



## Computational Studies of Energy and Expectation Values of Modified Yukawa Potential (MYP) for some Diatomic Molecules

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### Abstract:

The modified Yukawa potential energy function is known to be a very lofty model due to its potency in predicting the behaviour of different atoms and molecules. The aim of this study is to establish numerical energies and expectation values of some diatomic molecules confined in modified Yukawa potential. By employing the basic ideas of non-relativistic quantum mechanics, the radial Schrödinger equation (SE) with modified Yukawa potential (MYP) is solved using the asymptotic iteration method (AIM). We explicitly obtained the energy value expression and their corresponding normalized eigen - functions in closed form for some diatomic molecules (DMs) such as hydrogen dimer ( $H_2$ ), lithium hydride ( $LiH$ ) and hydrogen chloride ( $HCl$ ), with the help of

the Greene - Aldrich-type approximation scheme. Using the Hellman-Feynman theorem (HFT), we obtained the expressions for the expectation values of the selected DMs. The numerical results of the energies and expectation values of the DMs with varying quantum numbers are further presented. In addition, the graphical plots of the energies and expectation values as functions of quantum numbers have been discussed extensively. It is observed that the energies and expectation values of MYP depend greatly on the quantum numbers for the selected DMs. Our results show a great correlation when compared to other works in available literature.

**Keywords:** Schrödinger equation (SE), Modified Yukawa Potential (MYP), Expectation Values, Diatomic molecules (DMs), Energy values

### 1. Introduction

Potential energy functions are known to be very lofty functions used in exciting interactions amongst atoms and molecules, due to their

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potency in predicting the behaviour of these atoms and molecules (Oluwadare *et al.*, 2022a). Over the years, these models have been employed to study different phenomena, not limited to molecular spectra, vibrations and dynamics (Huber and Herzberg, 1979), spin-orbit interaction, relativistic corrections and diamagnetic susceptibility (Khordad *et al.*, 2012; Donfack and Fotue, 2021), optical properties (Liu *et al.*, 2012), interband light absorption and interband optical transitions (Saravanan *et al.*, 2015), energy and relativistic effects in weakly bound nuclei (Rezvani and Shojaei, 2017; Rezvani and Shojaei, 2018), energy confinement on quantum dots (Okorie, 2017; Okorie and Iboh, 2018), external magnetic fields, Aharonov-Bohm flux fields (Rajabi and Hamzavi, 2013; Ikhdair and Falaye, 2014), interactions between the magnetic and electric fields (Chen *et al.*, 2022), thermodynamic properties (Duc *et al.*, 2018; Ikot *et al.*, 2019; Chabi and Boumali, 2020; Oluwadare *et al.*, 2022b), spin and pseudospin symmetries (Oyewumi and Oluwadare, 2017), two-body effects (Arda, 2017; Oluwadare and Oyewumi, 2018a) and prediction of thermochemical properties (Qin *et al.*, 2021). Various techniques, not limited to factorization method (Dong, 2007), Nikiforov-Uvarov (NU) method (Nikiforov and Uvarov, 1998), asymptotic iteration method (AIM) (Ciftci *et al.*, 2005; Bayrak and Boztosun, 2007), NU Functional Analysis (NUFA) method (Ikot *et al.*, 2021), exact and proper quantization rule (Dong *et al.*, 2007; Dong and Cruz-Irisson, 2012), have been employed to solve different wave functions with potential energy functions of interest. Okorie and his collaborators (2018) used the modified factorization method to solve the Schrödinger equation with modified Yukawa potential model. They obtained the energy spectra and thermodynamic properties with the help of Pekeris approximation scheme.

Numerous studies have been carried out as regards potential energy functions with

diatomic molecules. Readers can refer to Onate *et al.* (2022) and Khordad *et al.* (2022). In addition, the studies of expectation values of various diatomic molecules have been of interest in recent times (Oyewumi, 2005; Falaye *et al.*, 2014; Okon *et al.*, 2017; Oluwadare and Oyewumi, 2018b; Ikot *et al.*, 2019). Most recent study on expectation values was carried out by Eyube and his collaborators (Eyube *et al.*, 2022). In their study, they obtained the expectation values and kinetic energies of improved deformed exponential-type potential (IDEP) for some DMs using Heymann Feymann theorem (HFT) (Feymann, 1939).

In view of this development, we are motivated to compute the energies and expectation values of modified Yukawa potential for some diatomic molecules. Similar study has not been carried out by any author to the best of our knowledge. The modified Yukawa potential was defined by Ikhdair and Hamzavi (2012) and Ikot *et al.* (2013) as:

$$V(r) = -V_0 \left( 1 - \frac{1}{r} e^{-\alpha r} \right)^2 = -\frac{A}{r^2} e^{-2\alpha r} + \frac{B}{r} e^{-\alpha r} - C \quad (1a)$$

where

$$A = C = V_o, B = 2V_o, V_0 = d_e r_e^2 \quad (1b)$$

Here,  $d_e$ ,  $r_e$  and  $\alpha$  represent the dissociation energy, equilibrium bond length and screening parameter, respectively, of the diatomic molecular systems. The MYP, also known as generalized inversely quadratic Yukawa potential, has great relevance in various aspects of Physics (Oyewumi *et al.*, 2014).

