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ANALYTICAL SOLUTIONS OF SCHRÖDINGER EQUATION WITH NEW SOLVABLE POTENTIAL FAMILY $V(r)=\frac{A}{r^2}-\frac{B}{r}+Cr^{\delta+1}$ VIA NIKIFOROV-UVAROV (NU) METHOD

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ABSTRACT

In this paper, we have presented the exact solutions of the Schrödinger equation with the family of potentials $\boldsymbol{V(r)=\frac{A}{r^2}-\frac{B}{r}+Cr^{\delta+1}}$. We have obtained the energy eigenvalues and the corresponding wave functions expressed in terms of the associated Laguerre polynomials for $\delta=-1,-2\ and=-3$ using the Nikiforov-Uvarov (NU) method. The energy levels for each case is computed for diatomic molecules H_2, CO, NO and N_2 for various values of n and l. We have also computed the expectation values of $<r^{-2}>$,$<r^{-1}>$ and the Virial theorem using the Hellmann-Feynman theorem (HFT).

Keywords: Schrödinger equation, Energy eigenvalue, Eigenfunction, Diatomic molecules, Hellmann-Feynman theorem
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1. INTRODUCTION

One of the important tasks of quantum mechanics is to find the exact solutions of the wave equations (nonrelativistic and relativistic) for certain potentials of physical importance as these solutions contain all necessary information regarding the quantum system under consideration. In this regard, considerable efforts have been made in recent years in obtaining the exact analytical solutions of Schrödinger equation with potentials of interest [1–6].

It is well known that the exact solutions of those wave equations are only possible in a few simple cases such as the coulomb, the harmonic oscillator, pseudoharmonic and Mie-type potentials [7–12]. For an arbitrary $l-state$, most quantum systems could be only treated by approximation methods. For the rotating Morse potential some semiclassical and/or numerical solutions have been obtained using the Pekeris approximation [13–16]. In recent years, many authors have studied the nonrelativistic and relativistic wave equation with certain potentials for the $l=0$ and $l\neq 0$ cases. Other exact or approximate solutions of these models have been addressed analytically in references [15–17]. Many authors have studied wave equations with various potentials such as Morse [18], the Hulthén [19, 20, 21], the Pφschl-Teller [22, 23], Woods-Saxon [24], Kratzer-type [25, 26], Rosen-Morse [27, 28], Scarf [29], Eckert [30] and non-central ring-shape Kratzer [31].

In this way, different analytical techniques have been used to obtain the solutions of the wave equations. This list includes the supersymmetry (SUSY) quantum mechanics and shape invariance [32], variational technique [33], path integral approach [34], asymptotic iteration method (AIM) [35], exact quantization rule (EQR) [11,15], hypervirial perturbation [36], shifted $\frac{1}{N}$ expansion (SE) [37], algebraic approach [38, 39], etc. Recently, an alternative method for solving Schrödinger equation has been proposed [40, 41]. The method is called the Nikiforov-Uvarov. This method is based on solving the second order linear differential equations by reducing them to a generalized equation of hypergeometric type. This method has shown its power in calculating the exact energy levels many quantum systems. In this work, we apply the NU method to study a new solvable potential family of the form [42]

$$V(r)=\frac{A}{r^2}-\frac{B}{r}+Cr^{\delta+1} \tag{1}$$

This potential yields several potentials when the parameters of the potential are adjusted.

(i) By choosing $A=0$ and $\delta=1$, potential in Eq. (1) reduces to coulomb plus harmonic oscillator potential, which is applied to examine the Zeeman quadratic effect [43] and the magnetic field effect in the hydrogen atom [44].

(ii) The Goĺdmen-Krirchenkokv potential is obtained when $A\neq 0, B=0\ and\ \delta=1$. When $A=0, B=1\ and\ \delta=1$, the potential in Eq. (1) becomes spiked harmonic oscillator potential [45].

(iii)The coulomb plus linear potential, i.e. the well-known Cornell (alternatively called Funnel) potential, is obtained by choosing $A = 0$ and $\delta = 0$ [46].

The potential of Eq. (1) can be used to study diatomic molecules. The knowledge of molecular spectra provides us with a valuable source to study atoms and molecules. The data on spectral characteristics allows us to detect the presence of particular characteristic and essential components of matter [47]. Especially, molecular spectra can be used to understand the motion of electrons in molecule as well as the vibration and rotation of the nuclei [47]. The chemical interactions between atoms and molecules are used to investigate the physical properties of individual molecules. The aim of this present paper is to obtain the analytical solution of this new solvable potential family for values of δ ranging from -1 to -3 via the NU method and then use the results to calculate the energy eigenvalues of selected diatomic molecules, H_2, CO, NO and N_2 for any n and l quantum numbers.

