the partial derivative of (54) with respect to  $l$  gives

$$\left\langle \Psi(l) \left| \frac{\partial H(l)}{\partial l} \right| \Psi(l) \right\rangle = \frac{\hbar^2}{2\mu} (2l+1) \langle r^{-2} \rangle. \quad (57)$$

Equating (56) to (57) gives the expectation values of  $\langle r^{-2} \rangle$  for different orbital quantum number. Hence,

$$\begin{aligned} \langle r^{-2} \rangle &= \frac{-8\alpha^2}{(2l+1)} \left\{ \left( \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right] [(2l+1) + (4n+2)(2l+1)] \right. \right. \\ &\quad \left. \left. - \left[ \frac{(2\mu B/\hbar^2 - \mu A/\hbar^2 \alpha - \mu V_0/2\hbar^2 \alpha^2 + l(l+1))(4l+2)}{\sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} + \frac{(n^2 + n + 1/2)(4l+2)}{\sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} + \left(n + \frac{1}{2}\right)(4l+2) \right] \right) \right. \\ &\quad \left. \times \left( \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right]^2 \right)^{-1} \right\} \\ &\quad \times \left\{ \frac{(2\mu B/\hbar^2 - \mu A/\hbar^2 \alpha - \mu V_0/2\hbar^2 \alpha^2 + l(l+1)) + (n^2 + n + 1/2) + (n+1/2)\sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}}{\left[ 1 + 2n + \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1} \right]} \right\}. \end{aligned} \quad (58)$$

5.2. Expectation Value of  $\langle r^{-1} \rangle$ . Taking the partial derivative of (28) with respect to  $A$  gives

$$\begin{aligned} \frac{\partial E_{nl}}{\partial A} &= \frac{4\alpha}{\left[ 1 + 2n + \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1} \right]^2} \left\{ \left( \frac{2\mu B}{\hbar^2} \right. \right. \\ &\quad \left. \left. - \frac{\mu A}{\hbar^2 \alpha} - \frac{\mu V_0}{2\hbar^2 \alpha^2} + l(l+1) \right) + \left( n^2 + n + \frac{1}{2} \right) + \left( n + \frac{1}{2} \right) \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right\}. \end{aligned} \quad (59)$$

Also, taking the partial derivative of (54) with respect to  $A$  gives

$$\left\langle \Psi(A) \left| \frac{\partial H(A)}{\partial A} \right| \Psi(A) \right\rangle = -e^{-\alpha r} \langle r^{-1} \rangle. \quad (60)$$

Equating (59) to (60) then gives

$$\begin{aligned} \langle r^{-1} \rangle &= \frac{-4\alpha e^{\alpha r}}{\left[ 1 + 2n + \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1} \right]^2} \left\{ \left( \frac{2\mu B}{\hbar^2} \right. \right. \\ &\quad \left. \left. - \frac{\mu A}{\hbar^2 \alpha} - \frac{\mu V_0}{2\hbar^2 \alpha^2} + l(l+1) \right) + \left( n^2 + n + \frac{1}{2} \right) + \left( n + \frac{1}{2} \right) \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right\}. \end{aligned} \quad (61)$$

5.3. Expectation Values for  $\langle T \rangle$  and  $\langle p^2 \rangle$ . Taking the partial derivative of (28) with respect to  $\mu$ , this then gives

$$\begin{aligned} \frac{\partial E_n(\mu)}{\partial \mu} &= \frac{-4\hbar^2 \alpha^2}{\mu} \left\{ \left( \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right] \left[ \frac{2B}{\hbar^2} - \frac{A}{\hbar^2 \alpha} - \frac{v_0}{2\hbar^2 \alpha^2} + \frac{(n+1/2)4B}{\hbar^2 \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} \right] \right. \right. \\ &\quad \left. \left. - \left[ \frac{(2\mu B/\hbar^2 - \mu A/\hbar^2 \alpha - \mu V_0/2\hbar^2 \alpha^2 + l(l+1))4B}{\hbar^2 \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} + \frac{(n^2 + n + 1/2)(4B)}{\hbar^2 \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} + \frac{(n+1/2)(4B)}{\hbar^2} \right] \right) \right. \\ &\quad \left. \times \left( \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right]^2 \right)^{-1} \right\} \end{aligned}$$

$$\times \left\{ \frac{\left(2\mu B/\hbar^2 - \mu A/\hbar^2 \alpha - \mu V_0/2\hbar^2 \alpha^2 + l(l+1)\right) + \left(n^2 + n + 1/2\right) + (n+1/2) \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}}{\left[1 + 2n + \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}\right]} \right\}$$

$$+ \frac{2\hbar^2 \alpha^2}{\mu^2} \left\{ \frac{\left(2\mu B/\hbar^2 - \mu A/\hbar^2 \alpha - \mu V_0/2\hbar^2 \alpha^2 + l(l+1)\right) + \left(n^2 + n + 1/2\right) + (n+1/2) \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}}{\left[1 + 2n + \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}\right]} \right\}^2. \quad (62)$$

However, taking the partial derivative of (54) with respect to  $\mu$  gives

$$\left\langle \Psi(\mu) \left| \frac{\partial H(A)}{\partial A} \right| \Psi(\mu) \right\rangle = -\frac{\hbar^2}{2\mu^2} \frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu^2} \frac{l(l+1)}{r^2}$$

$$= \frac{1}{\mu} \left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} \right) \Rightarrow \quad (63)$$

$$-\frac{1}{\mu} \left( \frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} \right) \Rightarrow$$

$$-\frac{1}{\mu} \langle T \rangle = -\frac{1}{\mu} (H - V).$$

Hence,

$$\left\langle \Psi(\mu) \left| \frac{\partial H(A)}{\partial A} \right| \Psi(\mu) \right\rangle = -\frac{1}{\mu} \langle T \rangle \quad (64)$$

$$\Rightarrow -\frac{1}{\mu} (H - V).$$

From the relation  $T = p^2/2\mu$ , substituting for  $T$  in (64) gives

$$\left\langle \Psi(\mu) \left| \frac{\partial H(A)}{\partial A} \right| \Psi(\mu) \right\rangle = -\frac{1}{\mu} (H - V) \quad (65)$$

$$= -\frac{1}{2\mu^2} \langle p^2 \rangle.$$

Equating (62) to (64) gives the expectation value of  $\langle T \rangle$ . Therefore,