In order to achieve our aim, the radial Schrödinger equation (SE) with modified Yukawa potential (MYP) will be solved using the asymptotic iteration method (AIM). Thereafter, the energy value expression and their corresponding normalized eigen-functions in closed form will be established for some

diatomic molecules (DMs) such as hydrogen dimer ( $H_2$ ), lithium hydride ( $LiH$ ) and hydrogen chloride ( $HCl$ ). Also, expressions for expectation values for the selected diatomic molecules will be obtained using the Hellman-Feynman theorem (HFT). The numerical results of the energies and expectation values of the

DMs with varying quantum numbers will be further presented. In addition, the graphical plots of the energies and expectation values as functions of quantum numbers will be discussed extensively. Correlation of the results obtained will be compared to other works in available literature.

## 2. Solution of the Radial Schrödinger Equation with Modified Yukwa Potential (MYP)

The radial contribution of the SE according to Ikot *et al.* (2018) is defined as

$$\frac{d^2\psi_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[ E_{nl} - V(r) - \frac{\hbar^2 l(l+1)}{2\mu r^2} \right] \psi_{nl}(r) = 0 \quad (2)$$

Here,  $\mu$  is the reduced mass,  $E_{nl}$  is the energy spectrum,  $\hbar$  is the reduced Planck's constant and  $n$  and  $l$  are the radial and orbital angular momentum quantum numbers respectively. These quantum numbers can also be referred to as vibrational and rotational quantum numbers, respectively (Zhang, 2011). By substituting equation (1a) into equation (2), we obtained

$$\left[ \frac{d^2}{dr^2} + \frac{2\mu E_{nl}}{\hbar^2} - \frac{2\mu A e^{-2\alpha r}}{\hbar^2 r^2} - \frac{2\mu B e^{-\alpha r}}{\hbar^2 r} - \frac{2\mu C}{\hbar^2} - \frac{l(l+1)}{r^2} \right] \psi_{nl}(r) = 0 \quad (3)$$

Due to the fact that equation (3) cannot be solved analytically for  $l \neq 0$  as a result of the centrifugal term, we employed the Greene-Aldrich approximation scheme given by Greene and Aldrich (1976) in equation (4):

$$\frac{1}{r^2} \approx \frac{4\alpha^2 e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2}; \Rightarrow \frac{1}{r} \approx \frac{2\alpha e^{-\alpha r}}{(1 - e^{-2\alpha r})} \quad (4)$$

By substituting equation (4) and introducing a coordinate transformation of the form  $z = e^{-2\alpha r}$ , equation (3) becomes:

$$\left[ z(1-z) \frac{d^2}{dz^2} + (1-z) \frac{d}{dz} - \frac{\varepsilon_{nl}(1-z)}{z} + \frac{Pz}{(1-z)} - Q - \frac{R}{(1-z)} \right] \psi_{nl}(z) = 0 \quad (5)$$

$$\text{where } -\varepsilon_{nl} = \frac{\mu}{2\hbar^2\alpha^2} (E_{nl} + C); P = \frac{2\mu A}{\hbar^2}; Q = \frac{\mu B}{\hbar^2\alpha}; R = l(l+1) \quad (6)$$

We propose the following ansatz:

$$\psi_{nl}(z) = z^w (1-z)^v f_{nl}(z) \quad (7)$$

By using the AIM method to solve equation (5), equation (5) was transformed into the following form proposed by Ciftci *et al.* (2005) and Bayrak and Boztosun (2007) in equation (8):

$$\frac{d^2 y}{dz^2} = \lambda_0(z) \frac{dy}{dz} + S_0(z) y(z) \quad (8)$$

By substituting equation (7) into equation (5), one obtains

$$\frac{d^2 f_{nl}}{dz^2} = \frac{[(2w+2v+1)z - (1+2w)]}{z(1-z)} \frac{df_{nl}}{dz} + \frac{(w+v+\phi)(w+v-\phi)}{z(1-z)} f_{nl}(z) \quad (9)$$

where

$$w = \pm \sqrt{-\frac{\mu}{2\hbar^2 \alpha^2} (E_{nl} + C)}; \quad v = \frac{1}{2} \left( 1 \pm \sqrt{(1+2l)^2 - \frac{8\mu A}{\hbar^2}} \right); \quad (10)$$

$$\phi = \sqrt{-\left( \frac{\mu}{2\hbar^2 \alpha^2} (E_{nl} + C) + \frac{\mu B}{\hbar^2 \alpha} + \frac{2\mu A}{\hbar^2} \right)}$$

By comparing equation (8) with equation (9), we have

$$\lambda_0(z) = \frac{[(2w+2v+1)z - (1+2w)]}{z(1-z)}, \quad S_0(z) = \frac{[v^2 + 2wv + P + Q]}{z(1-z)} \quad (11)$$

By invoking the quantization condition used in AIM method (Ciftci *et al.*, 2005; Bayrak and Boztosun, 2007), we obtained

$$S_0 \lambda_1 - S_1 \lambda_0 = 0; \Rightarrow w_0 = -\frac{1}{2} \left[ \frac{v^2 + P + Q}{v} \right]$$

$$S_1 \lambda_2 - S_2 \lambda_1 = 0; \Rightarrow w_1 = -\frac{1}{2} \left[ \frac{v^2 + 2v + 1 + P + Q}{(1+v)} \right] \quad (12)$$

$$S_2 \lambda_3 - S_3 \lambda_2 = 0; \Rightarrow w_2 = -\frac{1}{2} \left[ \frac{v^2 + 4v + 4 + P + Q}{(2+v)} \right]$$

For arbitrary  $n$ , one obtains

$$w_n = -\frac{1}{2} \left[ \frac{v^2 + 2vn + n^2 + P + Q}{(n+v)} \right] \quad (13)$$

