Approximate Solutions of Schrödinger 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 Schrödinger 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.
The proposed quantum interaction potential is given by

\[ V(r) = -V_0 e^{-2\alpha r} \left( 1 - e^{-2\alpha r} \right) - \frac{A e^{-\alpha r}}{r} + \frac{B}{r^2} + C, \]

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 \( \ell = 0, 1, 2, 3, 4, \) 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
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

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

$\bar{\tau}(s)$ is a polynomial of degree one while $\sigma(s)$ and $\bar{\sigma}(s)$ 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
\[ \frac{\phi^1(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}, \tag{5} \]
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
\[ \chi_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} \left[ \sigma''(s) \rho(s) \right]. \tag{6} \]

$B_n$ is the normalization constant and the weight function $\rho(s)$ satisfies the condition
\[ \frac{d}{ds} \left( \sigma(s) \rho(s) \right) = \tau(s) \rho(s) \tag{7} \]
such that
\[ \tau(s) = \bar{\tau}(s) + 2\pi(s). \tag{8} \]

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,
\[ \frac{d\tau(s)}{ds} < 0. \tag{9} \]

Therefore, the function $\pi(s)$ and the parameter $\lambda$ required for the NU method are defined as follows:
\[ \pi(s) = \frac{\sigma' - \bar{\sigma}}{2} \pm \sqrt{\left(\frac{\sigma' - \bar{\sigma}}{2}\right)^2 - \bar{\sigma} + k\sigma}, \tag{10} \]
\[ \lambda = k + n'(s). \tag{11} \]

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
\[ \lambda = n d\tau \frac{ds}{ds} - \frac{n(n-1)\sigma''}{2}, \quad n = 0, 1, 2, \ldots, \tag{12} \]
where $\tau(s)$ is as defined in (8) and, on comparing (11) and (12), we obtain the energy eigenvalues.

### 3. Radial Solution of Schrödinger Equation

The Schrödinger wave equation is given by
\[ \frac{d^2\psi(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[ E - V(r) - \frac{\hbar^2l(l+1)}{2\mu r^2} \right] \psi(r) = 0. \tag{13} \]

Substituting (1) into (13) gives
\[ \frac{d^2\psi(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[ E + \frac{V_0 e^{-2\alpha r}}{1 - e^{-2\alpha r}} + \frac{A e^{-\alpha r}}{r} - \frac{B}{r^2} - C - \frac{\hbar^2 l(l+1)}{2\mu r^2} \right] \psi(r) = 0. \tag{14} \]

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
\[ \frac{1}{r^2} = \frac{4\alpha^2 e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} \iff \frac{1}{r} = \frac{2\alpha e^{-\alpha r}}{(1 - e^{-2\alpha r})}. \tag{15} \]

Substituting (15) into (14) with the transformation $s = e^{-2\alpha r}$ gives
\[ \frac{d^2\psi(s)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{d\psi(s)}{ds} + \frac{1}{s^2(1-s)^2} \left[ -\epsilon^2 (1-s)^2 \right. \]
\[ \left. + \delta^2 s (1-s) + \sigma_1 s (1-s) - \sigma_3 s - \sigma_3 (1-s)^2 - sl(l+1) \right] \psi(s) = 0, \tag{16} \]

where
\[ \epsilon^2 = -\frac{\mu E}{2\hbar^2 \alpha^2}, \]
\[ \delta^2 = \frac{\mu V_0}{2\hbar^2 \alpha^2}, \]
\[ \sigma_1 = \frac{\mu A}{\hbar^2 \alpha}, \]
\[ \sigma_2 = \frac{2\mu B}{\hbar^2}, \]
\[ \sigma_3 = \frac{\mu c}{2\hbar^2 \alpha}. \tag{17} \]

Simplifying (16) further reduced to
\[ \frac{d^2\psi(s)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{d\psi(s)}{ds} \]
\[ + \frac{1}{s^2(1-s)^2} \left[ -\left(\epsilon^2 + \delta^2 + \sigma_1 + \sigma_3\right)s^2 \right. \]
\[ \left. + \left(2\epsilon^2 + \delta^2 + \sigma_1 - \sigma_3 + 2\sigma_3 - l(l+1)\right)s \right. \]
\[ \left. - \left(\epsilon^2 + \sigma_3\right)\right] \psi(s) = 0. \tag{18} \]

Comparing (18) to (2) we obtained the following:
\[ \sigma(s) = s(1-s), \]
\[ \bar{\sigma}(s) = -\left(\epsilon^2 + \delta^2 + \sigma_1 + \sigma_3\right)s^2 \]
\[ + \left(2\epsilon^2 + \delta^2 + \sigma_1 - \sigma_3 + 2\sigma_3 - l(l+1)\right)s \]
\[ - \left(\epsilon^2 + \sigma_3\right), \tag{19} \]
\[ \tau(s) = (1-s). \]
Then, using (10), the polynomial equation $\pi(s)$ then becomes

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

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

$$
a = \left(\frac{1}{4} + e^2 + \delta^2 + \sigma_1 + \sigma_3 - k\right),
$$
$$
b = -\left(2e^2 + \delta^2 + \sigma_1 - \sigma_2 + 2\sigma_3 - l(l + 1) - k\right),
$$
$$
c = -(e^2 + \sigma_3).
$$

Hence,

$$
k_1 = -\left(\sigma_2 - \sigma_1 - \delta^2 + l(l + 1)\right) + \sqrt{(e^2 + \sigma_3)(4e^2 + 4l(l + 1) + 1)},
$$
$$
k_2 = -\left(\sigma_2 - \sigma_1 - \delta^2 + l(l + 1)\right) - \sqrt{(e^2 + \sigma_3)(4e^2 + 4l(l + 1) + 1)}.
$$

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

$$
\pi(s) = \frac{-s}{2} \pm \begin{cases} 
\frac{1}{2}\sqrt{(4\sigma_2 + 4l(l + 1) + 1) + \sqrt{(e^2 + \sigma_3)}}, & k_1 = -\left(\sigma_2 - \sigma_1 - \delta^2 + l(l + 1)\right) + \sqrt{(e^2 + \sigma_3)(4e^2 + 4l(l + 1) + 1)} \\
\frac{1}{2}\sqrt{(4\sigma_2 + 4l(l + 1) + 1) - \sqrt{(e^2 + \sigma_3)}}, & k_2 = -\left(\sigma_2 - \sigma_1 - \delta^2 + l(l + 1)\right) - \sqrt{(e^2 + \sigma_3)(4e^2 + 4l(l + 1) + 1)}
\end{cases}
$$