$$\langle T \rangle = 4\hbar^2 \alpha^2 \left\{ \left( \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right] \left[ \frac{2B}{\hbar^2} - \frac{A}{\hbar^2 \alpha} - \frac{v_0}{2\hbar^2 \alpha^2} + \frac{(n+1/2)4B}{\hbar^2 \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} \right] \right. \right.$$

$$\left. - \left[ \frac{(2\mu B/\hbar^2 - \mu A/\hbar^2 \alpha - \mu V_0/2\hbar^2 \alpha^2 + l(l+1))4B}{\hbar^2 \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} + \frac{(n^2 + n + 1/2)(4B)}{\hbar^2 \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} + \frac{(n+1/2)(4B)}{\hbar^2} \right] \right)$$

$$\times \left( \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right]^2 \right)^{-1} \left. \right\} \quad (66)$$

$$\times \left\{ \frac{\left(2\mu B/\hbar^2 - \mu A/\hbar^2 \alpha - \mu V_0/2\hbar^2 \alpha^2 + l(l+1)\right) + \left(n^2 + n + 1/2\right) + (n+1/2) \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}}{\left[1 + 2n + \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}\right]} \right\}$$

$$- \frac{2\hbar^2 \alpha^2}{\mu} \left\{ \frac{\left(2\mu B/\hbar^2 - \mu A/\hbar^2 \alpha - \mu V_0/2\hbar^2 \alpha^2 + l(l+1)\right) + \left(n^2 + n + 1/2\right) + (n+1/2) \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}}{\left[1 + 2n + \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}\right]} \right\}^2.$$

TABLE I: Molecular parameter using Nikiforov-Uvarov method.

Molecule	A (Å)	B (1/Å)	C (Å)	$\alpha$	$\mu$ (amu)
Hydrogen (H <sub>2</sub> )	0.7416	1.9426	1.440558	0.20990	0.5039100
Lithium hydride (LiH)	1.5956	1.1280	1.7998368	1.55000	0.8801221
Hydrogen chloride (HCl)	1.2746	1.8677	2.38057	0.20039	0.9801045
Carbon (II) oxide (CO)	1.1283	2.2994	2.59441	0.39000	6.8606719

Also, equating (62) to (65) gives  $\langle p^2 \rangle$ . Thus,

$$\langle p^2 \rangle = 8\hbar^2\alpha^2\mu \left\{ \left( \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right] \right. \right. \\ \left. \left. + \frac{2B}{\hbar^2} - \frac{A}{\hbar^2\alpha} - \frac{v_0}{2\hbar^2\alpha^2} \right. \right. \\ \left. \left. + \frac{(n+1/2)4B}{\hbar^2\sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} \right. \right. \\ \left. \left. - \left[ \frac{(2\mu B/\hbar^2 - \mu A/\hbar^2\alpha - \mu V_0/2\hbar^2\alpha^2 + l(l+1))4B}{\hbar^2\sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} \right. \right. \right. \\ \left. \left. \left. + \frac{(n^2 + n + 1/2)(4B)}{\hbar^2\sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} + \frac{(n+1/2)(4B)}{\hbar^2} \right] \right) \right\} \\ \times \left( \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right]^2 \right)^{-1} \\ \times \left\{ \left( \left( \frac{2\mu B}{\hbar^2} - \frac{\mu A}{\hbar^2\alpha} - \frac{\mu V_0}{2\hbar^2\alpha^2} + l(l+1) \right) + \left( n^2 + n \right. \right. \right. \\ \left. \left. \left. + \frac{1}{2} \right) + \left( n + \frac{1}{2} \right) \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right) \times \left( \left[ 1 + 2n \right. \right. \right. \\ \left. \left. \left. + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right] \right)^{-1} \right\} - 4\hbar^2\alpha^2 \left\{ \left( \left( \frac{2\mu B}{\hbar^2} \right. \right. \right. \\ \left. \left. \left. - \frac{\mu A}{\hbar^2\alpha} - \frac{\mu V_0}{2\hbar^2\alpha^2} + l(l+1) \right) + \left( n^2 + n + \frac{1}{2} \right) + \left( n \right. \right. \right.$$

$$\left. \left. \left. + \frac{1}{2} \right) \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right) \times \left( \left[ 1 + 2n \right. \right. \right. \\ \left. \left. \left. + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1} \right] \right)^{-1} \right\}^2. \quad (67)$$

## 6. Numerical Solutions for the Different Expectation Values

MATLAB algorithm is developed to solve numerically equations (58), (61), (66), and (67) for expectation values of  $\langle r^{-2} \rangle$ ,  $\langle r^{-1} \rangle$ ,  $\langle T \rangle$ , and  $\langle p^2 \rangle$ , respectively, for the different diatomic molecules. The diatomic molecules considered in this work are hydrogen, lithium hydride, hydrogen chloride, and carbon (ii) oxide. Table 1 is the spectroscopic constant used in the numerical computation of the expectation values. Tables 2–17 show the numerical expectation values of  $\langle r^{-2} \rangle$ ,  $\langle r^{-1} \rangle$ ,  $\langle T \rangle$ , and  $\langle p^2 \rangle$ , respectively, for the four different diatomic molecules.. These tables show that some of the expectation values increase with an increase in quantum state while some decrease with an increase in quantum state. Tables 2–5 show the expectation values of  $\langle r^{-2} \rangle$  for the diatomic molecules which decrease with an increase in quantum state for LiH but increase with an increase in quantum state for H<sub>2</sub>, HCl, and CO, respectively. The expectation value  $\langle r^{-1} \rangle$  decreases with an increase in quantum state for all the diatomic molecules as shown in Tables 6–9. The expectation value  $\langle T \rangle$  decreases with an increase in quantum state for H<sub>2</sub> and LiH, respectively, but increases with an increase in quantum state for HCl and CO as shown in Tables 10–13. Finally, the expectation value  $\langle p^2 \rangle$  increases with an increase in quantum state for H<sub>2</sub> and CO but decreases with an increase in quantum state for LiH and HCl as shown in Tables 14–17, respectively.