By putting equations (6) and (10) into equation (13), the non-relativistic energy expression of MYP becomes:

$$E_{nl} = C - \frac{2\hbar^2 \alpha^2}{\mu} \left[ \frac{(n+v)}{2} + \frac{\gamma}{2(n+v)} \right]^2 \quad (14)$$

where

$$\gamma = \left( \frac{2\mu A}{\hbar^2} + \frac{\mu B}{\hbar^2 \alpha} \right) \quad (15)$$

The solution to the hypergeometric Gauss differential equation, as given in equation (9) is obtained as

$$f_{n\ell}(z) = f_{n\ell} z^w (1-z)^v {}_2F_1(a, b, c, z) \quad (16)$$

where

$$a = w + v + \phi; \quad b = w + v - \phi; \quad c = 1 + 2w \quad (17)$$

The unnormalized wave function of MYP of equation (16) can also be written in terms of the Jacobi polynomials as

$$f_{n\ell}(z) = N_{n\ell} z^w (1-z)^v \frac{n! \Gamma(1+2w)}{\Gamma(1+n+2w)} P_n^{(2w, 2v)}(1-2z) \quad (18)$$

Here, we have used the definition of Gradshteyn and Ryzhik(2007) given in equation (19):

$$P_n^{(\sigma, \delta)}(1-2z) = \frac{\Gamma(1+n+\sigma)}{n! \Gamma(1+\sigma)} {}_2F_1(-n, 1+n+\sigma+\delta; 1+\sigma; z) \quad (19)$$

With the help of the quantum condition of finiteness (where  $a = -n$  or  $b = -n$ ,  $n = 0, 1, 2, \dots$ ), the unnormalized eigenfunction of MYP can be obtained as

$$f_{n\ell}(z) = N_{n\ell} z^w (1-z)^v {}_2F_1(-n, n+2(w+v), 1+2w, z) \quad (20)$$

To find the normalization constant  $N_{n\ell}$ , we employed the normalization condition of the wave function:

$$\int_0^{\infty} |R_{n\ell}(r)|^2 dr = 1 \quad (21)$$

By substituting equation (20) into equation (21) and carrying out change of limits, we obtained

$$\frac{|N_{n\ell}|^2}{2\alpha} I_{n\ell} = 1 \quad (22)$$

Here, we have defined  $I_{n\ell}$  to be

$$I_{n\ell} = \int_0^1 z^{2w-1} (1-z)^{2v} [{}_2F_1(-n, n+2w+2v, 1+2w, z)]^2 dz, \quad z = e^{-2\alpha r} \quad (23)$$

We evaluated the integral  $I_{n\ell}$ , using the Mathematica software programme as given below:

$$\begin{aligned}
n=0 &\Rightarrow I_{0\ell} = \frac{\Gamma(2w)\Gamma(1+2v)}{\Gamma(1+2w+2v)}, \\
n=1 &\Rightarrow I_{1\ell} = \frac{(1+v)}{(1+2w)(1+w+v)} \frac{\Gamma(2w)\Gamma(1+2v)}{\Gamma(1+2w+2v)}, \\
n=2 &\Rightarrow I_{2\ell} = \frac{(2+v)}{(1+w)(1+2w)(2+w+v)} \frac{\Gamma(2w)\Gamma(2+2v)}{\Gamma(2+2w+2v)}, \\
n=3 &\Rightarrow I_{3\ell} = \frac{6(3+v)}{(3+w+v)} \frac{\Gamma(2w)\Gamma(1+2w)\Gamma(3+2v)}{\Gamma(4+2w)\Gamma(3+2w+2v)}, \\
n=m &\Rightarrow I_{m\ell} = \frac{m!(m+v)}{(m+w+v)} \frac{\Gamma(2w)\Gamma(1+2w)\Gamma(m+2v)}{\Gamma(1+m+2w)\Gamma(m+2w+2v)}
\end{aligned} \tag{24}$$

Therefore, the normalization constant was obtained as

$$N_{n\ell} = \sqrt{\left( \frac{2\alpha(n+w+v)\Gamma(1+n+2w)\Gamma(n+2w+2v)}{n!(n+v)\Gamma(2w)\Gamma(1+2w)\Gamma(n+2v)} \right)} \tag{25}$$

Hence, the normalized wave function of MYP was therefore obtained as

$$f_{n\ell}(z) = \sqrt{\left( \frac{2\alpha(n+w+v)\Gamma(1+n+2w)\Gamma(n+2w+2v)}{n!(n+v)\Gamma(2w)\Gamma(1+2w)\Gamma(n+2v)} \right)} z^w (1-z)^v {}_2F_1(-n, n+2(w+v), 1+2w, z) \tag{26}$$

### 3. Computation of Expectation Values for Modified Yukawa Potential (MYP)

In this section, we employed the Hellman-Feynman theorem (HFT), which is a technique used in obtaining the expectation values of quantum systems for any given quantum number. The HFT has been known to relate the derivative of the energy values with respect to any parameter (say  $q$ ) and the expectation value of the Hamiltonian with respect to that same parameter (Okon *et al.*, 2022). The HFT is defined as

$$\frac{\partial E_{n\ell}(q)}{\partial q} = \left\langle \psi_{n\ell}(q) \left| \frac{\partial H(q)}{\partial q} \right| \psi_{n\ell}(q) \right\rangle, \tag{27}$$

provided the normalized eigenfunctions  $\psi_{n\ell}(q)$  are continuous with respect to the chosen parameter  $q$ .