The contents of this paper is as follows: In section 2, we present the (NU) method. In section 3, solutions of Schrödinger equation with the new solvable potential are calculated. In section 4, the radial solutions of the Schrödinger equation are presented. Expectation values and the results of the corresponding Virial theorem are presented in section 5. Discussions and applications to diatomic molecules are given in section 6. Finally, a brief conclusion is presented in section 7.

2. NIKIFOROV-UVAROV METHOD

The differential equations with hypergeometric-type solutions can be solved by the NU method [40]. In this method, the one-dimensional Schrödinger equation, by the coordinate transformation $x = x(s)$, appears as

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

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most of second degree, and $\tilde{\tau}(s)$ is a polynomial, at most of first degree. In order to obtain a particular solution to Eq. (2), we consider the wave function in the form

$$\psi(s) = \phi(s)y(s) \tag{3}$$

and substitute Eq. (3) into Eq. (2) to obtain

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0 \tag{4}$$

where the other wave function is defined as the logarithmic derivative [40]

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)} \tag{5}$$

and

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s), \tau'(s) < 0 \tag{6}$$

The condition $\tau'(s) < 0$ is the physical condition guarantee of the physical meaning of the energy eigenvalues. The condition $\tau'(s) > 0$ has been comprehensively discussed in [40]. The λ in Eq. (4) satisfies the second order differential equation.

$$\lambda = \lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s), n = 0, 1, 2 \ldots\ldots \tag{7}$$

where the first-order derivative must be negative. It is to be noted that λ or λ_n are obtained from a particular solution of the form $y(s) = y_n(s)$ which is a polynomial of degree n. The second part $y_n(s)$ of the wave function in Eq. (3) is the hypergeometric-type function whose polynomial solution is connected by Rodriques relation.

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n}[\sigma^n(s)\rho(s)] \tag{8}$$

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

$$\frac{d}{ds}[\sigma(s)\rho(s)] = \tau(s)\rho(s) \tag{9}$$

On the other hand, in order to find the eigenfunctions $\phi_n(s)$, $y_n(s)$ and λ_n in Eq. (7), we need to calculate the functions

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

$$k = \lambda - \pi'(s) \tag{11}$$

In principle, since $\pi(s)$ has to be a polynomial of degree at most one, the expression under the square root sign in Eq. (10) can be set to the square of a polynomial of first degree [40], which is possible only if its discriminant is zero. Thus, the equation for k obtained from the solution of Eq. (10) is further substituted in Eq. (11). In addition, the energy eigenvalues are obtained from Eqs. (7) and (11).

3. THE CORRESPONDING SCHRÖDINGER EQUATION

In the spherical coordinates, the Schrödinger equation is,

$$\frac{-\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2 sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

$$\psi_{n,l,m} + V(r)\psi_{n,l,m} = E_{n,l,m}\psi_{n,l,m} \tag{12}$$

where $V(r)$ is potential of equation (1). In other to find exact solution of Eq. (12), we write total wave function as

$$\psi_{n,l,m}(r,\theta,\varphi) = R_{n,l}(r)\Theta(\theta)\phi(\varphi) \tag{13}$$

Substitution of Eq. (13) into Eq. (12) yields the decouples equations

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2\mu}{\hbar^2}\left[E_{n,l} - V(r) - \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}\right]R_{n,l}(r) = 0 \tag{14}$$

$$\frac{d^2\Theta(\theta)}{d\theta^2} + \cot(\theta)\frac{d\Theta(\theta)}{d\theta} + \left[\lambda - \frac{m^2}{sin^2\theta}\right]\Theta(\theta) = 0 \tag{15}$$

$$\frac{d^2\phi(\varphi)}{d\varphi^2} + m^2\phi(\varphi) = 0 \tag{16}$$

Eqs. (15) and (16) are spherical harmonics $Y_{lm}(\theta,\varphi) = \Theta(\theta)\phi(\varphi)$ whose solution is well known [30].

4. THE SOLUTIONS OF THE RADIAL SCHΦDINGER EQUATION

The radial equation of the potential of Eq. (1) using Eq. (14) becomes

$$\frac{d^2R_{n,l}(r)}{dr^2} + \frac{2}{r}\frac{dR_{n,l}(r)}{dr} + \frac{2\mu}{\hbar^2}\left[E_{n,l} - \frac{A}{r^2} + \frac{B}{r} - Cr^{\delta+1} - \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}\right]R_{n,l}(r) = 0 \tag{17}$$

Now we want to solve Eq. (17) for different values of δ (from $\delta = -1, -2\ and - 3$).