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

$$
\lambda = k + \pi'(s)
$$

$$
= -\frac{1}{2} - \left(\frac{1}{2}\sqrt{(4\sigma_2 + 4l(l + 1) + 1) - \sqrt{(e^2 + \sigma_3)}}\right) + \sqrt{(e^2 + \sigma_3)}
$$

$$
- \left(\sigma_2 - \sigma_1 - \delta^2 + l(l + 1)\right).
$$

Using (12)

$$
\lambda_n = n^2 + n + n\sqrt{(4\sigma_2 + 4l(l + 1) + 1)}
$$

$$
- 2n\sqrt{(e^2 + \sigma_3)}.
$$

Equating (25) and (26) gives the result

$$
\epsilon^2 = \left[\left(n^2 + n + 1/2\right) + \left(n + 1/2\right)\sqrt{(4\sigma_2 + 4l(l + 1) + 1) + \left(\sigma_2 - \sigma_1 - \delta^2 + l(l + 1)\right)}\right]^2 - \sigma_3.
$$
Substituting parameters of (17) into (27) gives

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

(28)

+ c

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

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

\[
\sigma(s) = s - s^2,
\]

\[
\pi(s) = \frac{s}{2} - \left[ \frac{1}{2} \sqrt{4\sigma_2 + 4l (l + 1) + 1} + \sqrt{\varepsilon^2 + \sigma_3} \right] s
\]

then

\[
\pi(s) = -\frac{1}{2} (1 - s)
\]

\[
\frac{\pi(s)}{\sigma(s)} = -\frac{1}{2} (1 - s)
\]

\[
\phi_1(s) = \pi(s) = -\frac{1}{2} (1 - s)
\]

(30)

which then leads to

\[
\ln \phi(s) = \ln \left[ 1 - s \right]^{1/2} + \ln \left[ 1 - s \right]^{(1/2) \sqrt{(4\sigma_2 + 4l (l + 1) + 1)}}
\]

\[+ \ln \left[ 1 - s \right]^{\varepsilon^2 + \sigma_3} + \ln [s]^{\varepsilon^2 + \sigma_3} \]

(34)

Equation (34) can further be reduced to

\[
\ln \phi(s) = \ln \left[ 1 - s \right]^{(1/2 + (1/2) \sqrt{(4\sigma_2 + 4l (l + 1) + 1)})} \cdot [s]^{\varepsilon^2 + \sigma_3}
\]

(35)

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

(36)

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

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

(37)

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)

\[
\frac{d}{ds} \left( \sigma(s) \rho(s) \right) = \tau(s) \rho(s) \Rightarrow
\]

\[
\int \frac{\rho'(s)}{\rho(s)} ds = \int \frac{\tau(s) - \sigma'(s)}{\sigma(s)} ds.
\]
Substituting the parameters gives

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

Integrating (38) gives

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

Hence the total wave function is given by

$$\Psi_n (s) = \phi (s) Y_n (s) = B_n(s) \cdot P_n \left[ \frac{1}{\left( \sqrt{(e^2 + \sigma_3)} \right)} \sqrt{(1 - s) \left( (1 - s)^{1/2} \right)} \right].$$  \hspace{1cm} (44)

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

$$Y_n (s) = B_n (s) \cdot P_n \left[ \frac{1}{\left( \sqrt{(e^2 + \sigma_3)} \right)} \sqrt{(1 - s) \left( (1 - s)^{1/2} \right)} \right].$$  \hspace{1cm} (42)

Let us define standard associated Laguerre polynomial as

$$\chi_n (s) = B_n (s) s^{-\nu} \left( 1 - s \right)^{-\mu} \frac{d^n}{ds^n} \left[ s^{\nu + \mu} \left( 1 - s \right)^{\nu + \mu} \right]$$

$$= p_n^{[\nu + \mu]} \left( 1 - s \right).$$

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

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

$$= B_n(s) \cdot P_n \left[ \frac{1}{\left( \sqrt{(e^2 + \sigma_3)} \right)} \sqrt{(1 - s) \left( (1 - s)^{1/2} \right)} \right] \left( 1 - e^{-2ar} \right)^{\mu} (e^{-2ar}) \sqrt{\left( \frac{\mu}{(e^2 + \sigma_3)} \right)}.$$

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

$$\Psi_n (s) = \frac{1}{\sqrt{51}} \left( s \right) \frac{1}{\left( \sqrt{(e^2 + \sigma_3)} \right)} \sqrt{(1 - s) \left( (1 - s)^{1/2} \right)} \sqrt{\left( \frac{\mu}{(e^2 + \sigma_3)} \right)}.$$  \hspace{1cm} (44c)
where the normalization constant is given as

\[ B_n = 1/\sqrt{s_1}, \]

where

\[ s_1 = (-1)^s \frac{\Gamma(n - 2\xi_1 - 4\Lambda + 1)\Gamma(n + 2\xi_1 - 4\Lambda + 1)}{2\alpha\Gamma(n + 1)\Gamma(1 - 2\xi_1 - 4\Lambda)} \times \frac{\Gamma(n + r + 1 - 8\Lambda)}{\Gamma(n + 1 - 8\Lambda)} \]

\[ \times \sum_{p=0}^{n} \sum_{r=0}^{n} (-1)^{p+r} \frac{\Gamma(\alpha_0 + 1)\Gamma(\Lambda + 2)}{\alpha_0\Gamma(\alpha_0 + \Lambda + 2)}. \]

(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

\[ V(r) = -V_0 e^{-\alpha r} \left( 1 - e^{-\alpha r} \right). \]

(45)

The energy of this potential is given as

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

(46)

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

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

(47a)

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

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

(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.

\[ V(r) = -\frac{A e^{-\alpha r}}{r}. \]

(48)

The corresponding energy equation for this potential is given as

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

(49a)
Equation (49a) can further be simplified as

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

(49b)