The effective Hamiltonian of the modified Yukawa potential (MYP) model is given by

$$\hat{H} = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} - \frac{A}{r^2} e^{-2ar} + \frac{B}{r} e^{-ar} - C \tag{28}$$

By employing  $q=l$  and  $q=\mu$  in equation (27), the expectation values of  $\langle r^{-2} \rangle_{n\ell}$ ,  $\langle T \rangle_{n\ell}$  and  $\langle P^2 \rangle_{n\ell}$  were obtained respectively, as

$$\langle r^{-2} \rangle_{n\ell} = -8\alpha^2 \left( \frac{n+v}{2} + \frac{\gamma}{2(n+v)} \right) \left( \frac{1}{\zeta} - \frac{\gamma}{2\zeta(n+v)^2} \right) \tag{29}$$

$$\langle T \rangle_{nl} = \frac{-2\hbar^2\alpha^2}{\mu} \left( \frac{n+v}{2} + \frac{\gamma}{2(n+v)} \right)^2 \quad (30)$$

$$\langle P^2 \rangle_{nl} = -4\hbar^2\alpha^2 \left( \frac{n+v}{2} + \frac{\gamma}{2(n+v)} \right)^2 \quad (31)$$

where

$$\gamma = \sqrt{(1+2l)^2 - \frac{8\mu A}{\hbar^2}} \quad (32)$$

The following relations have been employed in obtaining equations (30) and (31), respectively:

$$\left\langle \psi_{nl}(\mu) \left| \frac{\partial H(\mu)}{\partial \mu} \right| \psi_{nl}(\mu) \right\rangle = -\frac{1}{\mu} \langle T \rangle_{nl} \quad \text{and} \quad \langle T \rangle_{nl} = \frac{1}{2\mu} \langle P^2 \rangle_{nl} \quad (33)$$

#### 4. Special Case for Modified Yukawa Potential (MYP)

The modified Yukawa potential can be reduced to a special case when its potential parameter is adjusted. As  $\alpha \rightarrow 0$ , the MYP in equation (1a) becomes the pseudoCoulomb potential given as

$$V^{ps}(r) = -\frac{A}{r^2} + \frac{B}{r} - C \quad (34)$$

and its corresponding energy equation becomes:

$$E_{nl}^{ps} = C - \frac{\mu B^2}{2\hbar^2(n+v)^2} \quad (35)$$

In addition, the expectation values of  $\langle r^{-2} \rangle_{nl}$ ,  $\langle r^{-1} \rangle_{nl}$ ,  $\langle T \rangle_{nl}$  and  $\langle P^2 \rangle_{nl}$  were analysed using the HFT. These include:

$$\langle r^{-2} \rangle_{nl} = \frac{2\mu^2 B^2}{\hbar^4 (n+\gamma)^3 \zeta} \quad (36)$$

$$\langle r^{-1} \rangle_{nl} = \frac{-\mu B}{\hbar^2 (n+\gamma)^2} \quad (37)$$

$$\langle T \rangle_{nl} = \frac{\mu B^2}{2\hbar^2 (n+\gamma)^2} \quad (38)$$

$$\langle P^2 \rangle_{nl} = \frac{\mu^2 B^2}{\hbar^2 (n+\gamma)^2} \quad (39)$$

#### 5. Results and Discussion

In this work, the radial SE of equation (2) is solved using the AIM and the eigensolutions of MYP are given in equations (14) and (26), respectively. The corresponding numerical results for some hydrogen-related DMs (*HCl*, *LiH* and *H<sub>2</sub>*) were obtained using the spectroscopic parameters in Table 1. We have

used the following conversions in our analysis, with the help of a Mathematica and Maple programming softwares (Edet et al., 2020):

$$1 \text{ amu} = 931.494028 \text{ MeV}c^{-2}$$

$$1 \text{ cm}^{-1} = 1.239841875 \times 10^{-4} \text{ eV}$$

$$\text{and } \hbar c = 1973.29 \text{ eV } \overset{\circ}{\text{A}}$$

With the help of the spectroscopic parameters defined, various energies and expectation values were computed at different quantum states for the selected DMs, as shown in Tables 2 – 4. In these tables, the energies increase with increase in the quantum numbers. There is also increase in  $\langle T \rangle_{nl}$  and  $\langle P^2 \rangle_{nl}$  expectation values as the quantum numbers increases. Conversely, the expectation values of  $\langle r^{-2} \rangle_{nl}$  decrease with increase in quantum numbers. These trends are similar for all the chosen DMs. By adjusting the MYP model of equation (1a), we obtain the pseudo Coulomb potential as presented in equation (34). The energy expression of the pseudo Coulomb potential and its expectation

values expressions of  $\langle r^{-2} \rangle_{nl}$ ,  $\langle T \rangle_{nl}$  and  $\langle P^2 \rangle_{nl}$  were obtained in equations 35 – 39, respectively. The numerical values of the energies of pseudo Coulomb potential and their corresponding expectation values  $\langle r^{-2} \rangle_{nl}$ ,  $\langle T \rangle_{nl}$  and  $\langle P^2 \rangle_{nl}$  are shown in Tables 5 – 7, for the chosen DMs. Here, the energies increase with increase in the quantum numbers. There is also a decrease in  $\langle r^{-2} \rangle_{nl}$ ,  $\langle T \rangle_{nl}$  and  $\langle P^2 \rangle_{nl}$  expectation values as the quantum numbers increases. In addition, these trends are similar for all the chosen DMs.