(i) Case I : $\delta = -1$

Using $\delta = -1$ in Eq. (17), we have

$$\frac{d^2R_{n,l}(r)}{dr^2} + \frac{2}{r}\frac{dR_{n,l}(r)}{dr} + \frac{2\mu}{\hbar^2}\left[E_{n,l} - \frac{A}{r^2} + \frac{B}{r} - C - \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}\right]R_{n,l}(r) = 0 \tag{18}$$

Simplifying Eq.(18), we obtain

$$\frac{d^2R_{n,l}(r)}{dr^2} + \frac{2}{r}\frac{dR_{n,l}(r)}{dr} + \frac{1}{r^2}(-\varepsilon^2r^2 + \alpha^2r - \beta^2)R_{n,l}(r) = 0 \tag{19}$$

where the used dimensionless parameters are

$$\varepsilon^2 = -\frac{2\mu}{\hbar^2}(E_{n,l} - C), \alpha^2 = \frac{2\mu}{\hbar^2}B, \beta^2 = \frac{2\mu}{\hbar^2}\left[A + \frac{\hbar^2}{2\mu}l(l+1)\right] \tag{20}$$

Now comparing Eq. (19) with Eq. (2), we have

$$\bar{\tau} = 2, \sigma(r) = r, \bar{\sigma}(r) = -\varepsilon^2r^2 + \alpha^2r - \beta^2 \tag{21}$$

Now substituting Eq. (21) into Eq. (10), we find

$$\pi(r) = -\tfrac{1}{2} \pm \sqrt{\varepsilon^2 r^2 + (k - \alpha^2) r + \left(\beta^2 + \tfrac{1}{4}\right)} \tag{22}$$

and we get two possible functions for each root as

$$\pi(r) = -\tfrac{1}{2} \pm \begin{cases} \varepsilon r + \tfrac{1}{2}\sqrt{1 + 4\beta^2}\; for\; k = \alpha^2 + \varepsilon\sqrt{1 + 4\beta^2} \\ \varepsilon r - \tfrac{1}{2}\sqrt{1 + 4\beta^2}\; for\; k = \alpha^2 - \varepsilon\sqrt{1 + 4\beta^2} \end{cases} \tag{23}$$

From the four possible forms of the polynomial $\pi(r)$, we select the case with $\tau'(r) < 0$, and by using Eq. (6), we obtain

$$\tau(r) = 1 - 2\varepsilon r + \sqrt{1 + 4\beta^2}$$

$$\tau'(r) = -2\varepsilon \tag{24}$$

Therefore, the appropriate $\pi(r)$ and k values are

$$\pi(r) = -\tfrac{1}{2} - \left(\varepsilon r - \tfrac{1}{2}\sqrt{1 + 4\beta^2}\right) \tag{25}$$

and

$$k = \alpha^2 - \varepsilon\sqrt{1 + 4\beta^2} \tag{26}$$

The parameter, $\lambda = k + \pi'(r)$ is obtained as

$$\lambda = \alpha^2 - \varepsilon\left(1 + \sqrt{1 + 4\beta^2}\right) \tag{27}$$

and from the definition of λ_n from Eq. (7), we obtain

$$\lambda_n = 2n\varepsilon \tag{28}$$

On comparing Eq.(27) and Eq.(28), we obtain the energy relation as

$$\alpha^2 - \varepsilon\left(1 + \sqrt{1 + 4\beta^2}\right) = 2n\varepsilon \tag{29}$$

which gives the energy spectrum as

$$E_{n,l} = C - \frac{\mu}{2\hbar^2} \frac{B^2}{\left[n + \tfrac{1}{2} + \sqrt{\frac{2\mu A}{\hbar^2} + (l + \tfrac{1}{2})^2}\right]^2} \tag{30}$$

From Eq. (9),we obtain the weight function as,

$$\rho(r) = r^{\nu} e^{-2\varepsilon r} \tag{31}$$

where $\nu = \sqrt{1 + 4\beta^2}$.

Let us now calculate the corresponding wave function. Substituting Eq. (31) into the Rodriques relation of Eq. (8), we get

$$y_n(r) = B_n r^{-\nu} e^{2\varepsilon r} \frac{d^n}{dr^n}\left[e^{-2\varepsilon r} r^{(n+\nu)}\right] \tag{32}$$

Eq. (32) can be expressed in terms of associated Laquerre polynomial as

$$y_n(r) = B_n L_n^{\nu}(2\varepsilon r) \tag{33}$$

The other part of the wave function in Eq. (5) is found as

$$\phi(r) = r^{\frac{1}{2}(\nu-1)} e^{-\frac{2\varepsilon r}{2}} \tag{34}$$

Combining Eqs. (33) and (34) together, we obtain the radial wave function of the case $\delta = -1$ as

$$R_{n,l}(r) = C_n r^{\frac{1}{2}(\nu-1)} e^{-\varepsilon r} L_n^{\nu}(2\varepsilon r) \tag{35}$$

where C_n is the new normalization constant. Therefore, the total wave function becomes

$$\psi_{n,l,m}(r,\theta,\varphi) = C_n r^{\frac{1}{2}(\nu-1)} e^{-\varepsilon r} L_n^{\nu}(2\varepsilon r) Y_{lm}(\theta,\varphi) \tag{36}$$