## 7. Normalizing the Wave Function of Quantum Interaction Potential Using Confluent Hypergeometric Functions

The wave function is given in

$$\Psi_n(s) = B_n(s) P_n^{[(2\sqrt{(\mu C/2\hbar^2\alpha^2 - \mu E/2\hbar^2\alpha^2)} - 4\sqrt{(8\mu B/\hbar^2 + 4l(l+1)+1)}, (-2\sqrt{(\mu C/2\hbar^2\alpha^2 - \mu E/2\hbar^2\alpha^2)} - 4\sqrt{(8\mu B/\hbar^2 + 4l(l+1)+1)})]} (1-s) \\ \times [1-s]^{(1/2+(1/2)\sqrt{(8\mu B/\hbar^2 + 4l(l+1)+1)})} (s)^{\sqrt{((\mu C/2\hbar^2\alpha^2 - \mu E/2\hbar^2\alpha^2))}}. \quad (44)$$

TABLE 2: Expectation values of  $\langle r^{-2} \rangle$  for hydrogen molecule.

$n$	$l$	$\langle r^{-2} \rangle_{nl} (\text{\AA}^{-2})$
0	0	-2.0357926925
1	0	-0.3696297856
2	0	-0.0592081872
3	0	-0.0012360898
4	0	-0.0104609211
5	0	-0.0408431125
6	0	-0.0781701991
7	0	-0.1174681786
8	0	-0.1568879315
0	1	-0.5500657326
1	1	-0.1011084016
2	1	-0.0093831431
3	1	-0.0017047903
4	1	-0.0190389837
5	1	-0.0445644291
6	1	-0.0726573984
7	1	-0.1012658894
8	1	-0.1296232040
0	2	-0.1008800199
1	2	-0.0120707336
2	2	-0.0002713032
3	2	-0.0106774421
4	2	-0.0282925702
5	2	-0.0482198274
6	2	-0.0686930232
7	2	-0.0890515939
8	2	-0.1090597335
0	3	-0.0119105671
1	3	-0.0000320975
2	3	-0.0070284422
3	3	-0.0201151142
4	3	-0.0351718504
5	3	-0.0507225834
6	3	-0.0662155593
7	3	-0.0814518703
8	3	-0.0963742259

TABLE 3: Expectation values of  $\langle r^{-2} \rangle$  for lithium hydride molecule.

$n$	$l$	$\langle r^{-2} \rangle_{nl} (\text{\AA}^{-2})$
0	0	-2.5067716077
1	0	-4.3311151186
2	0	-6.0543340693
3	0	-7.7327455626
4	0	-9.3878653299
5	0	-11.0294166762
6	0	-12.6623937821
7	0	-14.2896150748
8	0	-15.9127886181
0	1	-2.5804875135
1	1	-3.8567374113
2	1	-5.0875482240
3	1	-6.2962032770
4	1	-7.4925183938
5	1	-8.6812844732
6	1	-9.8651049570
7	1	-11.0455127066
8	1	-12.2234677505
0	2	-2.5968121549
1	2	-3.4838614479
2	2	-4.3529311128
3	2	-5.2122003606
4	2	-6.0655656768
5	2	-6.9151070951
6	2	-7.7620329080
7	2	-8.6070919545
8	2	-9.4507726300
0	3	-2.5853004074
1	3	-3.2472911138
2	3	-3.9014155691
3	3	-4.5508403180
4	3	-5.1972396752
5	3	-5.8415792817
6	3	-6.4844542567
7	3	-7.1262510136
8	3	-7.7672312288

Basically to normalize a wave function we get the integral of wave function and its complex conjugate to be equal to one. That is,

$$\int_0^{\infty} \Psi(r) \Psi^*(r) dr = 1. \quad (68)$$

In a situation where  $\Psi(r)$  and its complex conjugate are real function, then (68) can be expressed as

$$\int_0^{\infty} |\Psi(r)|^2 dr = 1. \quad (69)$$

Considering the fact that  $s = e^{-2\alpha r}$  then when  $r = 0$ ,  $s = 1$  and when  $r = \infty$ ,  $s = 0$ ,

Hence the wave function will be physically valid for  $s \in [0, 1]$  and  $r \in (0, \infty)$ .

However from (44) let

$$\xi_1 = \sqrt{\left(\frac{\mu c}{2\hbar^2 \alpha^2} - \frac{\mu E}{2\hbar^2 \alpha^2}\right)}, \quad (70)$$

$$\Lambda = \sqrt{\left(\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1\right)}.$$

Equation (44) can then be expressed as

$$\Psi_n(s) = B_n(s) (s)^{\xi_1} [1-s]^{(1/2+(1/2)\Lambda)} \times P_n^{[(2\xi_1-4\Lambda), (-2\xi_1-4\Lambda)]}(1-s). \quad (71)$$

TABLE 4: Expectation values of  $\langle r^{-2} \rangle$  for hydrogen chloride molecule.

$n$	$l$	$\langle r^{-2} \rangle_{nl} (\text{\AA}^{-2})$
0	0	-3.3684130731
1	0	-0.9463978738
2	0	-0.2983665406
3	0	-0.0858762881
4	0	-0.0155115416
5	0	-0.0000100220
6	0	-0.0080075039
7	0	-0.0266967106
8	0	-0.0503597253
0	1	-1.4968915458
1	1	-0.4550672530
2	1	-0.1414988910
3	1	-0.0355399041
4	1	-0.0034391544
5	1	-0.0014140351
6	1	-0.0126923268
7	1	-0.0301145909
8	1	-0.0503830973
0	2	-0.4870936532
1	2	-0.1534956468
2	2	-0.0423781577
3	2	-0.0064304364
4	2	-0.0001287810
5	2	-0.0066922782
6	2	-0.0191475545
7	2	-0.0343426512
8	2	-0.0507669460
0	3	-0.1460080210
1	3	-0.0419218285
2	3	-0.0074968794
3	3	-0.0000019647
4	3	-0.0040520781
5	3	-0.0133574528
6	3	-0.0251076232
7	3	-0.0379661955
8	3	-0.0512710657

TABLE 5: Expectation values of  $\langle r^{-2} \rangle$  for carbon (11) oxide molecule.