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

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

(49c)

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

\[ E_{nl} = a = \alpha, \]
\[ 2m = \mu, \]
\[ A = V_0, \]
\[ \hbar = 1. \]  

(50)

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

\[ V(r) = \frac{B}{r^2}. \]  

(51)

The corresponding energy for this potential is given as

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

(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

\[ \frac{\partial E_n}{\partial q} = \left\langle \Psi(q) \left| \frac{\partial H(q)}{\partial q} \right| \Psi(q) \right\rangle. \]  

(53)

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

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

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

(56)
Taking the partial derivative of (54) with respect to \( l \) gives

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

Thus,

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

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

\[
\langle r^{-2} \rangle = -4\alpha e^{\alpha r} \left[ 1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l + 1) + 1} \right] - \frac{\mu A}{\hbar^2 \alpha} - \frac{\mu V_0}{2\hbar^2 \alpha^2} + l(l + 1) \right] + \left( n^2 + n + \frac{1}{2} \right) + \left( n + \frac{1}{2} \right) \left( n + \frac{1}{2} \right) \left( n + \frac{1}{2} \right) \right] \left[ 1 + 2n + \sqrt{8\mu B/\hbar^2 + 4l(l + 1) + 1} \right]^{-1}.
\] (59)

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

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

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

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

Equating (59) to (60) then gives

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

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

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

\[
\left\langle \Psi(\mu) \frac{\partial H(A)}{\partial A} \Psi(\mu) \right\rangle = -\frac{\hbar^2}{2\mu^2} \frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2}
\]
\[
= \frac{1}{\mu} \left(-\frac{\hbar^2}{2\mu^2} \frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2}\right) \Rightarrow
\]
\[
-\frac{1}{\mu} \left(\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2}\right) \Rightarrow
\]
\[
-\frac{1}{\mu} \langle T \rangle = -\frac{1}{\mu} (H - V).
\]

Hence,

\[
\left\langle \Psi(\mu) \frac{\partial H(A)}{\partial A} \Psi(\mu) \right\rangle = -\frac{1}{\mu} (H - V).
\]

(64)

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

\[
\left\langle \Psi(\mu) \frac{\partial H(A)}{\partial A} \Psi(\mu) \right\rangle = -\frac{1}{2\mu} \left\langle p^2 \right\rangle.
\]

(65)

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

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

(66)
Also, equating (62) to (65) gives $\langle p^2 \rangle$. Thus,

$$\langle p^2 \rangle = 8\hbar^2 \alpha^2 \mu \left(1 + 2n + \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1}\right)$$

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

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

$$+ \frac{(n^2 + n + 1/2)4B}{\hbar^2\sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}} + \frac{(n + 1/2)4B}{\hbar^2\sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}}\right\}}$$

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

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

$$+ \frac{1}{2} + \frac{1}{2} + \frac{8\mu B}{\hbar^2} + 4l(l+1) + 1\right\} \times \left[1 + 2n$$

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

$$- \frac{\mu A}{\hbar^2\alpha} - \frac{\mu V_0}{2\hbar^2\alpha^2} + I(l+1) + (n^2 + n + \frac{1}{2}) + (n$$

$$+ \left\{\frac{\sqrt{\mu c/2\hbar^2\alpha^2 - \mu E/2\hbar^2\alpha^2}}{4} - 4\sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}\right\}\right\}$$

$$\times (1 - s)$$

$$\times (s)\left\{\sqrt{(\mu c/2\hbar^2\alpha^2 - \mu E/2\hbar^2\alpha^2)}\right\}$$

$$\times (1 - s) \left(1/2 + (1/2) \sqrt{8\mu B/\hbar^2 + 4l(l+1) + 1}\right)$$

$$\times (s)\sqrt{(\mu c/2\hbar^2\alpha^2 - \mu E/2\hbar^2\alpha^2)}.$$

### 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$_2$, 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$_2$ 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$_2$ 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
### Table 2: Expectation values of $\langle r^{-2} \rangle$ for hydrogen molecule.

| $n$ | $l$ | $\langle r^{-2} \rangle_{el}$ (Å$^{-2}$) |
|-----|-----|-----------------------------------|
| 0   | 0   | -2.0357926925                    |
| 1   | 0   | -0.3696297856                    |
| 2   | 0   | -0.0592081872                    |
| 3   | 0   | -0.0012360988                    |
| 4   | 0   | -0.0104609211                    |
| 5   | 0   | -0.040843125                     |
| 6   | 0   | -0.0781701991                    |
| 7   | 0   | -0.1174681786                    |
| 8   | 0   | -0.156879315                     |
| 0   | 1   | -0.5500657326                    |
| 1   | 1   | -0.1011084016                    |
| 2   | 1   | -0.009381431                     |
| 3   | 1   | -0.00170747903                   |
| 4   | 1   | -0.01903889872                   |
| 5   | 1   | -0.0445644429                    |
| 6   | 1   | -0.0726573984                    |
| 7   | 1   | -0.1012658894                    |
| 8   | 1   | -0.1296232040                    |
| 0   | 2   | -0.1068000999                    |
| 1   | 2   | -0.012070336                     |
| 2   | 2   | -0.0002713032                    |
| 3   | 2   | -0.0106774421                    |
| 4   | 2   | -0.0282925702                    |
| 5   | 2   | -0.0482198274                    |
| 6   | 2   | -0.0686930232                    |
| 7   | 2   | -0.089051593                     |
| 8   | 2   | -0.1090597335                    |
| 0   | 3   | -0.0119105671                    |
| 1   | 3   | -0.0000320975                    |
| 2   | 3   | -0.0070284422                    |
| 3   | 3   | -0.020151142                     |
| 4   | 3   | -0.0351851804                    |
| 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.