(ii) Case II : $\boldsymbol{\delta = -2}$

For $\delta = -2$ into Eq. (17), we have

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2}{r}\frac{dR_{nl}(r)}{dr} + \frac{1}{r^2}\left[-\varepsilon_1^2 r^2 + \alpha_1^2 r - \beta^2\right] R_{nl}(r) = 0, \tag{37}$$

where

$$\varepsilon_1^2 = \frac{-2\mu E}{\hbar^2}, \alpha_1^2 = \frac{2\mu}{\hbar^2}(B - C) \ and\ \beta^2 = \frac{2\mu A}{\hbar^2} + l(l+1) \tag{38}$$

Solving Eq. (37) by the NU method and following the same procedure of section 4(a), we obtain the spectrum as

$$E_{n,l} = \frac{-\mu}{2\hbar^2} \frac{(B-C)^2}{\left[n + ½ + \sqrt{\frac{2\mu A}{\hbar^2} + (l + ½)^2}\right]^2} \tag{39}$$

and the corresponding radial wave function as

$$R_{n,l}(r) = A_n r^{\frac{1}{2}(\nu-1)} e^{-\varepsilon_1 r} L_n^{\nu}(2\varepsilon_1 r), \tag{40}$$

(iii) Case III : $\delta = -3$

Substituting $\delta = -3$ into Eq. (18), we obtain

$$\frac{d^2R_{nl}(r)}{dr^2} + \frac{2}{r}\frac{dR_{nl}(r)}{dr} + \frac{1}{r^2}[-\varepsilon_1^2 r^2 + \alpha^2 r - \beta_1^2]R_{nl}(r) = 0 \tag{41}$$

where

$$\beta_1^2 = \frac{2\mu}{\hbar^2}(A + C) + l(l+1) \tag{42}$$

By solving Eq. (41), we obtain the energy eigenvalues as

$$E_{n,l} = \frac{-\mu}{2\hbar^2}\frac{B^2}{\left[n + ½ + \sqrt{\frac{2\mu}{\hbar^2}(A+C) + (l+½)^2}\right]^2} \tag{43}$$

and the associated wave function becomes

$$R_{nl}(r) = N_n r^{½(\Lambda-1)} e^{-\varepsilon_1 r} L_n^{\Lambda}(2\varepsilon_1 r) \tag{44}$$

where $\Lambda = \sqrt{1 + 4\beta_1^2}$ and N_n is the normalization constant.

5. EXPECTATION VALUES AND THE VIRIAL THEOREM

Some useful expectation values $\langle r^{-2}\rangle, \langle r^{-1}\rangle$ and the Virial theorem for the considered potential family for arbitrary quantum numbers $n \; and \; l$ can be obtained via the Hellmann-Feynman theorem (HFT) [48,49]. Assuming that the Hamiltonian $\hat{H}$ for a particular quantum mechanical system as a function of some parameter q and letting $E(q) and \; \Psi(q)$ be the eigenvalues and eigenfunctions of the Hamiltonian $\hat{H}$. The HFT theorem then states that

$$\frac{\partial E(q)}{\partial q} = \left\langle \Psi(q) \middle| \frac{\partial \hat{H}(q)}{\partial q} \middle| \Psi(q) \right\rangle. \tag{45}$$

Before proceeding further, it should be noted that the expectation values in fact give the radial probability density of a particle in a potential and we can therefore estimate the appropriate position of a particle in a potential. Even in some cases the NMR experiment works by means of this kind of result. The effective Hamiltonian for the family of the new solvable potential is

$$\hat{H} = \frac{-\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + \frac{A}{r^2} - \frac{B}{r} + Cr^{\delta+1}. \tag{46}$$

(i) Case I: $\boldsymbol{\delta = -1}$.
For case I, Eq. (46) becomes

$$\hat{H} = \frac{-\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + \frac{A}{r^2} - \frac{B}{r} + C. \tag{47}$$

In order to calculate the term $\langle r^{-2}\rangle$, we set $q = \frac{\hbar^2 l(l+1)}{2\mu} + A$ in Eq. (45) and using Eqs. (30) and (47), we have

$$\langle r^{-2}\rangle = \frac{\left(\frac{\mu B}{\hbar^2}\right)^2}{\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^3\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}}\,. \tag{48}$$

Similarly, we find the expectation value for the term $\langle r^{-1}\rangle$ by setting $q = B$ in Eq. (45) and using Eqs. (30), (47),we obtain

$$\langle r^{-1}\rangle = \frac{\left(\frac{\mu B}{\hbar^2}\right)}{\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^2} \tag{49}$$