$n$	$l$	$\langle r^{-2} \rangle_{nl} (\text{\AA}^{-2})$
0	0	-5.4124527704
1	0	-3.0306606674
2	0	-1.7478304736
3	0	-1.0168948372
4	0	-0.5850753187
5	0	-0.3251871304
6	0	-0.1688134583
7	0	-0.07711780105
8	0	-0.02706175743
0	1	-4.7293036688
1	1	-2.6662325623
2	1	-1.5422086726
3	1	-0.8968395046
4	1	-0.5138531529
5	1	-0.2830295670
6	1	-0.1444688867
7	1	-0.0638852202
8	1	-0.0207992373
0	2	-3.6765597149
1	2	-2.0956762231
2	2	-1.2170016580
3	2	-0.7058809007
4	2	-0.4003901614
5	2	-0.2160772200
6	2	-0.0106187105
7	2	-0.0435491137
8	2	-0.0117284027
0	3	-2.6130004021
1	3	-1.5063610220
2	3	-0.8764213217
3	3	-0.5044821669
4	3	-0.2806791571
5	3	-0.1459868053
6	3	-0.0669337108
7	3	-0.2368085249
8	3	0.0040288991

Substituting (71) into (69) gives

$$-\frac{B_n^2}{2\alpha} \int_0^1 (s)^{2\xi_1-1} [1-s]^{(1+\lambda)} \times |P_n^{(2\xi_1-4\lambda), (-2\xi_1-4\lambda)}(1-s)|^2 ds = 1. \quad (72)$$

Jacobi polynomial  $P_n^{(\rho, \nu)}(\xi_1)$  can be expressed in two different hypergeometric functions by

$$P_n^{(\rho, \nu)}(\xi_1) = 2^{-n} \sum_{p=0}^n (-1)^{n-p} \binom{n+\rho}{p} \binom{n+\nu}{p} (1-\xi_1)^{n-p} (1+\xi_1)^p, \quad (73)$$

$$P_n^{(\rho, \nu)}(\xi_1) = \frac{\Gamma(n+\rho+1)}{n! \Gamma(n+\rho+\nu+1)} \sum_{r=0}^n \binom{n}{r} \frac{\Gamma(n+\rho+\nu+r+1)}{\Gamma(r+\rho+1)} \left(\frac{\xi_1-1}{2}\right)^r, \quad (74)$$

where

$$\binom{n}{r} = {}^n C_r = \frac{n!}{(n-r)!r!} = \frac{\Gamma(n+1)}{\Gamma(n-r+1)\Gamma(r+1)}. \quad (75)$$

Equations (73) and (74) are used simultaneously in evaluating the Jacobi polynomial.

TABLE 6: Expectation values of  $\langle r^{-1} \rangle$  for hydrogen molecule.

$n$	$l$	$\langle r^{-1} \rangle_{nl} (\text{\AA}^{-1})$
0	0	1.2603680546
1	0	0.4379795401
2	0	0.1517172611
3	0	0.1960018427
4	0	-0.0520387537
5	0	-0.0951819716
6	0	-0.0123158672
7	0	-0.0142326424
8	0	-0.1560297050
0	1	0.6791360070
1	1	0.2467913485
2	1	0.0664104304
3	1	-0.0256311394
4	1	-0.0788474859
5	1	-0.1123603234
6	1	-0.1348197402
7	1	-0.1506017288
8	1	-0.1621130507
0	2	0.2992866512
1	2	0.9089728082
2	2	-0.1229187417
3	2	-0.7079611201
4	2	-0.1071332977
5	2	-0.1312363775
6	2	-0.1480391542
7	2	-0.1602175908
8	2	-0.1693251067
0	3	0.1047211078
1	3	-0.0489334886
2	3	-0.0663845048
3	3	-0.1042945872
4	3	-0.1293034551
5	3	-0.1466642182
6	3	-0.1592049675
7	3	-0.1685578998
8	3	-0.1757185637

TABLE 7: Expectation values of  $\langle r^{-1} \rangle$  for lithium hydride molecule.

$n$	$l$	$\langle r^{-1} \rangle_{nl} (\text{\AA}^{-1})$
0	0	-1.6004003285
1	0	-1.7169221172
2	0	-1.7576288115
3	0	-1.7764517192
4	0	-1.7866702782
5	0	-1.7928291806
6	0	-1.7968253335
7	0	-1.7995644507
8	0	-1.8015233696
0	1	-1.6824412202
1	1	-1.7440039428
2	1	-1.7697345550
3	1	-1.7828775641
4	1	-1.7904817568
5	1	-1.7952728019
6	1	-1.7984847995
7	1	-1.8007424714
8	1	-1.8023895794
0	2	-1.7364379965
1	2	-1.7662014135
2	2	-1.7809515122
3	2	-1.7893186518
4	2	-1.7945174323
5	2	-1.7979668174
6	2	-1.8003719661
7	2	-1.8021154796
8	2	-1.8034195262
0	3	-1.7642012758
1	3	-1.7798804427
2	3	-1.7886797501
3	3	-1.7941062087
4	3	-1.7976867501
5	3	-1.8001727144
6	3	-1.8019687138
7	3	-1.8033083180
8	3	-1.8043340174

Considering the Jacobi polynomial of (72)

$$\begin{aligned}
 & P_n^{[(2\xi_1-4\wedge), (-2\xi_1-4\wedge)]} (1-s) \\
 & \quad \Downarrow \\
 & \rho = (2\xi_1 - 4\wedge), \\
 & \nu = (-2\xi_1 - 4\wedge), \\
 & \xi = (1-s).
 \end{aligned} \tag{76}$$

Using (73) then the Jacobi polynomial becomes

$$\begin{aligned}
 P_n^{[(2\xi_1-4\wedge), (-2\xi_1-4\wedge)]} (1-s) &= 2^{-n} \sum_{p=0}^n (-1)^{n-p} \\
 & \cdot \binom{n+2\xi_1-4\wedge}{p} \binom{n-2\xi_1-4\wedge}{n-p} (s)^{n-p} (2-s)^p \implies
 \end{aligned}$$

$$\begin{aligned}
 & P_n^{[(2\xi_1-4\wedge), (-2\xi_1-4\wedge)]} (1-s) = 2^{-n} (s)^{n-p} (2-s)^p \\
 & \cdot \sum_{p=0}^n (-1)^{n-p} \binom{n+2\xi_1-4\wedge}{p} \binom{n-2\xi_1-4\wedge}{n-p}.
 \end{aligned} \tag{77}$$

The summation sign in (73) can be evaluated simultaneously for  $p = 0$  and  $p = 0, n$  as a partial sum.