| $n$ | $l$ | $\langle r^{-2} \rangle_{el}$ (Å$^{-2}$) |
|-----|-----|-----------------------------------|
| 0   | 0   | -2.5067716077                    |
| 1   | 0   | -4.331151186                     |
| 2   | 0   | -6.0543340693                    |
| 3   | 0   | -7.732755626                     |
| 4   | 0   | -9.3878635299                    |
| 5   | 0   | -11.029466762                    |
| 6   | 0   | -12.6623937821                   |
| 7   | 0   | -14.2896150748                   |
| 8   | 0   | -15.8912886181                   |
| 0   | 1   | -2.580487535                     |
| 1   | 1   | -3.8567374113                    |
| 2   | 1   | -5.0875482240                    |
| 3   | 1   | -6.2962037702                    |
| 4   | 1   | -7.4925183938                    |
| 5   | 1   | -8.6812844732                    |
| 6   | 1   | -9.8651049570                    |
| 7   | 1   | -11.045127066                    |
| 8   | 1   | -12.2234677505                   |
| 0   | 2   | -2.5968121549                    |
| 1   | 2   | -3.4838644792                    |
| 2   | 2   | -4.352931128                     |
| 3   | 2   | -5.2122003606                    |
| 4   | 2   | -6.0655657689                    |
| 5   | 2   | -6.9150709513                    |
| 6   | 2   | -7.7620392900                    |
| 7   | 2   | -8.6070919545                    |
| 8   | 2   | -9.4507726300                    |
| 0   | 3   | -2.5853004074                    |
| 1   | 3   | -3.247921138                     |
| 2   | 3   | -3.904155691                     |
| 3   | 3   | -4.5508403180                    |
| 4   | 3   | -5.1972396752                    |
| 5   | 3   | -5.8415792817                    |
| 6   | 3   | -6.4844525672                    |
| 7   | 3   | -7.262510136                     |
| 8   | 3   | -7.767232288                     |

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

$$
\xi_1 = \sqrt{\left( \frac{\mu c}{2\hbar^2 \alpha^2} - \frac{\mu E}{2\hbar^2 \alpha^2} \right)} \wedge = \sqrt{\frac{8\mu B}{\hbar^2} + 4l(l+1) + 1}. \quad (70)
$$

Equation (44) can then be expressed as

$$
\Psi_n(s) = B_n(s) \xi_1^{l} \left[ 1 - s \right]^{(1/2+l)(1/2)} \times \psi_n^{(2\xi_1-4\lambda),(2-2\xi_1-4\lambda)} (1-s). \quad (71)
$$
Table 4: Expectation values of \( \langle r^{-2} \rangle \) for hydrogen chloride molecule.

| \( n \) | \( l \) | \( \langle r^{-2} \rangle_{nl} \) (Å\(^{-2}\)) |
|---|---|---|
| 0 | 0 | -3.3684130731 |
| 1 | 0 | -0.9469378738 |
| 2 | 0 | -0.2983655406 |
| 3 | 0 | -0.0858726882 |
| 4 | 0 | -0.0155115416 |
| 5 | 0 | -0.0000012220 |
| 6 | 0 | -0.0080075039 |
| 7 | 0 | -0.0266967106 |
| 8 | 0 | -0.0503972535 |
| 0 | 1 | -1.4986915458 |
| 1 | 1 | -0.4550672530 |
| 2 | 1 | -0.1414988910 |
| 3 | 1 | -0.0353990416 |
| 4 | 1 | -0.0034391544 |
| 5 | 1 | -0.0014403531 |
| 6 | 1 | -0.0126923268 |
| 7 | 1 | -0.0301459097 |
| 8 | 1 | -0.0503830973 |
| 0 | 2 | -0.4870935323 |
| 1 | 2 | -0.1534956468 |
| 2 | 2 | -0.0423781577 |
| 3 | 2 | -0.0064034364 |
| 4 | 2 | -0.0002878180 |
| 5 | 2 | -0.0066922782 |
| 6 | 2 | -0.0194755454 |
| 7 | 2 | -0.0343426512 |
| 8 | 2 | -0.0507696946 |
| 0 | 3 | -0.1460080210 |
| 1 | 3 | -0.0419218285 |
| 2 | 3 | -0.0074968794 |
| 3 | 3 | -0.0000196467 |
| 4 | 3 | -0.0040520781 |
| 5 | 3 | -0.0133574532 |
| 6 | 3 | -0.0251076232 |
| 7 | 3 | -0.0379661955 |
| 8 | 3 | -0.0512701657 |

Substituting (71) into (69) gives

\[
- \frac{B_2^2}{2\alpha} \int_0^1 (s)_{2\ell - 1} [1 - s]^{(1 + \lambda)} \times \left[ \Gamma_n^{(2\ell - 4\xi)} (1 - s) \right]^2 \ ds = 1. \tag{72}
\]

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

\[
P_n^{(\rho,\nu)}(\xi) = 2^n \sum_{p=0}^{n} (-1)^n \rho^{-p} \binom{n + \rho - p}{p} \binom{n + \nu}{p} (1 - \xi)^p (1 + \xi)^p, \tag{73}
\]

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

| \( n \) | \( l \) | \( \langle r^{-2} \rangle_{nl} \) (Å\(^{-2}\)) |
|---|---|---|
| 0 | 0 | -3.4125427704 |
| 1 | 0 | -3.0306606764 |
| 2 | 0 | -1.7478304736 |
| 3 | 0 | -1.0168948372 |
| 4 | 0 | -0.5850753187 |
| 5 | 0 | -0.3251871304 |
| 6 | 0 | -0.1688134583 |
| 7 | 0 | -0.0771780105 |
| 0 | 1 | -4.7293036688 |
| 1 | 1 | -2.6662352623 |
| 2 | 1 | -1.5422086726 |
| 3 | 1 | -0.8968395046 |
| 4 | 1 | -0.5138531529 |
| 5 | 1 | -0.2830295670 |
| 6 | 1 | -0.1444688867 |
| 7 | 1 | -0.0638852202 |
| 0 | 2 | -3.6765597149 |
| 1 | 2 | -2.0956762249 |
| 2 | 2 | -1.270016580 |
| 3 | 2 | -0.7058809007 |
| 4 | 2 | -0.4003901614 |
| 5 | 2 | -0.2160772200 |
| 6 | 2 | -0.106187105 |
| 7 | 2 | -0.043549137 |
| 8 | 2 | -0.0117284027 |
| 0 | 3 | -2.6130040241 |
| 1 | 3 | -1.5063610220 |
| 2 | 3 | -0.8764213217 |
| 3 | 3 | -0.5044821669 |
| 4 | 3 | -0.2806791571 |
| 5 | 3 | -0.1459868053 |
| 6 | 3 | -0.069337108 |
| 7 | 3 | -0.2368085249 |
| 8 | 3 | 0.0040288991 |

\[
P_n^{(\rho,\nu)}(\xi) = \frac{\Gamma(n + \rho + 1)}{n! \Gamma(n + \rho + 1 + \nu + r + 1)} \sum_{r=0}^{n} \binom{n}{r} \frac{\Gamma(n + \rho + v + r + 1)}{\Gamma(r + \rho + 1)} \left( \frac{\xi - 1}{2} \right)^r, \tag{74}
\]

where

\[
\binom{n}{r} = \frac{n!}{(n-r)!r!} = \frac{\Gamma(n+1)}{\Gamma(n-r+1)\Gamma(r+1)}. \tag{75}
\]

