

**ROTATIONAL-VIBRATIONAL EIGEN SOLUTIONS OF THE D-DIMENSIONAL SCHRÖDINGER EQUATION FOR THE IMPROVED WEI POTENTIAL***¹Eyube, E. S., ²Yabwa, D. and ³Wadata, U.¹Department of Physics, School of Physical Sciences, Modibbo Adama University of Technology, Yola, Nigeria²Department of Physics, Faculty of Science, Taraba State University, Jalingo, Nigeria³Department of Physics, School of Sciences, Aminu Saleh College of Education, Azare, Nigeria* Corresponding Author: Email Address: edwineyubes@mautech.edu.ng; Tel.: +2348036870057**ABSTRACT**

In this present study, we have employed the techniques of exact quantization rule and ansatz solution method to obtain closed form expressions for the rotational-vibrational eigensolutions of the D-dimensional Schrödinger equation for the improved Wei potential, for cases of $h' \neq 0$ and $h' = 0$. By using our derived energy equation and choosing arbitrary values of n and ℓ , we have computed the bound state rotational-vibrational energies of CO, H₂ and LiH for various quantum states. The mean absolute percentage deviation (MAPD) and the Lippincott criterion were used as a goodness-of-fit indices to compare our result with the Rydberg-Klein-Rees (RKR) and improved Tietz potential data in the literature. MAPD of 0.2862%, 0.2896% and 0.0662% relative to the RKR data for CO were obtained. For the improved Wei and Morse potential, our computed energy eigenvalues for CO, H₂ and LiH are in excellent agreement with existing results in the literature.

Keywords: Improved Wei potential, Morse potential, exact quantization rule, ansatz solution, RKR data, D-dimensions

INTRODUCTION

Extensive literature review reveals that wave functions are of tremendous importance in both relativistic and nonrelativistic quantum mechanics because they completely define the quantum mechanical system under review (Yanar *et al.*, 2020; Hamzavi *et al.*, 2012), information such as energy of the system, momentum, frequency of vibration, speed and wavelength are readily obtainable if the wave function of the system is known (Eyube *et al.*, 2019a). Obtaining the wave function of a quantum mechanical system requires solving the Schrödinger equation for a given potential energy function (Eyube *et al.*, 2019b). The Coulomb and harmonic oscillator potentials are known to give exact solution with the Schrödinger equation for all quantum states $n\ell$ (Qiang *et al.*, 2009) where n is the vibrational quantum number and ℓ is the rotational quantum number, similarly, few other potential energy functions such as Eckart, Hulthén and Morse potentials give exact solution only for the s-wave ($\ell = 0$) state (Ikhdair, 2011; Serrano *et al.*, 2010). Most of the other known potential energy models have no exact solution with the Schrödinger equation for all values of n and ℓ , with these class of potential energy functions only approximate numerical (Nasser *et al.*, 2012; Lucha and Schöberl, 1999) or approximate analytical (Khodja *et al.*, 2019; Eyube *et al.*, 2019c; Ferreira and Bezerra, 2017) solutions are possible. Solving the Schrödinger equation by approximate analytical method is quite a challenge, it involves applying an appropriate approximation scheme (Ferreira and Prudente, 2017; Greene and Aldrich, 1976; Pekeris, 1934) to deal with the centrifugal term of the effective potential energy function, followed by a suitable solution technique. Different solution methods have been used by researchers to solve the Schrödinger equation, some of the solution techniques include: asymptotic iteration method (Falaye *et al.*, 2013), generalized pseudospectral method (Roy, 2013), exact