**Table 1:** Spectroscopic parameters for the selected hydrogen-related diatomic molecules (Osobonye *et al.*, 2021)

Molecules	$d_e$ (eV)	$r_e$ (Å)	$\alpha$ (Å <sup>-1</sup> )	$\mu$ (amu)
HCl	4.6190	1.2746	1.8677	0.9801045
LiH	2.5152	1.5956	1.1280	0.8801221
H <sub>2</sub>	4.7446	0.7416	1.9426	0.5039100

**Table 2:** Energy eigenvalues and expectation values of HCl diatomic molecule corresponding to MYP with various quantum numbers

$n$	$l$	$E_{nl}$ (eV)	$\langle r^{-2} \rangle_{nl}$ (Å <sup>-2</sup> )	$\langle T \rangle_{nl}$ (eV)	$\langle P^2 \rangle_{nl}$ (eV/c) <sup>2</sup> × 10 <sup>-6</sup>
0	0	-160.1824468	-4.328190593	-167.6865974	-3.402031235
1	0	-159.1009823	-4.747496626	-166.6051329	-3.380090447
	1	-159.0837158	-4.753020134	-166.5878664	-3.379740144
2	0	-158.1296473	-5.144863346	-165.6337979	-3.360383972
	1	-158.1141842	-5.149920279	-165.6183348	-3.360070254
	2	-158.0833595	-5.160004165	-165.5875101	-3.359444882
3	0	-157.2624257	-5.522095447	-164.7665763	-3.342789750
	1	-157.2486685	-5.526720414	-164.7528191	-3.342510645
	2	-157.2212497	-5.535942857	-164.7254003	-3.341954370
	3	-157.1803594	-5.549708058	-164.6845100	-3.341124788
	0	-156.4937687	-5.880826614	-163.9979193	-3.327195211
4	1	-156.4816277	-5.885051038	-163.9857783	-3.326948895
	2	-156.4574356	-5.893474677	-163.9615862	-3.326458085
	3	-156.4213712	-5.906047345	-163.9255218	-3.325726409
	4	-156.3737010	-5.922694541	-163.8778516	-3.324759274

**Table 3:** Energy eigenvalues and expectation values of LiH diatomic molecule corresponding to MYP with various quantum numbers



$n$	$l$	$E_{nl}$ (eV)	$\langle r^{-2} \rangle_{nl}$ ( $\text{\AA}^{-2}$ )	$\langle T \rangle_{nl}$ (eV)	$\langle P^2 \rangle_{nl}$ ( $\text{eV}/c$ ) <sup>2</sup> $\times 10^{-6}$
0	0	-61.08923144	-0.5472982078	-67.49277812	-1.229611149
1	0	-60.35431808	-0.7942256306	-66.75786476	-1.216222196
	1	-60.34080696	-0.7985232117	-66.74435364	-1.215976044
2	0	-59.68304890	-1.025299242	-66.08659558	-1.203992738
	1	-59.67072148	-1.029220913	-66.07426816	-1.203768152
3	2	-59.64614626	-1.037035294	-66.04969294	-1.203320430
	0	-59.07130494	-1.241979642	-65.47485162	-1.192847735
	1	-59.06008558	-1.245557266	-65.46363226	-1.192643336
4	2	-59.03772118	-1.252686130	-65.44126786	-1.192235892
	3	-59.00435954	-1.263313822	-65.40790622	-1.191628096
	0	-58.51532894	-1.445571936	-64.91887562	-1.182718736
	1	-58.50514866	-1.448834078	-64.90869534	-1.182533268
4	2	-58.48485736	-1.455334326	-64.88840404	-1.182163592
	3	-58.45459308	-1.465024911	-64.85813976	-1.181612225
	4	-58.41456086	-1.477835146	-64.81810754	-1.180882902

**Table 4:** Energy eigenvalues and expectation values of  $H_2$  diatomic molecule corresponding to MYP with various quantum numbers

$n$	$l$	$E_{nl}$ (eV)	$\langle r^{-2} \rangle_{nl}$ ( $\text{\AA}^{-2}$ )	$\langle T \rangle_{nl}$ (eV)	$\langle P^2 \rangle_{nl}$ ( $\text{eV}/c$ ) <sup>2</sup> $\times 10^{-7}$
0	0	-59.18162872	-5.145529763	-61.79101904	-6.445340944
1	0	-58.39575510	-6.121637050	-61.00514542	-6.363367488
	1	-58.36881534	-6.148363135	-60.97820566	-6.360557436
2	0	-57.81227844	-6.989187262	-60.42166876	-6.302505796
	1	-57.79288444	-7.010649162	-60.40227476	-6.300482832
3	2	-57.75502954	-7.052853154	-60.36441986	-6.296534236
	0	-57.40768274	-7.767478241	-60.01707306	-6.260302944
	1	-57.39498440	-7.784498083	-60.00437472	-6.258978396
4	2	-57.37039720	-7.817952562	-59.97978752	-6.256413736
	3	-57.33550476	-7.866709221	-59.94489508	-6.252774152
	0	-57.16235778	-8.471930280	-59.77174810	-6.234713416
4	1	-57.15564364	-8.485171208	-59.76503396	-6.234013072
	2	-57.14291940	-8.511179112	-59.75230972	-6.232685824
	3	-57.12556290	-8.549036912	-59.73495322	-6.230875388
	4	-57.10556706	-8.597442648	-59.71495738	-6.228789648

**Table 5:** Energy eigenvalues and expectation values of  $HCl$  diatomic molecule corresponding to Pseudo-Coulomb potential with various quantum numbers