Equations (73) and (74) are used simultaneously in evaluating the Jacobi polynomial.
Table 6: Expectation values of $\langle r^{-1}\rangle$ for hydrogen molecule.

| $n$ | $l$ | $\langle r^{-1}\rangle_{nl}$ (Å$^{-1}$) |
|-----|-----|---------------------------------|
| 0   | 0   | 1.2603680546                   |
| 1   | 0   | 0.437975401                   |
| 2   | 0   | 0.151717261                   |
| 3   | 0   | 0.1960018427                  |
| 4   | 0   | -0.0520387537                 |
| 5   | 0   | -0.095189716                  |
| 6   | 0   | -0.0123158672                 |
| 7   | 0   | -0.0142326424                 |
| 8   | 0   | -0.1560297050                 |
| 0   | 1   | 0.6791360070                  |
| 1   | 1   | 0.246793485                   |
| 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   | -0.707961201                  |
| 4   | 2   | -0.1071332977                 |
| 5   | 2   | -0.1312363775                 |
| 6   | 2   | -0.1480391542                 |
| 7   | 2   | -0.1602175908                 |
| 8   | 2   | -0.1693251067                 |
| 0   | 3   | 0.104721078                   |
| 1   | 3   | -0.0489334886                 |
| 2   | 3   | -0.0663845048                 |
| 3   | 3   | -0.1042945872                 |
| 4   | 3   | -0.129304551                  |
| 5   | 3   | -0.1466642182                 |
| 6   | 3   | -0.1592049675                 |
| 7   | 3   | -0.1685578998                 |
| 8   | 3   | -0.1757185637                 |

Considering the Jacobi polynomial of (72)

$$p_n^{(2\xi_1 - 4\Lambda), (-2\xi_1 - 4\Lambda)} (1 - s)$$

\[ \rho = (2\xi_1 - 4\Lambda), \quad \nu = (-2\xi_1 - 4\Lambda), \quad \xi = (1 - s). \]

Using (73) then the Jacobi polynomial becomes

$$p_n^{(2\xi_1 - 4\Lambda), (-2\xi_1 - 4\Lambda)} (1 - s) = 2^{-n} \sum_{p=0}^{n} (-1)^{n-p} \binom{n + 2\xi_1 - 4\Lambda}{p} \binom{n - 2\xi_1 - 4\Lambda}{n-p} (s)^{n-p} (2-s)^p$$

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

| $n$ | $l$ | $\langle r^{-1}\rangle_{nl}$ (Å$^{-1}$) |
|-----|-----|---------------------------------|
| 0   | 0   | -1.6004003285                   |
| 1   | 0   | -1.7169221172                  |
| 2   | 0   | -1.757628815                   |
| 3   | 0   | -1.776451792                   |
| 4   | 0   | -1.7866702782                  |
| 5   | 0   | -1.7928291806                  |
| 6   | 0   | -1.7968253335                  |
| 7   | 0   | -1.795644507                   |
| 8   | 0   | -1.8015233696                  |
| 0   | 1   | -1.6824412202                  |
| 1   | 1   | -1.7440039428                  |
| 2   | 1   | -1.7697345550                  |
| 3   | 1   | -1.7828775641                  |
| 4   | 1   | -1.7904817685                  |
| 5   | 1   | -1.7952728019                  |
| 6   | 1   | -1.7984847995                  |
| 7   | 1   | -1.8007424714                  |
| 8   | 1   | -1.8023895794                  |
| 0   | 2   | -1.7364379965                  |
| 1   | 2   | -1.7662041335                  |
| 2   | 2   | -1.7809515222                  |
| 3   | 2   | -1.7893186518                  |
| 4   | 2   | -1.7945147323                  |
| 5   | 2   | -1.797668174                   |
| 6   | 2   | -1.800379661                   |
| 7   | 2   | -1.802154796                   |
| 8   | 2   | -1.803495262                   |
| 0   | 3   | -1.7642012758                  |
| 1   | 3   | -1.7198804427                  |
| 2   | 3   | -1.7886797501                  |
| 3   | 3   | -1.7941062087                  |
| 4   | 3   | -1.7976867501                  |
| 5   | 3   | -1.8001727144                  |
| 6   | 3   | -1.8019687138                  |
| 7   | 3   | -1.803308380                   |
| 8   | 3   | -1.8043340174                  |

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

Evaluating it for $p = 0$

$$\sum_{p=0}^{n} (-1)^{n-p} \binom{n + 2\xi_1 - 4\Lambda}{p} \binom{n - 2\xi_1 - 4\Lambda}{n-p} (s)^{n-p} (2-s)^p$$
Table 8: Expectation values of \( \langle r^{-1} \rangle \) for hydrogen chloride molecule.