Evaluating it for  $p = 0$

$$\begin{aligned}
 & \sum_{p=0}^n (-1)^{n-p} \binom{n+2\xi_1-4\wedge}{p} \binom{n-2\xi_1-4\wedge}{n-p} \\
 &= \sum_{p=0}^n (-1)^{n-p} \binom{n+2\xi_1-4\wedge}{0} \binom{n-2\xi_1-4\wedge}{n}
 \end{aligned}$$



TABLE 8: Expectation values of  $\langle r^{-1} \rangle$  for hydrogen chloride molecule.

$n$	$l$	$\langle r^{-1} \rangle_{nl} (\text{\AA}^{-1})$
0	0	1.6729006170
1	0	0.7484646279
2	0	0.3703627204
3	0	0.1796456609
4	0	0.0702095120
5	0	0.0166105989
6	0	-0.4409486494
7	0	-0.0761475106
8	0	-0.0994688026
0	1	1.1368069123
1	1	0.5412411880
2	1	0.2694738513
3	1	0.1231413170
4	1	0.0354355317
5	1	-0.0212411621
6	1	-0.0599699313
7	1	-0.0876003075
8	1	-0.1080007236
0	2	0.6614557236
1	2	0.3289571474
2	2	0.1568012770
3	2	0.0562991328
4	2	-0.0074281360
5	2	-0.0503567338
6	2	-0.0806430409
7	2	-0.1028045106
8	2	-0.1195073036
0	3	0.3674917640
1	3	0.1780764140
2	3	0.0692601602
3	3	0.0010437052
4	3	-0.0445186237
5	3	-0.0764508536
6	3	-0.0996933551
7	3	-0.1171352594
8	3	-0.1305576611

TABLE 9: Expectation values of  $\langle r^{-1} \rangle$  for carbon (11) oxide molecule.

$n$	$l$	$\langle r^{-1} \rangle_{nl} (\text{\AA}^{-1})$
0	0	2.3183952626
1	0	1.6087565101
2	0	1.1442089011
3	0	0.8236269179
4	0	0.5931311104
5	0	0.4218775175
6	0	0.2911757802
7	0	0.1891645008
8	0	0.1080220439
0	1	2.1698058118
1	1	1.5137194441
2	1	1.0797914397
3	1	0.7779687438
4	1	0.5596010388
5	1	0.3965336986
6	1	0.2715561482
7	1	0.1736671893
8	1	0.0955685247
0	2	1.9172571191
1	2	1.3495663209
2	2	0.9671517266
3	2	0.6973560297
4	2	0.4999374576
5	2	0.3511456004
6	2	0.2362292864
7	2	0.1456344871
8	2	0.0729524039
0	3	1.6206607845
1	3	1.1522380728
2	3	0.8292959293
3	3	0.5972813496
4	3	0.4250064850
5	3	0.2935928640
6	3	0.1910702660
7	3	0.1095511163
8	3	0.0436667613

$$\begin{aligned}
 &= (-1)^n \frac{(n + 2\xi_1 - 4 \wedge)!}{[(n + 2\xi_1 - 4 \wedge) - 0]!0!} \frac{(n - 2\xi_1 - 4 \wedge)!}{[(-2\xi_1 - 4 \wedge)]!n!} \\
 &= (-1)^n \frac{\Gamma(n - 2\xi_1 - 4 \wedge + 1)}{\Gamma(n + 1) \Gamma(1 - 2\xi_1 - 4 \wedge)}.
 \end{aligned} \tag{78}$$

For  $p = 0, n$

$$\sum_{p=0}^n (-1)^{n-p} \binom{n + 2\xi_1 - 4 \wedge}{p} \binom{n - 2\xi_1 - 4 \wedge}{n-p} = (-1)^p \frac{(n + 2\xi_1 - 4 \wedge)!}{[(n + 2\xi_1 - 4 \wedge - p)]!p!}$$

$$\begin{aligned}
 &\frac{(n - 2\xi_1 - 4 \wedge)!}{[(n - 2\xi_1 - 4 \wedge) - (n - p)]! (n - p)!} = \sum_{p=0}^n (-1)^p \\
 &\frac{\Gamma(n + 2\xi_1 - 4 \wedge) \Gamma(n - 2\xi_1 - 4 \wedge)}{p! (n - p)! \Gamma(n + 2\xi_1 - 4 \wedge - p + 1) \Gamma(p - 2\xi_1 - 4 \wedge + 1)}.
 \end{aligned} \tag{79}$$

Substituting (78) and (79) into (73) gives

$$\begin{aligned}
 &P_n^{[(2\xi_1 - 4 \wedge), (-2\xi_1 - 4 \wedge)]} (1 - s) \\
 &= (-1)^n \frac{\Gamma(n - 2\xi_1 - 4 \wedge + 1)}{\Gamma(n + 1) \Gamma(1 - 2\xi_1 - 4 \wedge)} \sum_{p=0}^n (-1)^p \frac{\Gamma(n + 2\xi_1 - 4 \wedge + 1) \Gamma(n - 2\xi_1 - 4 \wedge + 1) 2^{-n} (s)^{n-p} (2 - s)^p}{p! (n - p)! \Gamma(n + 2\xi_1 - 4 \wedge - p + 1) \Gamma(p - 2\xi_1 - 4 \wedge + 1)}.
 \end{aligned} \tag{80}$$

TABLE 10: Expectation values of  $\langle T \rangle$  for hydrogen molecule.

$n$	$l$	$\langle T \rangle_{nl}$ (eV)
0	0	-5.7775010957
1	0	-0.1575248128
2	0	0.3833647660
3	0	0.1004688440
4	0	-0.4051760492
5	0	-1.0142757581
6	0	-1.7009007969
7	0	-2.4609241866
8	0	-3.2955155097
0	1	-1.1305296358
1	1	0.4062543383
2	1	0.2903023018
3	1	-0.1806436110
4	1	-0.7793821663
5	1	-1.4584654527
6	1	-2.2092740425
7	1	-3.0323596290
8	1	-3.9301708526
0	2	0.3945367735
1	2	0.3765550363
2	2	-0.0842946033
3	2	-0.6872416982
4	2	-1.3716032980
5	2	-2.1263145693
6	2	-2.9517276048
7	2	-3.8505394856
8	2	-4.8255106670
0	3	0.4231977151
1	3	-0.0331938070
2	3	-0.6403179766
3	3	-1.3293878653
4	3	-2.0879210976
5	3	-2.9161860233
6	3	-3.8170461261
7	3	-4.7934410194
8	3	-5.8478274746

TABLE 11: Expectation values of  $\langle T \rangle$  for lithium hydride molecule.