$n$	$l$	$E_{nl}$ (eV)	$\langle r^{-2} \rangle_{nl}$ ( $\text{\AA}^{-2}$ )	$\langle T \rangle_{nl}$ (eV)	$\langle P^2 \rangle_{nl}$ ( $\text{eV}/c$ ) <sup>2</sup> $\times 10^{-7}$
0	0	0.1254411140	0.9749960998	7.378709505	1.496995025
1	0	0.3660790240	0.9276915674	7.138071595	1.448174327
	1	0.3700335090	0.9266574796	7.134117110	1.447372040
2	0	0.5951343590	0.8833983450	6.909016260	1.401703504
	1	0.5989000640	0.8824254940	6.905250555	1.400939518
2	2	0.6064190490	0.8804846286	6.897731570	1.399414063

0	0	0.8133387040	0.8418805798	6.690811915	1.357434135
1	0	0.8169274540	0.8409643964	6.687223165	1.356706049
2	0	0.8240932490	0.8391365402	6.680057370	1.355252250
3	3	0.8348127740	0.8364059896	6.669337845	1.353077468
0	0	1.021366784	0.8029242418	6.482783835	1.315229330
1	0	1.024789484	0.8020605650	6.479361135	1.314534930
2	0	1.031623874	0.8003374236	6.472526745	1.313148368
3	0	1.041847954	0.7977632008	6.462302665	1.311074103
4	4	1.055428974	0.7943503610	6.448721645	1.308318780

**Table 6:** Energy eigenvalues and expectation values of  $LiH$  diatomic molecule corresponding to Pseudo-Coulomb potential with various quantum numbers

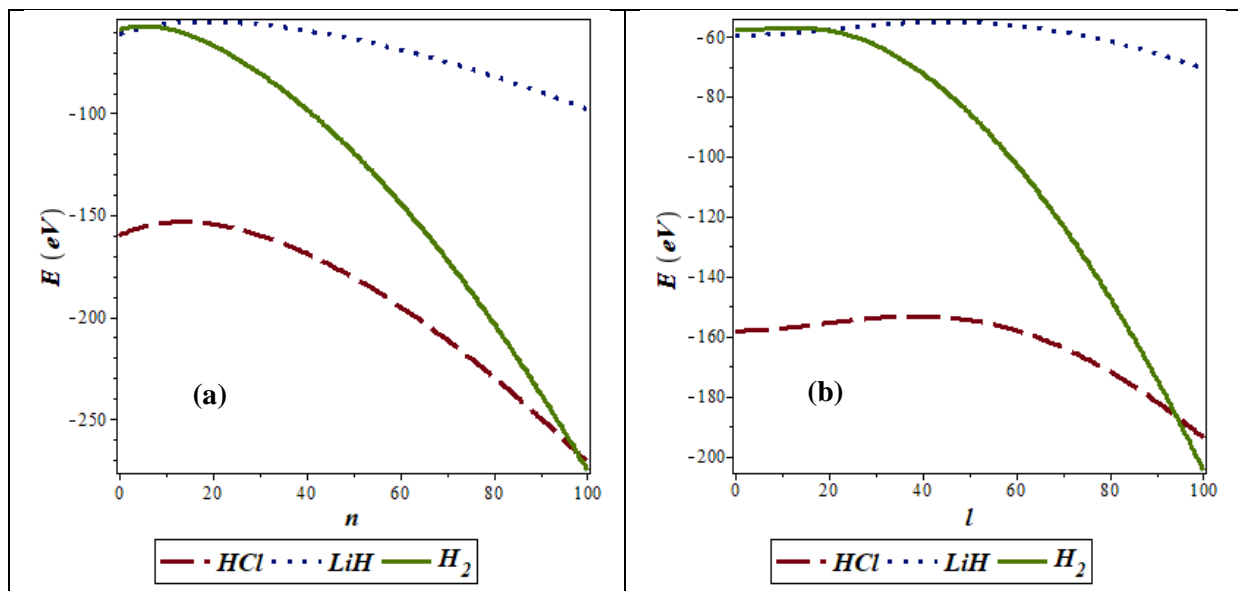
$n$	$l$	$E_{nl}$ (eV)	$\langle r^{-2} \rangle_{nl}$ ( $\text{\AA}^{-2}$ )	$\langle T \rangle_{nl}$ (eV)	$\langle P^2 \rangle_{nl}$ ( $eV/c$ ) <sup>2</sup> $\times 10^{-7}$
0	0	0.1221358080	0.9714820948	6.281410870	1.144373228
1	0	0.3550634230	0.9179493578	6.048483255	1.101937519
1	1	0.3594201630	0.9166178936	6.044126515	1.101143790
2	0	0.5752710780	0.8682786412	5.828275600	1.061819183
2	1	0.5793921180	0.8670364370	5.824154560	1.061068396
2	2	0.5876165430	0.8645600540	5.815930135	1.059570036
3	0	0.7836683730	0.8221278594	5.619878305	1.023852509
3	1	0.7875704030	0.8209673924	5.615976275	1.023141620
3	2	0.7953579780	0.8186538730	5.608188700	1.021722848
3	3	0.8069982430	0.8152020464	5.596548435	1.019602177
4	0	0.9810850030	0.7791906544	5.422461675	0.9878863358
4	1	0.9847832780	0.7781051582	5.418763400	0.9872125688
4	2	0.9921644080	0.7759410278	5.411382270	0.9858678445
4	3	1.003197643	0.7727119088	5.400349035	0.9838577640
4	4	1.017837338	0.7684380108	5.385709340	0.9811906444

**Table 7:** Energy eigenvalues and expectation values of  $H_2$  diatomic molecule corresponding to Pseudo-Coulomb potential with various quantum numbers