| \( n \) | \( l \) | \( \langle r^{-1} \rangle_{nl} (\text{Å}^{-1}) \) |
|---|---|---|
| 0 | 0 | 1.629706170 |
| 1 | 0 | 0.7484646279 |
| 2 | 0 | 0.3703627204 |
| 3 | 0 | 0.1796456609 |
| 4 | 0 | 0.0702995120 |
| 5 | 0 | 0.0165105899 |
| 6 | 0 | -0.4409464949 |
| 7 | 0 | -0.0761475106 |
| 8 | 0 | -0.0994688026 |
| 0 | 1 | 1.1368069123 |
| 1 | 1 | 0.5412411880 |
| 2 | 1 | 0.2694738513 |
| 3 | 1 | 0.123413170 |
| 4 | 1 | 0.0354355337 |
| 5 | 1 | -0.0212411621 |
| 6 | 1 | -0.0599699133 |
| 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 |

\[
\langle r^{-1} \rangle_{nl} = (-1)^{n-l} \frac{(n + 2 \xi_1 - 4 \Lambda)!}{[(n + 2 \xi_1 - 4 \Lambda) - 0]!} \frac{(n - 2 \xi_1 - 4 \Lambda)!}{[(n - 2 \xi_1 - 4 \Lambda) + 1]!} \\
= (-1)^{n-l} \frac{\Gamma(n - 2 \xi_1 - 4 \Lambda + 1)}{\Gamma(n + 1) \Gamma(1 - 2 \xi_1 - 4 \Lambda)}.
\]

(78)

For \( p = 0, n \)

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

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

\[
\rho_n^p(2\xi_1 - 4\Lambda)(-2\xi_1 - 4\Lambda)](1-s) = (-1)^n \frac{\Gamma(n - 2 \xi_1 - 4 \Lambda + 1)}{\Gamma(n + 1) \Gamma(1 - 2 \xi_1 - 4 \Lambda)} \sum_{p=0}^{n} (-1)^p \frac{2n^p(2-s)^p}{p!(n-p)!\Gamma(n + 2 \xi_1 - 4 \Lambda - p + 1) \Gamma(p - 2 \xi_1 - 4 \Lambda + 1)}.
\]

(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    | -1.700907969                |
| 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    | 0.376550363                 |
| 2    | 2    | -0.0842496033               |
| 3    | 2    | -0.6872416982               |
| 4    | 2    | -1.3760329800               |
| 5    | 2    | -2.1263145693               |
| 6    | 2    | -2.9517276048               |
| 7    | 2    | -3.8503398566               |
| 8    | 2    | -4.8455016676               |
| 0    | 3    | 0.423977151                 |
| 1    | 3    | -0.0331938070               |
| 2    | 3    | -0.6403179766               |
| 3    | 3    | -1.3293878653               |
| 4    | 3    | -2.0879210976               |
| 5    | 3    | -2.916860233                |
| 6    | 3    | -3.8170461261               |
| 7    | 3    | -4.7934410194               |
| 8    | 3    | -5.8478274746               |

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

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

(81)

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

\[
[P_n^{(2\xi_1 - 4\lambda, -2\xi_1 - 4\lambda)}(1-s)]^2 = (80) \times \left(-1\right)^n \frac{\Gamma(n + 2\xi_1 - 4\Lambda + 1)}{\Gamma(n + 1) \Gamma(1 - 2\xi_1 - 4\Lambda)} \times \sum_{p=0}^{n} \left(-1\right)^{p} 
\cdot \frac{\Gamma(n + 2\xi_1 - 4\Lambda + 1)}{\Gamma(n + 1 - 8\Lambda)} \times \frac{\Gamma(n + 2\xi_1 - 4\Lambda)}{\Gamma(n + 1 - 8\Lambda)} \times \Gamma(n + r + 1 - 8\Lambda) \times \sum_{r=0}^{n} \left(\frac{-1}{2}\right)^r 
\cdot \frac{\Gamma(n + r + 1 - 8\Lambda)}{\Gamma(n + r - 1 + 8\Lambda)} \Gamma(r + 2\xi_1 - 4\Lambda + 1) s^r.
\]

\[
(82)
\]

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    | -39.089487134               |
| 5    | 0    | -54.8817584651              |
| 6    | 0    | -73.434205101               |
| 7    | 0    | -94.7369941855              |
| 8    | 0    | -118.7841018590             |
| 0    | 1    | -7.808669292               |
| 1    | 1    | -14.271409244               |
| 2    | 1    | -23.685411210               |
| 3    | 1    | -35.9457058061              |
| 4    | 1    | -51.002483523               |
| 5    | 1    | -68.831106737               |
| 6    | 1    | -89.416929911               |
| 7    | 1    | -112.751669680              |
| 8    | 1    | -138.830077540              |
| 0    | 2    | -14.239153700               |
| 1    | 2    | -23.446771704               |
| 2    | 2    | -35.526170800               |
| 3    | 2    | -50.415740033               |
| 4    | 2    | -68.084482670               |
| 5    | 2    | -88.514260654               |
| 6    | 2    | -111.6984397090             |
| 7    | 2    | -137.6272527440             |
| 8    | 2    | -166.297720400              |
| 0    | 3    | -23.4729539098              |
| 1    | 3    | -35.489861236               |
| 2    | 3    | -50.325408181               |
| 3    | 3    | -67.949620490               |
| 4    | 3    | -88.329650796               |
| 5    | 3    | -133.468304780              |
| 6    | 3    | -137.354231380              |
| 7    | 3    | -165.982763447              |
| 8    | 3    | -197.350617564              |
Table 12: Expectation values of $\langle T \rangle$ for hydrogen chloride molecule.

| $n$ | $l$ | $\langle T \rangle$ (eV) |
|-----|-----|-------------------------|
| 0   | 0   | -16.8602470534         |
| 1   | 0   | -3.817340938           |
| 2   | 0   | -0.7264968799          |
| 3   | 0   | 0.8107812272           |
| 4   | 0   | 0.1808796145           |
| 5   | 0   | 0.0076433944           |
| 6   | 0   | -0.2925912249          |
| 7   | 0   | -0.6554441904          |
| 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   | -2.7518967983          |
| 0   | 2   | -0.371965298           |
| 1   | 2   | 0.1982728862           |
| 2   | 2   | 0.1926154142           |
| 3   | 2   | -0.409008669           |
| 4   | 2   | -0.3834013618          |
| 5   | 2   | -0.7902268789          |
| 6   | 2   | -1.2436082882          |
| 7   | 2   | -1.736979570           |
| 8   | 2   | -0.5275303052          |
| 0   | 3   | 0.1879629685           |
| 1   | 3   | 0.2257165907           |
| 2   | 3   | 0.0056050075           |
| 3   | 3   | -0.3335743383          |
| 4   | 3   | -0.740542881           |
| 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.