$n$	$l$	$\langle T \rangle_{nl}$ (eV)
0	0	-4.2305585674
1	0	-8.5398534703
2	0	-15.8689882670
3	0	-26.0744836125
4	0	-39.0894871134
5	0	-54.8817584651
6	0	-73.4342035101
7	0	-94.7369941855
8	0	-118.7841018590
0	1	-7.8088669292
1	1	-14.2714091244
2	1	-23.6854511210
3	1	-35.9457058061
4	1	-51.0026938513
5	1	-68.8311306737
6	1	-89.4169299119
7	1	-112.7516689680
8	1	-138.8300177540
0	2	-14.2391535700
1	2	-23.4467711704
2	2	-35.5261470800
3	2	-50.4157170230
4	2	-68.0844826720
5	2	-88.5154126054
6	2	-111.6984397090
7	2	-137.6272527440
8	2	-166.2977020400
0	3	-23.4729539098
1	3	-35.4898681236
2	3	-50.3254081811
3	3	-67.9449624090
4	3	-88.3296507196
5	3	-111.4683804780
6	3	-137.3542318380
7	3	-165.9826734470
8	3	-197.3506175640

Using the second expression for the Jacobi polynomial that is (74) then

$$P_n^{[(2\xi_1-4\lambda),(-2\xi_1-4\lambda)]}(1-s) = \frac{\Gamma(n+2\xi_1-4\lambda+1)}{\Gamma(n+1-8\lambda)} \sum_{r=0}^n \left(-\frac{1}{2}\right)^r \frac{\Gamma(n+r+1-8\lambda)}{r!(n-r)!\Gamma(r+2\xi_1-4\lambda+1)} s^r. \quad (81)$$

Then the square of the Jacobi polynomial in (72) then becomes

$$[P_n^{[(2\xi_1-4\lambda),(-2\xi_1-4\lambda)]}(1-s)]^2 = (80) \text{ multiplied by } (81).$$

$$\begin{aligned} [P_n^{[(2\xi_1-4\lambda),(-2\xi_1-4\lambda)]}(1-s)]^2 &= (-1)^n \frac{\Gamma(n-2\xi_1-4\lambda+1)}{\Gamma(n+1)\Gamma(1-2\xi_1-4\lambda)} \\ &\times \sum_{p=0}^n (-1)^p \\ &\times \frac{\Gamma(n+2\xi_1-4\lambda)\Gamma(n-2\xi_1-4\lambda)2^{-n}(s)^{n-p}(2-s)^p}{p!(n-p)!\Gamma(n+2\xi_1-4\lambda-p+1)\Gamma(p-2\xi_1-4\lambda+1)} \quad (82) \\ &\times \frac{\Gamma(n+2\xi_1-4\lambda+1)}{\Gamma(n+1-8\lambda)} \times \sum_{r=0}^n \left(-\frac{1}{2}\right)^r \\ &\times \frac{\Gamma(n+r+1-8\lambda)}{r!(n-r)!\Gamma(r+2\xi_1-4\lambda+1)} s^r. \end{aligned}$$

TABLE 12: Expectation values of  $\langle T \rangle$  for hydrogen chloride molecule.

$n$	$l$	$\langle T \rangle_{nl}$ (eV)
0	0	-16.8602470534
1	0	-3.8173740938
2	0	-0.7264968799
3	0	0.8170812272
4	0	0.1808796145
5	0	0.0076433944
6	0	-0.2925912249
7	0	-0.6654441904
8	0	-1.0891026610
0	1	-1.8259881179
1	1	-0.1652596937
2	1	0.2050704178
3	1	0.1331442742
4	1	-0.1233945608
5	1	-0.4738642417
6	1	-0.8832796542
7	1	-1.3374731433
8	1	-2.7518917695
0	2	-0.3749865298
1	2	0.1982728862
2	2	0.1926154142
3	2	-0.0409008669
4	2	-0.3834013618
5	2	-0.7902268789
6	2	-1.2436082882
7	2	-1.7363979570
8	2	-0.5275303052
0	3	0.1879629685
1	3	0.2257156907
2	3	0.0056050075
3	3	-0.3335743383
4	3	-0.7405492881
5	3	-1.1951594384
6	3	-1.6893574408
7	3	-2.2201023828
8	3	0.1879629685

TABLE 13: Expectation values of  $\langle T \rangle$  for carbon (11) oxide molecule.

$n$	$l$	$\langle T \rangle_{nl}$ (eV)
0	0	-129.9291130830
1	0	-75.6124342843
2	0	-45.8529997998
3	0	-28.4567951051
4	0	-17.7933612549
5	0	-11.0290843042
6	0	-6.6378456500
7	0	-3.7514369504
8	0	-1.8531332454
0	1	-117.6340205260
1	1	-69.0411092188
2	1	-42.0768329533
3	1	-26.1683200430
4	1	-16.3516907261
5	1	-10.0962337215
6	1	-6.0247765063
7	1	-3.3471874404
8	1	-1.5898907876
0	2	-97.7238969338
1	2	-58.1864276360
2	2	-35.7490746782
3	2	-22.2936665438
4	2	-13.8933817128
5	2	-8.4988638639
6	2	-4.9737074744
7	2	-2.6557694881
8	2	-1.1430395374
0	3	-76.0158584874
1	3	-46.0107012922
2	3	-28.5036356479
3	3	-17.7913843239
4	3	-11.0086725080
5	3	-6.6145424645
6	3	-3.7334128723
7	3	-1.8447253427
8	3	-0.6270405479

Equation (82) can be further simplified to

$$\begin{aligned}
 [P_n^{[(2\xi_1-4\wedge),(-2\xi_1-4\wedge)]} (1-s)]^2 &= (-1)^n \frac{\Gamma(n-2\xi_1-4\wedge+1)^2 \Gamma(n+2\xi_1-4\wedge+1)^2}{\Gamma(n+1)\Gamma(1-2\xi_1-4\wedge)} \times \frac{\Gamma(n+r+1-8\wedge)}{\Gamma(n+1-8\wedge)} \\
 &\cdot \sum_{p=0}^n \sum_{r=0}^n (-1)^{p+r} \frac{2^{-n-r} (s)^{n-p+r} (2-s)^p}{p!(n-p)!r!(n-r)!\Gamma(n+2\xi_1-4\wedge-p+1)\Gamma(p-2\xi_1-4\wedge+1)\Gamma(r+2\xi_1-4\wedge+1)}.
 \end{aligned} \tag{83}$$

TABLE 14: Expectation values of  $\langle p^2 \rangle$  for hydrogen molecule.