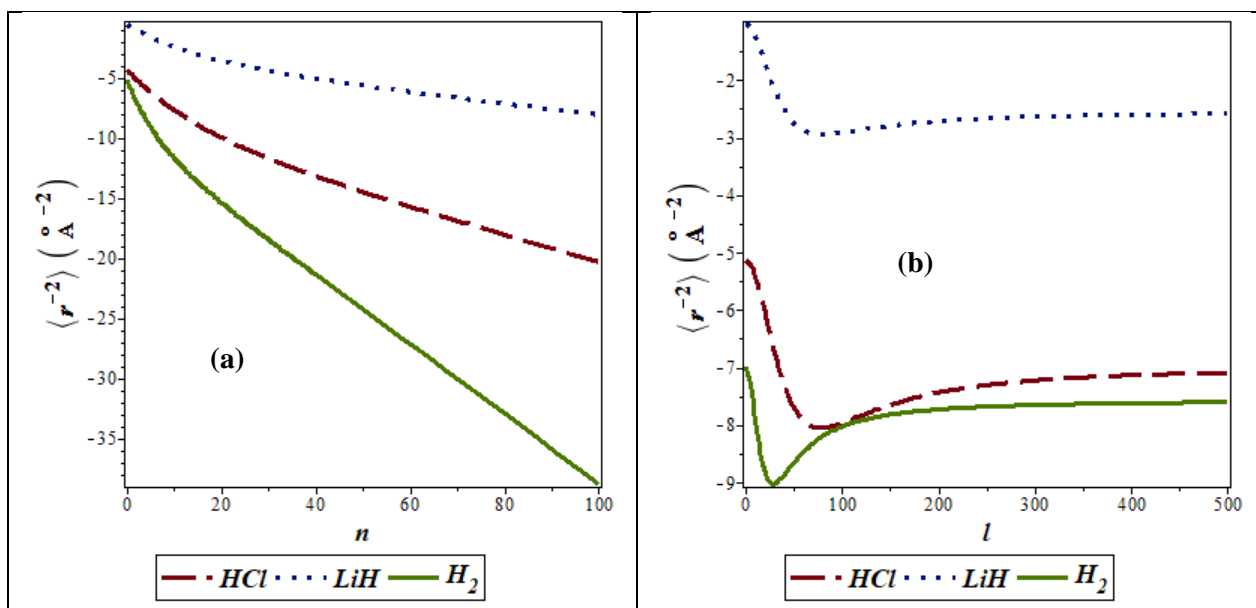
$n$	$l$	$E_{nl}$ (eV)	$\langle r^{-2} \rangle_{nl}$ ( $\text{\AA}^{-2}$ )	$\langle T \rangle_{nl}$ (eV)	$\langle P^2 \rangle_{nl}$ ( $eV/c$ ) <sup>2</sup> $\times 10^{-8}$
0	0	0.1019816310	0.9417656450	2.507408688	2.615445438
1	0	0.2870544910	0.8394458522	2.322335828	2.422398340
1	1	0.2939970860	0.8343597024	2.315393233	2.415156610
2	0	0.4523682690	0.7514274072	2.157022050	2.249961686
2	1	0.4585834160	0.7469960636	2.150806903	2.243478747
2	2	0.4709042480	0.7382516000	2.138486071	2.230627047
3	0	0.6006387750	0.6752964852	2.008751544	2.095302646
3	1	0.6062246570	0.6714156826	2.003165662	2.089476085
3	2	0.6173005430	0.6637554774	1.992089776	2.077922973
3	3	0.6336788240	0.6525127744	1.975711495	2.060839001
4	0	0.7341307700	0.6091121082	1.875259549	1.956058881
4	1	0.7391695470	0.6056971016	1.870220772	1.950802998

2	0.7491627170	0.5989545714	1.860227602	1.940379251
3	0.7639450970	0.5890544834	1.845445222	1.924959943
4	0.7832775770	0.5762397840	1.826112742	1.904794484

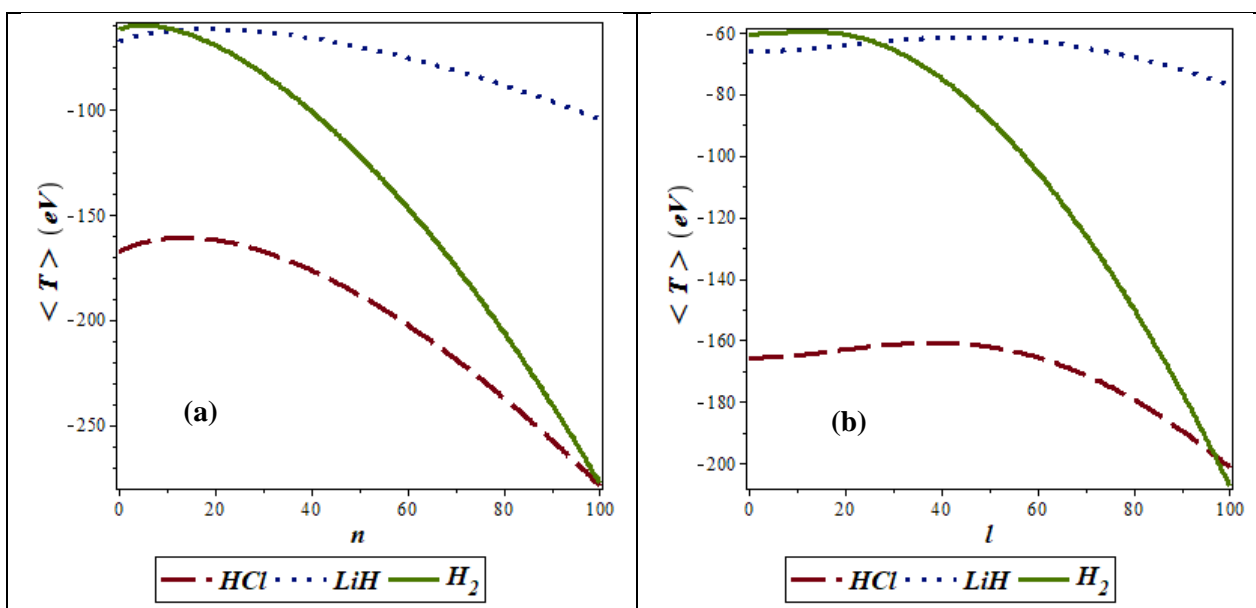
The variations of energy and different expectation values with principal and angular momentum quantum numbers are displayed in figures 1 – 4, for the chosen DMs. In figure 1(a and b), the energies increase with increase in both quantum numbers. With further increase of the quantum numbers, the energies of the chosen DMs decrease monotonously. This phenomenon is also observed in figures 3 (a and b) and 4(a and b) for the expectation values  $\langle T \rangle_{nl}$  and  $\langle P^2 \rangle_{nl}$ . In figure 2 (a and b), the expectation values  $\langle r^{-2} \rangle_{nl}$  decrease with increase in both quantum number. Further increase in the different quantum numbers result in a slow increase in the expectation values  $\langle r^{-2} \rangle_{nl}$ . These results are in perfect correlation with the results published by Oluwadare and Oyewumi (2018b).