Also, if we let $q = \mu$ and make use of the HFT theorem, we obtain the Virial theorem for the new solvable potential family as follows:

$$\langle\psi(\mu)\left|\frac{\partial H(\mu)}{\partial\mu}\right|\psi(\mu)\rangle = \frac{1}{\mu}\langle H - V\rangle = \frac{\partial E_{n,l}}{\partial\mu}, \tag{50}$$

$$\frac{\partial E_{n,l}}{\partial\mu} = \frac{-B^2}{2\hbar^2\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^2} + \frac{\mu B^2 A}{\hbar^4\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^3\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}} \tag{51}$$

With Eqs. (50) and (51), we obtain,

$$-\langle H - V\rangle = (1 - \Lambda)E_{n,l} - (1 - \Lambda)C, \tag{52}$$

where

$$\Lambda = \frac{2\mu A}{\hbar^2\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}} \tag{53}$$

Now, as

$$H = \langle T\rangle + \langle V\rangle = E_{n,l} \tag{54}$$

Combining Eqs (52) and (54), we obtain

$$-(2 - \Lambda)\langle T\rangle = (1 - \Lambda)\langle V\rangle - (1 - \Lambda)C \tag{55}$$

If $\Lambda = 0$ (ie. $A = 0$) and $C = 0$, we have the usual Viral theorem as

$$-2\langle T\rangle = \langle V\rangle \tag{56}$$

(ii) Case II: $\delta = -2$

The Hamiltonian in this case is

$$\hat{H} = \frac{-\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + \frac{A}{r^2} - \frac{B}{r} + \frac{C}{r} \tag{57}$$

To find $\langle r^{-2}\rangle$, we set $q = l$ and using Eqs. (39) and (57) ,we obtain $< r^{-2} >$ as

$$\langle r^{-2}\rangle = \frac{\left[\mu(B-C)/\hbar^2\right]^2}{\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^3\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}} \tag{58}$$

Similarly, to order to find $\langle r^{-1}\rangle$, we set $q = B$ in Eq. (45) and using Eqs. (39) and (57),we have

$$\langle r^{-1}\rangle = \frac{\mu(B-C)/\hbar^2}{\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^2} \tag{59}$$

The Virial theorem is obtained by setting $q = \mu$ in Eq. (45) and using Eqs. (39) and (57),we obtain

$$\langle\psi(\mu)\left|\frac{\partial H(\mu)}{\partial\mu}\right|\psi(\mu)\rangle = \frac{-1}{\mu}\langle H - V\rangle = \frac{\partial E_{n,l}}{\partial\mu}, \tag{60}$$

where

$$\frac{\partial E_{n,l}}{\partial\mu} = \frac{-(B-C)^2}{2\hbar^2\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^2} + \frac{\mu(B-C)^2 A}{\hbar^4\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^3\sqrt{\frac{2\mu A}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}} \tag{61}$$

Using Eqs. (60) and (61), we have

$$-\langle H - V\rangle = E_{n,l}(1-\Lambda) \tag{62}$$

Since

$$H = \langle T\rangle + \langle V\rangle = E_{n,l} \tag{63}$$

Substituting Eq. (63) into Eq. (60), we obtain the Virial theorem for our potential family as

$$-(2-\Lambda)\langle T\rangle = (1-\Lambda)\langle V\rangle \tag{64}$$

If $\Lambda = 0$, (ie. $A = 0$), we Eq. (56) is recovered.

(iii) Case III: $\delta = -3$

The Hamiltonian in this case is defined as

$$\hat{H} = \frac{-\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + \frac{A}{r^2} - \frac{B}{r} + \frac{C}{r^2} \tag{65}$$

In order to evaluate $\langle r^{-2}\rangle$, we let $q = l$ in Eq. (45) and using Eqs. (43) and (65), we have

$$\langle r^{-2}\rangle = \frac{\left[\mu B/\hbar^2\right]^2}{\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu(A+C)}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^3\sqrt{\frac{2\mu(A+C)}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}} \tag{66}$$

The same result can be obtained by setting $q = A = C$. Similarly, the expectation value for $\langle r^{-1}\rangle$, by setting $q = B$ in Eq. (45) and using Eqs. (43) and (65), is calculated as

$$\langle r^{-1}\rangle = \frac{\mu B/\hbar^2}{\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu(A+C)}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^2} \tag{67}$$

The Virial theorem is then obtained by setting $q = \mu$ in Eq. (45) and using Eqs. (43) and (65) as

$$\langle\psi(\mu)\left|\frac{\partial H(\mu)}{\partial\mu}\right|\psi(\mu)\rangle = \frac{-1}{\mu}\langle H - V\rangle = \frac{\partial E_{n,l}}{\partial\mu} \tag{68}$$

where

$$\frac{\partial E_{n,l}}{\partial\mu} = \frac{-B^2}{2\hbar^2\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu(A+C)}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^2} + \frac{\mu B^2(A+C)}{\hbar^4\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu(A+C)}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^3\sqrt{\frac{2\mu(A+C)}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}} \tag{69}$$