$n$	$l$	$\langle p^2 \rangle_{nl} \text{ (eV/c)}^2$
0	0	-5.8226811543
1	0	-0.1587566569
2	0	0.3863626785
3	0	0.1012545103
4	0	-0.4083445259
5	0	-1.0222073945
6	0	-1.7142018411
7	0	-2.4801686138
8	0	-3.3212864410
0	1	-1.1393703776
1	1	0.4094312472
2	1	0.2925724658
3	1	-0.1806436110
4	1	-0.7854769348
5	1	-1.4698706526
6	1	-2.2265505655
7	1	-3.0560726813
8	1	-3.9609047886
0	2	0.3945367735
1	2	0.3794996967
2	2	-0.8495378710
3	2	-0.6926159282
4	2	-1.3823292358
5	2	-2.1429423493
6	2	-2.9748101146
7	2	-3.8806507044
8	2	-4.8632461604
0	3	0.4265071213
1	3	-0.0334533826
2	3	-0.6453252632
3	3	-1.3397836784
4	3	-2.1042486406
5	3	-2.9389905980
6	3	-3.8468954268
7	3	-4.8309257282
8	3	-5.8935574854

TABLE 15: Expectation values of  $\langle p^2 \rangle$  for lithium hydride molecule.

$n$	$l$	$\langle p^2 \rangle_{nl} \text{ (eV/c)}^2$
0	0	-7.4468161811
1	0	-15.0322275400
2	0	-27.9332945570
3	0	-45.8974585468
4	0	-68.8070429723
5	0	-96.6052970237
6	0	-129.2621308100
7	0	-166.7602445400
8	0	-209.0890263500
0	1	13.7455127207
1	1	-25.1211651371
2	1	-41.6921779602
3	1	-35.9457058061
4	1	-89.7771960362
5	1	-121.1595985480
6	1	-157.3956322590
7	1	-198.4704713410
8	1	-244.3747335380
0	2	-14.2391535700
1	2	-41.2720429614
2	2	-62.5346943459
3	2	-88.7439734787
4	2	-119.8453157330
5	2	-155.8087416490
6	2	-196.6165306470
7	2	-242.2575734060
8	2	-292.7245654890
0	3	-41.3181309765
1	3	-62.4708345234
2	3	-88.5850078633
3	3	-119.5997260000
4	3	-155.4817553670
5	3	-196.2115702200
6	3	-241.7769899380
7	3	-292.1700382350
8	3	-347.3852799350

Substituting (83) into (72) gives

$$\begin{aligned}
& -(-1)^n \frac{\Gamma(n-2\xi_1-4\wedge+1)^2 \Gamma(n+2\xi_1-4\wedge+1)^2}{2\alpha\Gamma(n+1)\Gamma(1-2\xi_1-4\wedge)} \times \frac{\Gamma(n+r+1-8\wedge)}{\Gamma(n+1-8\wedge)} \\
& \cdot \sum_{p=0}^n \sum_{r=0}^n (-1)^{p+r} \frac{2^{-n-r} (2-s)^p B_n^2}{p!(n-p)!r!(n-r)!\Gamma(n+2\xi_1-4\wedge-p+1)\Gamma(p-2\xi_1-4\wedge+1)\Gamma(r+2\xi_1-4\wedge+1)} \quad (84) \\
& \times \int_0^1 (s)^{2\xi_1-1+n-p+r} [1-s]^{(1+\wedge)} ds = 1
\end{aligned}$$

TABLE 16: Expectation values of  $\langle p^2 \rangle$  for hydrogen chloride molecule.

$n$	$l$	$\langle p^2 \rangle_{nl} \text{ (eV/c)}^2$
0	0	-7.446816181
1	0	-15.0322275400
2	0	-27.9332945570
3	0	-45.8974585468
4	0	-68.8070429723
5	0	-96.6052970237
6	0	-129.2621308100
7	0	-166.7602445400
8	0	-209.0890263500
0	1	-13.7455127207
1	1	-25.1211651371
2	1	-41.6921779602
3	1	-35.9457058061
4	1	-89.7771960362
5	1	-121.1595985480
6	1	-157.3956322590
7	1	-198.4704713410
8	1	-244.3747335380
0	2	-14.2391535700
1	2	-41.2720429614
2	2	-62.5346943459
3	2	-88.7439734787
4	2	-119.8453157330
5	2	-155.8087416490
6	2	-196.6165306470
7	2	-242.2575734060
8	2	-292.7245654890
0	3	-41.3181309765
1	3	-62.4708345234
2	3	-88.5850078633
3	3	-119.5997260000
4	3	-155.481755367
5	3	-196.2115702200
6	3	-241.7769899380
7	3	-292.1700382350
8	3	-347.3852799350

TABLE 17: Expectation values of  $\langle p^2 \rangle$  for carbon (11) oxide molecule.

$n$	$l$	$\langle p^2 \rangle_{nl} \text{ (eV/c)}^2$
0	0	-1782.8020302400
1	0	-1037.5042063700
2	0	-629.1647745140
3	0	-390.4654690820
4	0	-244.1488271370
5	0	-151.333857537
6	0	-91.0801622550
7	0	-51.474756141
8	0	-25.4274783679
0	1	-1614.0968382200
1	1	-947.3367959250
2	1	-577.3506909670
3	1	-26.1683200430
4	1	-224.3671701640
5	1	-138.5338939770
6	1	-82.6680297618
7	1	-45.9279096337
8	1	-21.8154381022
0	2	-97.7238969338
1	2	-798.3959780860
2	2	-490.5253441900
3	2	-305.8990632100
4	2	-190.6358670260
5	2	-116.6158329860
6	2	-68.2459502172
7	2	-36.4407262008
8	2	-15.6840384698
0	3	-1043.0397285600
1	3	-631.3286509110
2	3	-391.1081842740
3	3	-244.1217009860
4	3	-151.0537802640
5	3	-90.7604112360
6	3	-51.2274415685
7	3	-25.3121106450
8	3	-8.6038389354

Confluent hypergeometric function can be defined as follows:

$${}_2F_1(\alpha_0, \beta_0 : \alpha_0 + 1; 1) = \alpha_0 \int_0^1 (s)^{\alpha_0-1} [1-s]^{-\beta_0} ds \quad (85)$$

$$= 1$$

assuming that

$$\gamma_0 = \alpha_0 + 1,$$

$$\text{then } {}_2F_1(\alpha_0, \beta_0 : \gamma_0; 1) = \alpha_0 \int_0^1 (s)^{\alpha_0-1} [1-s]^{-\beta_0} ds \quad (86)$$

$$= 1.$$

TABLE 18: Bound state energy of Hulthen potential in comparison to other works.