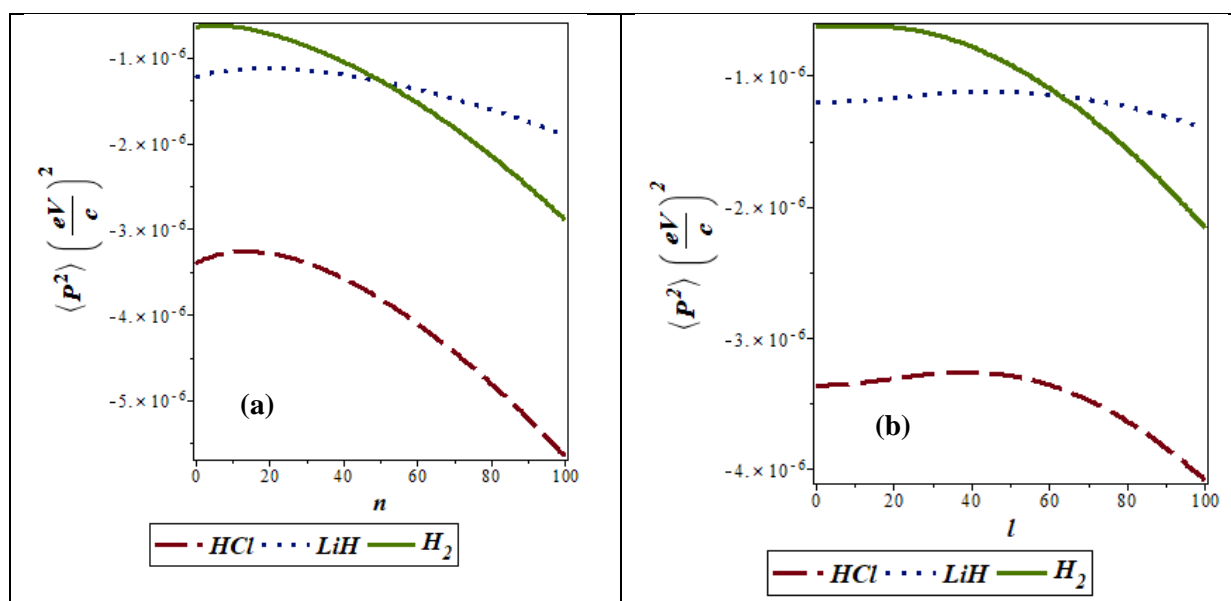
**Figure 1:** Graphical variation of energy values with (a) radial quantum number and (b) orbital angular momentum quantum number, corresponding to MYP for some DMs



**Figure 2:** Graphical variation of expectation values  $\langle r^{-2} \rangle$  with (a) radial quantum number and (b) orbital angular momentum quantum number, corresponding to MYP for some DMs



**Figure 3:** Graphical variation of expectation values  $\langle T \rangle$  with (a) radial quantum number and (b) orbital angular momentum quantum number, corresponding to MYP for some DMs



**Figure 4:** Graphical variation of expectation values  $\langle P^2 \rangle$  with (a) radial quantum number and (b) orbital angular momentum quantum number, corresponding to MYP for some DMs

## 6. Concluding Remarks

In this work, we have carried out a study of the radial Schrödinger equation for the modified Yukawa potential (MYP) model with the help of AIM. We obtained both analytical expression and computational values of the energy and expectation values  $\langle r^{-2} \rangle_{nl}$ ,  $\langle T \rangle_{nl}$  and  $\langle P^2 \rangle_{nl}$  with respect to various radial and orbital angular momentum quantum numbers for the selected diatomic molecules, using the Hellman-Feynman theorem (HFT). The nature of the computed results obtained for the chosen DMs have been discussed both numerically and graphically with regards to varying radial and orbital angular momentum quantum numbers. These results are clearly seen to be highly dependent on the chosen quantum numbers. A special case has also been considered in this study and our obtained results agreed well with existing ones in different literatures. Our results are expected to be very relevant in chemical Physics, quantum Physics, high energy Physics, etc.

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