Combining Eqs. (68) and (69), we get

$$-\langle H - V\rangle = E_{n,l}(1-\mathcal{G}), \tag{70}$$

where

$$\mathcal{G} = \frac{2\mu(A+C)}{\hbar^2\left[\left(n+\frac{1}{2}\right)+\sqrt{\frac{2\mu(A+C)}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}\right]^3\sqrt{\frac{2\mu(A+C)}{\hbar^2}+\left(l+\frac{1}{2}\right)^2}} \tag{71}$$

Since

$$H = \langle T\rangle + \langle V\rangle = E_{n,l} \tag{72}$$

Using Eqs. (70) and (72) we obtain the Virial theorem for this potential as

$$-(2-\mathcal{G})\langle T\rangle = (1-\mathcal{G})\langle V\rangle \tag{73}$$

If we now set $\mathcal{G} = 0$ (ie. $A = -C$), we obtain the ordinary Virial theorem as expected.

6. DISCUSSIONS AND APPLICATIONS TO DIATOMIC MOLECULES

We have obtained the energy spectra of the Schrödinger equation for the three cases of the of Eqs. (30), (39) and (43) for $\delta = -1, -2$ and -3 with $A = D_e r_e^2, B = 2D_e r_e \; and \; C = D_e$ [50], where D_e, r_e are the dissociation energy and distant from equilibrium position, respectively. We computed the energy eigenvalues for the diatomic molecules H_2, CO, NO and N_2 for different values of n and l .The reduced mass and spectroscopic constant of these selected diatomic molecules are given in Table (1) taken from Refs. [12, 51, 52]. The bound-state energies of the diatomic molecules given in Table (1) are computed using Eqs. (30), (39) and (43). Table (2) shows the exact bound-state energy eigenvalues for the selected diatomic molecules H_2, CO, NO and N_2 for various values of n and l for $\delta = -1$. Similarly, Table (3) and Table (4) show the exact bound-state energy eigenvalues for various n and l values for $\delta = -2 \; and \; \delta = -3$. In addition, according to what we expect from the quantum considerations, it is observed that the energy increases as *n, l* increase.

TABLE 1: Molecular constant of some selected molecules taken from Refs. [12, 51-52]

Molecules	D_e(eV)	r_e(Å)	μ(amu)
H_2	4.7446	0.7416	0.50391
CO	10.84507364	1.1282	6.860586
NO	8.043729855	1.1508	7.468441
N_2	11.93819382	1.094	7.00335

TABLE 2: Energy eigenvalues of Eq. (30) for some selected diatomic molecules for $\delta = -1$.

	n	l	H_2	CO	NO	N_2
$E_{nl}(eV)$	1	0	3.523819982	2.037437416	1.627871837	2.19024884
	2	0	4.036255553	3.086749363	2.448252803	3.325645911
		1	4.181922626	3.15535359	2.506229261	3.398064305
	3	0	4.282626735	3.959132563	3.120783141	4.273637870
		1	4.361777384	4.016519227	3.168650935	4.334456591
		2	4.447443522	4.128297137	3.261465224	4.453073450
	4	0	4.419692917	4.692238414	3.678968504	5.073308431
		1	4.467393967	4.740725685	3.718947487	5.124878233
		2	4.521586989	4.835265179	3.796563351	5.225551845
		3	4.565961226	4.97129629	3.907478683	5.370695809
	5	0	4.503709824	5.314210711	4.147334322	5.754059434
		1	4.534646748	5.355547576	4.18106697	5.798164508
		2	4.57108369	5.436218708	4.246629622	5.884338895
		3	4.602102221	5.552466628	4.340490863	6.008751015
		4	4.626606508	5.699217545	4.457965328	6.166200826

TABLE 3: Energy eigen state of Eq.(39) for some selected diatomic molecules for $\delta = -2$

	n	l	H_2	CO	NO	N_2
$E_{nl}(eV)$	1	0	-0.129566232	-2.730756917	-2.051871346	-2.873765424
	2	0	-0.07517941	-2.405423787	-1.789503289	-2.539042069
		1	-0.059719185	-2.384153441	-1.770961696	-2.517692597
	3	0	-0.049031058	-2.134946397	-1.574419707	-2.259567111
		1	-0.040630485	-2.117153992	-1.55911099	-2.241637308
		2	-0.031538397	-2.082497895	-1.529427823	-2.206668191
	4	0	-0.034483679	-1.907651148	-1.395905072	-2.023818385
		1	-0.029420977	-1.892617949	-1.383119295	-2.008615231
		2	-0.023669257	-1.863306522	-1.358296774	-1.978935914
		3	-0.018959643	-1.821130859	-1.322824669	-1.936146413
	5	0	-0.025566631	-1.714812217	-1.246115847	-1.823128015
		1	-0.022283173	-1.70199596	-1.235327725	-1.810125516
		2	-0.018415975	-1.67698434	-1.214359972	-1.784720677
		3	-0.015123855	-1.640942341	-1.184341978	-1.748043075
		4	-0.012523118	-1.595443064	-1.14677218	-1.70162572

Using the Hellmann-Feynmann theorem, we computed the expectation values. In Tables (5)-(7), we have presented the behavior of the terms $\langle r^{-2}\rangle$ and $\langle r^{-1}\rangle$ for some mentioned diatomic molecules for various n and l values for $\delta = -1, \delta = -2\ and\ \delta = -3$.