$n$	$l$	$\delta$	Present work	Arda and Sever, 2012
0	1	0.025	-0.1128125	-0.1128130
0	1	0.050	-0.1012500	-0.1012500
0	1	0.075	-0.0903125	-0.0903120
0	1	0.100	-0.0800000	-0.0800000
0	1	0.150	-0.0612500	-0.0612500

However,

$${}_2F_1(\alpha_0, \beta_0 : \gamma_0; 1) = \frac{\Gamma(\gamma_0)\Gamma(\gamma_0 - \alpha_0 - \beta_0)}{\Gamma(\gamma_0 - \alpha_0)\Gamma(\gamma_0 - \beta_0)}. \quad (87)$$

Considering

$$\int_0^1 (s)^{2\xi_1-1+n-p+r} [1-s]^{(1+\wedge)} ds, \tag{88}$$

$$\alpha_0 = 2\xi_1 + n - p + r,$$

$$\beta_0 = -(1 + \wedge)$$

therefore

$$\int_0^1 (s)^{2\xi_1-1+n-p+r} [1-s]^{(1+\wedge)} ds = \frac{\Gamma(\alpha_0 + 1) \Gamma(\wedge + 2)}{\alpha_0 \Gamma(\alpha_0 + \wedge + 2)}. \tag{89}$$

Substituting (89) into (84) gives

$$-(-1)^n \frac{\Gamma(n - 2\xi_1 - 4\wedge + 1)^2 \Gamma(n + 2\xi_1 - 4\wedge + 1)^2}{2\alpha \Gamma(n + 1) \Gamma(1 - 2\xi_1 - 4\wedge)} \times \frac{\Gamma(n + r + 1 - 8\wedge)}{\Gamma(n + 1 - 8\wedge)}$$

$$\cdot \sum_{p=0}^n \sum_{r=0}^n (-1)^{p+r} \frac{2^{-n-r} (2-s)^p B_n^2}{p! (n-p)! r! (n-r)! \Gamma(n + 2\xi_1 - 4\wedge - p + 1) \Gamma(p - 2\xi_1 - 4\wedge + 1) \Gamma(r + 2\xi_1 - 4\wedge + 1)}$$

$$\times \frac{\Gamma(\alpha_0 + 1) \Gamma(\wedge + 2)}{\alpha_0 \Gamma(\alpha_0 + \wedge + 2)} = 1. \tag{90}$$

Let

$$s_1 = -(-1)^n \frac{\Gamma(n - 2\xi_1 - 4\wedge + 1)^2 \Gamma(n + 2\xi_1 - 4\wedge + 1)^2}{2\alpha \Gamma(n + 1) \Gamma(1 - 2\xi_1 - 4\wedge)} \times \frac{\Gamma(n + r + 1 - 8\wedge)}{\Gamma(n + 1 - 8\wedge)}$$

$$\cdot \sum_{p=0}^n \sum_{r=0}^n (-1)^{p+r} \frac{2^{-n-r} (2-s)^p}{p! (n-p)! r! (n-r)! \Gamma(n + 2\xi_1 - 4\wedge - p + 1) \Gamma(p - 2\xi_1 - 4\wedge + 1) \Gamma(r + 2\xi_1 - 4\wedge + 1)}$$

$$\times \frac{\Gamma(\alpha_0 + 1) \Gamma(\wedge + 2)}{\alpha_0 \Gamma(\alpha_0 + \wedge + 2)}. \tag{91}$$

However,

$$B_n^2 s_1 = 1 \implies B_n = \frac{1}{\sqrt{s_1}}. \tag{92}$$

Hence, the normalized wave function then becomes

$$\Psi_n(s) = \frac{1}{\sqrt{s_1}} (s) P_n^{[(2\sqrt{(\mu c/2\hbar^2 \alpha^2 - \mu E/2\hbar^2 \alpha^2) - 4\sqrt{(8\mu B/\hbar^2 + 4l(l+1)+1)}), (-2\sqrt{(\mu c/2\hbar^2 \alpha^2 - \mu E/2\hbar^2 \alpha^2) - 4\sqrt{(8\mu B/\hbar^2 + 4l(l+1)+1)})]} (1-s)$$

$$\times [1-s]^{(1/2+(1/2)\sqrt{(8\mu B/\hbar^2 + 4l(l+1)+1)})} (s)^{\sqrt{((\mu c/2\hbar^2 \alpha^2 - \mu E/2\hbar^2 \alpha^2))}}. \tag{93}$$

### 8. Conclusion

In this work, we obtained analytical solution of Schrodinger equation with quantum interaction potential (HYIQP) and obtained the energy eigenvalue and the wave function using conventional Nikiforov-Uvarov method. Under some special cases, the potential reduced to three well-known potentials which are as follows: Hulthen, Yukawa, and inversely

quadratic potential. The result from these potentials is in agreement with that reported in existing literature. Expectation values for four diatomic molecules are computed using Hellmann-Feynman theorem. Numerical solutions of the expectation values are obtained by implementing MATLAB algorithm. However, by implementing mathematica algorithm, the wave function and probability density plots were obtained for four diatomic molecules with an increasing

orbital angular momentum. The quantum interaction potential model developed is suitable in studying bound state energies of diatomic molecules. Figure 1 shows the graph of the quantum interaction potential with different values of the screening parameter. However, Figure 2 shows the graph of the potential ( $F$ ) plotted against the individual potentials ( $F_1$ ,  $F_2$ , and  $F_3$ ). Some of the numerical expectation values either increase or decrease with an increase in quantum state.

## Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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