| $n$ | $l$ | $\langle T \rangle$ (eV) |
|-----|-----|-------------------------|
| 0   | 0   | -129.9291130830         |
| 1   | 0   | -75.6124342843          |
| 2   | 0   | -45.8529997998          |
| 3   | 0   | -28.4567950151          |
| 4   | 0   | -17.933612549           |
| 5   | 0   | -11.029843042           |
| 6   | 0   | -6.6378456500           |
| 7   | 0   | -3.7514369504           |
| 8   | 0   | -1.8533323454           |
| 0   | 1   | -17.6340205260          |
| 1   | 1   | -6.941012988            |
| 2   | 1   | -42.0768329333          |
| 3   | 1   | -26.1683200430          |
| 4   | 1   | -16.3516907261          |
| 5   | 1   | -10.0962337215          |
| 6   | 1   | -6.0247765063           |
| 7   | 1   | -3.347174404            |
| 8   | 1   | -1.5898907876           |
| 0   | 2   | -97.238969338           |
| 1   | 2   | -58.1864276360          |
| 2   | 2   | -35.7490746782          |
| 3   | 2   | -22.293665438           |
| 4   | 2   | -13.8933817128          |
| 5   | 2   | -8.4988638639           |
| 6   | 2   | -4.9737074744           |
| 7   | 2   | -2.6557694881           |
| 8   | 2   | -1.143095374            |
| 0   | 3   | -76.0158584874          |
| 1   | 3   | -46.0107012922          |
| 2   | 3   | -28.5036356479          |
| 3   | 3   | -17.913843239           |
| 4   | 3   | -11.008725080           |
| 5   | 3   | -6.645424645            |
| 6   | 3   | -3.7334128723           |
| 7   | 3   | -1.8447253427           |
| 8   | 3   | -0.6270405479           |

Equation (82) can be further simplified to

$$
\left[p_n^{2(\xi_1 - 4 \Lambda)} \right]^2 = (-1)^n \frac{\Gamma(n + \xi_1 - 4 \Lambda + 1)^2 \Gamma(n + 2\xi_1 - 4 \Lambda + 1)^2}{\Gamma(n + 1)^2 \Gamma(1 - 2\xi_1 - 4 \Lambda)^2} \times \frac{\Gamma(n + r + 1 - 8 \Lambda)}{\Gamma(n + 1 - 8 \Lambda)} \times \frac{\Gamma(n - p + 1 - 8 \Lambda)}{\Gamma(n - p - 8 \Lambda)} 
$$

$$
\sum_{p=0}^{n} \sum_{r=0}^{n} (-1)^{p+r} p!(n-p)!^r(n-r)! \Gamma(n + 2\xi_1 - 4 \Lambda - p + 1)^2 \Gamma(p - 2\xi_1 - 4 \Lambda + 1) \Gamma(r + 2\xi_1 - 4 \Lambda + 1) \Gamma(n + r + 1 - 8 \Lambda) \times \Gamma(n + 1 - 8 \Lambda) \Gamma(n - p + 1 - 8 \Lambda) \Gamma(n - p - 8 \Lambda) 
$$

$$
\frac{2^{n-r} (s)^{n-p+r} (2 - s)^p}{p! (n-p)!^r(n-r)! \Gamma(n + 2\xi_1 - 4 \Lambda - p + 1)^2 \Gamma(p - 2\xi_1 - 4 \Lambda + 1) \Gamma(r + 2\xi_1 - 4 \Lambda + 1) \Gamma(n + r + 1 - 8 \Lambda) \times \Gamma(n + 1 - 8 \Lambda) \Gamma(n - p + 1 - 8 \Lambda) \Gamma(n - p - 8 \Lambda)} 
$$

(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   | -0.1587565569                 |
| 2   | 0   | 0.3863626785                  |
| 3   | 0   | 0.1012545103                  |
| 4   | 0   | -0.4083445259                 |
| 5   | 0   | -1.0222073945                 |
| 6   | 0   | -1.7142018411                 |
| 7   | 0   | -2.4801686318                 |
| 8   | 0   | -3.3212864410                 |
| 0   | 1   | -1.46978706526                |
| 1   | 1   | -2.2655056555                 |
| 2   | 1   | -3.0560726813                 |
| 3   | 1   | -3.960947886                  |
| 4   | 1   | -3.45367735                  |
| 5   | 1   | -1.4697870652                |
| 6   | 1   | -2.2655056555                 |
| 7   | 1   | -3.0560726813                 |
| 8   | 1   | -3.960947886                  |
| 0   | 2   | 0.394312472                  |
| 1   | 2   | 0.2925724658                 |
| 2   | 2   | -0.1806436110                |
| 3   | 2   | -0.4083445259                |
| 4   | 2   | -1.0222073945                |
| 5   | 2   | -1.7142018411                |
| 6   | 2   | -2.4801686318                |
| 7   | 2   | -3.3212864410                |
| 8   | 2   | -4.139703776                 |
| 0   | 3   | 0.4094312472                  |
| 1   | 3   | 0.2925724658                 |
| 2   | 3   | -0.1806436110                |
| 3   | 3   | -0.4083445259                |
| 4   | 3   | -1.0222073945                |
| 5   | 3   | -1.7142018411                |
| 6   | 3   | -2.4801686318                |
| 7   | 3   | -3.3212864410                |
| 8   | 3   | -4.139703776                 |

Substituting (83) into (72) gives

\[
\begin{align*}
- (-1)^n \frac{\Gamma(n - 2\xi_1 - 4 - 1)\Gamma(n + 2\xi_1 - 4 + 1)^2}{2\alpha \Gamma(n + 1)\Gamma(1 - 2\xi_1 - 4 \wedge)} & \times \frac{\Gamma(n + r + 1 - 8 \wedge)}{\Gamma(n + 1 - 8 \wedge)} \\
\sum_{p=0}^{n} \sum_{r=0}^{n} (-1)^{p+r} & \frac{p!(n-p)!r!(n-r)!\Gamma(n + 2\xi_1 - 4 - p + 1)\Gamma(p + 2\xi_1 - 4 - p + 1)\Gamma(p + r + 1)}{2^{-n}r} B_n^2 B_n^2 \\
\int_{0}^{1} (s)^{2\xi_1 - 1 + n - p + r} [1 - s]^{(1 + n)} & ds = 1
\end{align*}
\]
Table 16: Expectation values of \( \langle p^2 \rangle \) for hydrogen chloride molecule.