It is seen in Tables (5)-(7) that the magnitude of the terms $\langle r^{-2}\rangle$ and $\langle r^{-1}\rangle$ for H_2, *CO, NO* and N_2 in condition $\delta = -1, \delta = -2\ and\ \delta = -3$ decreases as *n, l* increases and we can see the decreasing trend the terms $\langle r^{-2}\rangle$ and $\langle r^{-1}\rangle$ versus increasing *n, l,* decreases as the δ parameter increases.

TABLE 4: Energy eigen state of Eq. (43) for some selected molecules for $\delta = -3$.

	n	l	H_2	CO	NO	N_2
$E_{nl}(eV)$	1	0	-0.684990846	-5.188431118	-3.856018466	-5.59052238
	2	0	-0.449613958	-4.70374956	-3.465180783	-5.086520496
		1	-0.396697905	-4.679410923	-3.443750215	-5.062159189
	3	0	-0.317593639	-4.28394203	-3.130887698	-4.647724679
		1	-0.285721397	-4.262784138	-3.112478037	-4.626443345
		2	-0.240947064	-4.221118113	-3.076333417	-4.584485968
	4	0	-0.23621029	-3.917926953	-2.842735369	-4.263353299
		1	-0.215549452	-3.899418853	-2.826804496	-4.244653872
		2	-0.185738616	-3.862953464	-2.795507258	-4.207770926
		3	-0.156320956	-3.809590846	-2.749921971	-4.153700194
	5	0	-0.182526894	-3.596891682	-2.592607162	-3.924764376
		1	-0.168378769	-3.580608742	-2.57872931	-3.908245533
		2	-0.14754003	-3.548513275	-2.551450013	-3.875650638
		3	-0.126433467	-3.501511415	-2.511680323	-3.827834993
		4	-0.107781421	-3.918821564	-2.460689257	-3.766009709

TABLE 5: The terms $\langle r^{-2}\rangle$ and $\langle r^{-1}\rangle$ of Eqs. (48) and (49) for some selected diatomic molecules for $\delta = -1$.

	n	l	H_2	CO	NO	N_2
$\langle r^{-1}\rangle$	1	0	0.346950954	0.719847943	0.693102419	0.746375064
	2	0	0.201314551	0.634087698	0.604477012	0.659440632
		1	0.159915340	0.628480675	0.598213839	0.653895742
	3	0	0.131294797	0.562787835	0.531823844	0.586855327
		1	0.108799841	0.558097624	0.526652707	0.582198594
		2	0.084453155	0.548962018	0.516626019	0.573116407
$\langle r^{-2}\rangle$	1	0	0.226776180	0.574621245	0.537471311	0.616106699
	2	0	0.100232383	0.475055683	0.437752716	0.511662753
		1	0.054514310	0.466316211	0.428287787	0.502720259
	3	0	0.052791813	0.397225919	0.361252510	0.429553068
		1	0.030592694	0.390218524	0.353783429	0.422347913
		2	0.015509524	0.37676514	0.339545800	0.408486631

TABLE 6: The terms $\langle r^{-2}\rangle$ and $\langle r^{-1}\rangle$ of Eqs. (58) and (59) for some selected diatomic molecules for $\delta = -2$.

	n	l	H_2	CO	NO	N_2
$\langle r^{-1}\rangle$	1	0	0.113030408	0.400822973	0.3919630296	0.405253006
	2	0	0.065584676	0.353070282	0.341843621	0.358050946
		1	0.052097554	0.349948201	0.338301674	0.355040284
	3	0	0.042773494	0.313369365	0.300756828	0.318639913
		1	0.035445040	0.310757780	0.297832449	0.316111485
		2	0.027513325	0.305670927	0.292162159	0.311180206
$\langle r^{-2}\rangle$	1	0	0.024068657	0.178158010	0.171890023	0.181632758
	2	0	0.010638061	0.147288280	0.139998774	0.150841919
		1	0.005785820	0.144578657	0.136971771	0.148205607
	3	0	0.005603005	0.123157610	0.115533055	0.126635384
		1	0.003246924	0.120985007	0.113144349	0.124511251
		2	0.001646087	0.116813863	0.108590978	0.120424844

TABLE 7: The terms $\langle r^{-2}\rangle$ and $\langle r^{-1}\rangle$ of Eqs. (66) and (67) for some selected diatomic molecules for $\delta = -3$.