quantization rule (Falaye *et al.*, 2015; Ikhdair and Sever, 2009; Ma and Xu, 2005), proper quantization rule (Louis *et al.*, 2019; Dong and Cruz-Irrison, 2012) path integral approach (Khodja *et al.*, 2019), Laplace transform approach (Tsaur and Wang, 2014), Nikiforov-Uvarov method (Khordad and Mirhosseini, 2015; Ikot *et al.*, 2013; Yazarloo *et al.*, 2012) and ansatz solution method (Okorie *et al.*, 2020; Tang *et al.*, 2013). In the year 1990, Wei proposed a four parameter potential energy function which fits the experimental Rydberg-Klein-Rees (RKS) data more closely than the Morse potential, particularly when the potential domain extends to near the dissociation limit (Jia *et al.*, 2012), the Wei potential has been used to investigate the rotational-vibrating levels of diatomic molecules (Kunc and Gordillo-Vazquez, 1997). However, it is pertinent to note that the expressions derived by these authors for the energy eigenvalues and eigenfunctions are only restricted to the case $h' \neq 0$ as these expressions become infinite when $h' = 0$ which is not physically acceptable for a finite potential energy function. In the present study, we aimed at obtaining closed form expressions for the rotational-vibrational eigensolutions of the D-dimensional Schrödinger equation for the improved Wei potential via exact quantization rule (EQR) and ansatz solution method. As our specific objectives, we will consider cases of rotational-vibrational energies and radial wave functions for $h' \neq 0$ as well as $h' = 0$, we will compare results with those in the literature where they exist.

THEORETICAL APPROACH**Overview of the concepts of exact quantization rule**

Here we present in outline form, the basic concepts of EQR, a detailed description of the concept is given by Ma and Xu (2005). The EQR has been proposed to solve the one-dimensional Schrödinger equation given by:

$$\psi''_{n\ell}(x) + k_{n\ell}^2(x)\psi_{n\ell}(x) = 0 \quad (1)$$

where

$$k_{n\ell}(x) = \sqrt{\frac{2\mu}{\hbar^2} \{E_{n\ell} - V_{eff}(x)\}} \tag{2}$$

is the momentum of the system, μ as the mass, $E_{n\ell}$ is the energy eigenvalue, $V_{eff}(x)$ is the effective potential energy function which is a piecewise continuous real function of x and $\psi_{n\ell}(x)$ is the wave function. If we define the phase angle, $\varphi_{n\ell}(x)$ as:

$$\varphi_{n\ell}(x) = \psi'_{n\ell}(x) / \psi_{n\ell}(x) \tag{3}$$

Eq. (1) assumes the well-known Riccati differential equation given by:

$$\varphi'_{n\ell}(x) + \frac{2\mu}{\hbar^2} \{E_{n\ell} - V_{eff}(x)\} + \varphi_{n\ell}^2(x) = 0 \tag{4}$$

As a result of Sturm-Liouville theorem, $\varphi_{n\ell}(x)$ decreases monotonically with respect to x between two turning points determined by the equation $E_{n\ell} \geq V_{eff}(x)$. Particularly, x increases across a node of the wavefunction $\psi_{n\ell}(x)$, where $E_{n\ell} \geq V_{eff}(x)$, $\varphi_{n\ell}(x)$ decreases to $-\infty$ and jumps to $+\infty$ and then decreases again. By carefully studying the one-dimensional Schrödinger equation, Ma and Xu (2005) proposed an EQR given by:

$$\int_{x_{nA}}^{x_{nB}} k_{n\ell}(x) dx = N\pi + \int_{x_{nA}}^{x_{nB}} \varphi_{n\ell}(x) \left[\frac{dk_{n\ell}(x)}{dx} \right] \left[\frac{d\varphi_{n\ell}(x)}{dx} \right]^{-1} dx \tag{5}$$

where x_{nA} and x_{nB} are two turning points determined by solving the equation $E_{n\ell} = V_{eff}(x)$ and $x_{nA} < x_{nB}$. N is the number of nodes of $\varphi_{n\ell}(x)$ in the neighborhood of $E_{n\ell} \geq V_{eff}(x)$ and it is larger by one than the number of nodes n of the wavefunction $\psi_{n\ell}(x)$, clearly, $N = n + 1$. The first term, $N\pi$, is the contribution from the nodes of the wave function, and the second term is referred to as the quantum correction. The quantum correction is independent of the number of nodes for the exactly solvable systems (Ma and Xu, 2005), therefore, it can be evaluated for the ground state ($n = 0$), the second term in Eq. (5) can thus be represented by:

$$Q_c = \int_{x_{nA}}^{x_{nB}} \varphi_{n\ell}(x) \left[\frac{dk_{n\ell}(x)}{dx} \right] \left[\frac{d\varphi_{n\ell}(x)}{dx} \right]^{-1} dx \equiv \int_{x_{0A}}^{x_{0B}} \varphi_{0\ell}(x) \left[\frac{dk_{0\ell}(x)}{dx} \right] \left[\frac{d\varphi_{0\ell}(x)}{dx} \right]^{-1} dx \tag{6}$$

where Q_c is the quantum correction term. In three dimensional spherical coordinates, the EQR is given by:

$$\int_{r_{nA}}^{r_{nB}} k_{n\ell}(r) dr = N\pi + \int_{r_{nA}}^{r_{nB}} \varphi_{0\ell}(r) \left[\frac{dk_{0\ell}(r)}{dr} \right] \left[\frac{d\varphi_{0\ell}(r)}{dr} \right]^{-1} dr \tag{7}$$