| \( n \) | \( l \) | \( \langle p^2 \rangle \) (eV/c)^2 |
|---|---|---|
| 0 | 0 | -7.446816181 |
| 1 | 0 | -15.0322275400 |
| 2 | 0 | -27.93329345570 |
| 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 | -59.4570586016 |
| 4 | 1 | -89.7771963400 |
| 5 | 1 | -121.1595854800 |
| 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 | -242.2575340600 |
| 8 | 2 | -292.7246564890 |
| 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 |

Confluent hypergeometric function can be defined as follows:

\[
\mathbb{F}_1(\alpha_0,\beta_0;\gamma_0;1) = \alpha_0 \int_0^1 (s)^{\alpha_0 - 1} (1 - s)^{\beta_0} \, ds \tag{85}
\]

assuming that

\[
\gamma_0 = \alpha_0 + 1,
\]

then

\[
\mathbb{F}_1(\alpha_0,\beta_0;\gamma_0;1) = \alpha_0 \int_0^1 (s)^{\alpha_0 - 1} (1 - s)^{\beta_0} \, ds \tag{86}
\]

= 1.

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

| \( n \) | \( l \) | \( \langle p^2 \rangle \) (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 | -151.3338575370 |
| 6 | 0 | -91.0801622550 |
| 7 | 0 | -51.4747561410 |
| 8 | 0 | -25.4274783679 |
| 0 | 1 | -13.7455127207 |
| 1 | 1 | -25.1211651371 |
| 2 | 1 | -41.6921779602 |
| 3 | 1 | -59.4570586016 |
| 4 | 1 | -89.7771963400 |
| 5 | 1 | -121.1595854800 |
| 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 | -242.2575340600 |
| 8 | 2 | -292.7246564890 |
| 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 |

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 | -0.0930125 | -0.0930120 |
| 0 | 1 | 0.100 | -0.0800000 | -0.0800000 |
| 0 | 1 | 0.150 | -0.0612500 | -0.0612500 |

However,

\[
\mathbb{F}_1(\alpha_0,\beta_0;\gamma_0;1) = \frac{\Gamma(\gamma_0)}{\Gamma(\gamma_0 - \alpha_0 - \beta_0)} \frac{\Gamma(\gamma_0 - \alpha_0)}{\Gamma(\gamma_0 - \beta_0)} \tag{87}
\]
Considering
\[
\int_0^1 (s)^{2\xi_1 - 1 + n - p + r} [1 - s]^{(1 + \Lambda)} ds, \tag{88}
\]
therefore
\[
\int_0^1 (s)^{2\xi_1 - 1 + n - p + r} [1 - s]^{(1 + \Lambda)} ds
= \frac{\Gamma (\alpha_0 + 1) \Gamma (\Lambda + 2)}{\alpha_0 \Gamma (\alpha_0 + \Lambda + 2)}. \tag{89}
\]
Substituting (89) into (84) gives
\[
- (-1)^n \frac{\Gamma (n - 2\xi_1 - 4 + 1)^2 \Gamma (n + 2\xi_1 - 4 + 1)^2}{2\alpha \Gamma (n + 1) \Gamma (1 - 2\xi_1 - 4 \Lambda)} \times \frac{\Gamma (n + r + 1 - 8\Lambda)}{\Gamma (n + 1 - 8\Lambda)} \times \sum_{p=0}^{n} \sum_{r=0}^{n} (-1)^{p+r} \frac{2^{-n-r} (2 - s)^p B_n^2}{p! (n-p)! r! (n-r)! \Gamma (n + 2\xi_1 - 4 + 1) \Gamma (p - 2\xi_1 - 4 + 1) \Gamma (r + 2\xi_1 - 4 + 1)} \times \frac{\Gamma (\alpha_0 + 1) \Gamma (\Lambda + 2)}{\alpha_0 \Gamma (\alpha_0 + \Lambda + 2)} = 1. \tag{90}
\]
Let
\[
s_1 = - (-1)^n \frac{\Gamma (n - 2\xi_1 - 4 + 1)^2 \Gamma (n + 2\xi_1 - 4 + 1)^2}{2\alpha \Gamma (n + 1) \Gamma (1 - 2\xi_1 - 4 \Lambda)} \times \frac{\Gamma (n + r + 1 - 8\Lambda)}{\Gamma (n + 1 - 8\Lambda)} \times \sum_{p=0}^{n} \sum_{r=0}^{n} (-1)^{p+r} \frac{2^{-n-r} (2 - s)^p}{p! (n-p)! r! (n-r)! \Gamma (n + 2\xi_1 - 4 + 1) \Gamma (p - 2\xi_1 - 4 + 1) \Gamma (r + 2\xi_1 - 4 + 1)} \times \frac{\Gamma (\alpha_0 + 1) \Gamma (\Lambda + 2)}{\alpha_0 \Gamma (\alpha_0 + \Lambda + 2)}. \tag{91}
\]
However,
\[
B_n^2 s_1 = 1 \implies B_n = \frac{1}{\sqrt{s_1}}. \tag{92}
\]

Let
\[
\Psi_n (s) = \frac{1}{\sqrt{s_1}} \left( s \right)^{2(\sqrt{\mu c/2\hbar^2 + \mu E/2\hbar^2a^2}) - 4\sqrt{(\hbar^2 c/h + \hbar^2/4(1 + 1))}, (-2\sqrt{\mu c/2\hbar^2a^2 - \mu E/2\hbar^2a^2}) - 4\sqrt{(\hbar^2 c/h + \hbar^2/4(1 + 1))} (1 - s)} \times [1 - s]^{(1/2 \pm 1/2)(\sqrt{\hbar^2 c/h + \hbar^2/4(1 + 1))}} (s) \sqrt{(\mu c/2\hbar^2a^2 - \mu E/2\hbar^2a^2)} \right). \tag{93}
\]

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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