	n	l	H_2	CO	NO	N_2
$\langle r^{-1}\rangle$	1	0	0.194677357	0.424050378	0.416564039	0.428051913
	2	0	0.127782229	0.384437363	0.374342009	0.389461786
		1	0.112743258	0.382448167	0.372026875	0.387596503
	3	0	0.090261484	0.350126502	0.338228469	0.355864319
		1	0.081203255	0.348397268	0.336239682	0.354234862
		2	0.068478196	0.344991904	0.332334994	0.351022294
$\langle r^{-2}\rangle$	1	0	0.058437611	0.194479935	0.189094282	0.197563529
	2	0	0.031075990	0.167875378	0.161086292	0.171458645
		1	0.022934526	0.166084131	0.159026315	0.169767141
	3	0	0.018449007	0.145910349	0.138347391	0.149757568
		1	0.014018904	0.144404715	0.136640982	0.148327204
		2	0.009129678	0.141464118	0.133323881	0.145528621

The wavefunction for three states and for two diatomic molecules *H*$_2$, *CO* is plotted in Figures (1)-(3) for values of $= -1, \delta = -2\ and\ \delta = -3$, respectively. We can clearly see that the δ parameter affects only the shape of the wave function and not the node structure of the wavefunctions.

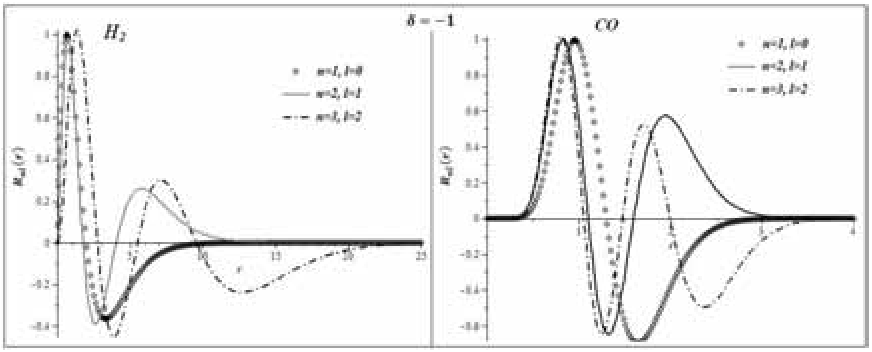

Figure 1: Behavior of wavefunctions for $\delta = -1$

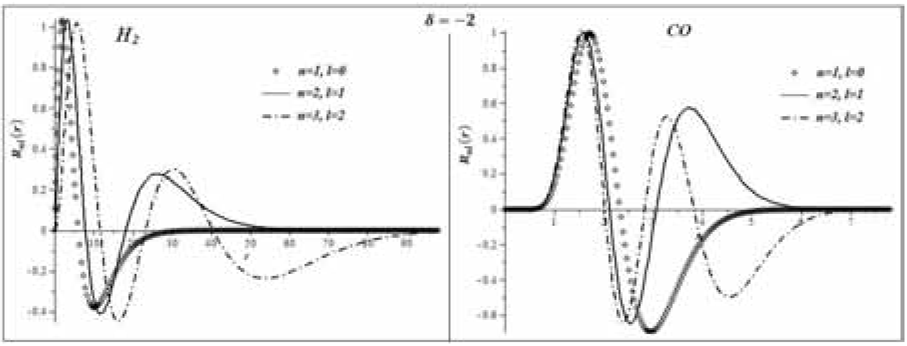

Figure 2: Behavior of wavefunctions for $\delta = -2$

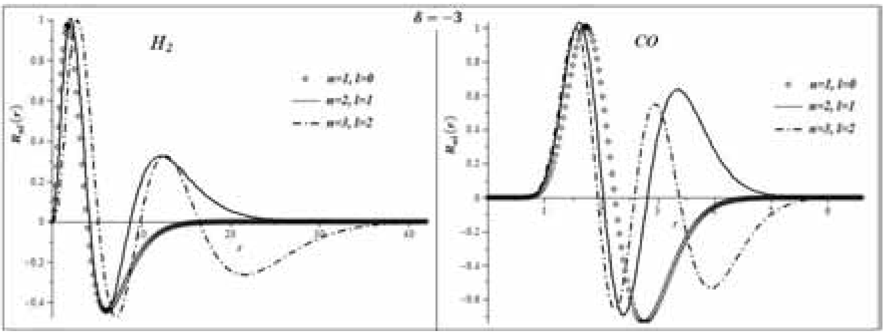

Figure 3: Behavior of wavefunctions for $\delta = -3$

7. CONCLUSIONS

In this work, we obtained the energy eigenvalues and the eigenfunctions of the Schrödinger equation with family of potentials for three different parameters of $\delta = -1, -2\ and - 3$ respectively. In each case we calculated the energies for the selected diatomic molecules as shown in Tables (2-4). Similarly, we also used the Hellmann-Feynmann theorem to compute the expectations values of the system.

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