In simplified form, Eq. (6) can be expressed as:

$$I = N\pi + Q_c \tag{8}$$

where the momentum integral is given by:

$$I = \int_{r_{nA}}^{r_{nB}} k_{n\ell}(r) dr \tag{9}$$

and the quantum correction is:

$$Q_c = \int_{r_{nA}}^{r_{nB}} \varphi_{0\ell}(r) \left[\frac{dk_{0\ell}(r)}{dr} \right] \left[\frac{d\varphi_{0\ell}(r)}{dr} \right]^{-1} dr \tag{10}$$

The radial Schrödinger equation in D-dimensional space Falaye *et al.* (2015) is written as:

$$\frac{d^2\psi_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \{E_{n\ell} - V_{eff}(r)\} \psi_{n\ell}(r) = 0 \tag{11}$$

$\psi_{n\ell}(r)$ is the radial wave function, r is the internuclear separation and $V_{eff}(r)$ is the effective potential defined in terms of a spherically symmetric potential $V(r)$ and a parameter Λ by:

$$V_{eff}(r) = V(r) + \frac{(\Lambda^2 - 1/4)\hbar^2}{2\mu r^2} \tag{12}$$

with Λ given in terms of spatial dimensions, $D \geq 2$ as:

$$\Lambda = \ell + \frac{1}{2}(D - 2) \tag{13}$$

Rotational-vibrational energy of the improved Wei potential

By choosing $V(r)$ to be the improved Wei potential (Jia *et al.*, 2012):

$$V(r) = D_e \left(1 - \frac{a}{e^{br} - H} \right)^2 \tag{14}$$

where D_e is the dissociation energy, r_e is the molecular bond length, r is the internuclear separation, $H = h' e^{br_e}$ and $a = (1 - h') e^{br_e}$. The parameters h' (dimensionless) and b (in m^{-1}) are determined through f_2 and f_3 the second and third derivatives of the potential energy function (Eq. (14)) at $r = r_e$ respectively (Jia *et al.*, 2012), therefore, by using the following relationship

$$\frac{d^2 V(r)}{dr^2} = f_2 = 4\pi^2 \mu c^2 \omega_e^2 \tag{15}$$

where ω_e is the equilibrium vibrational harmonic frequency (in m^{-1}), we find:

$$h' = 1 - \frac{b}{\pi c \omega_e} \left(\frac{D_e}{2\mu} \right)^{\frac{1}{2}} \tag{16}$$

also, employing the relationship between the vibrational-rotational coupling constant, α_e and f_3 (Jia *et al.*, 2012), viz:

$$\alpha_e = -\frac{6B_e^2}{\omega_e} \left(1 + \frac{r_e f_3}{3f_2} \right) \tag{17}$$

B_e being the rotational constant given by (Jia *et al.*, 2012):

$$B_e = \frac{\hbar}{4\pi c \mu r_e^2} \tag{18}$$

using Eqs. (16) – (18) and obtaining f_3 from (14), get:

$$b = \pi c \omega_e \left(\frac{8\mu}{D_e} \right)^{\frac{1}{2}} - \frac{8\pi^2 c^2 \mu^2 r_e^3 \alpha_e \omega_e}{3\hbar^2} - \frac{1}{r_e} \tag{19}$$

Putting Eq. (14) in (12), we have the effective improved Wei potential given by:

$$V_{eff}(r) = D_e \left(1 - \frac{a}{e^{br} - H} \right)^2 + \frac{(\Lambda^2 - 1/4)\hbar^2}{2\mu r^2} \tag{20}$$

Eq. (1) when used with the effective potential of Eq. (20) has exact solution only for the s-wave ($\ell = 0$) case, to obtain analytical solution for all quantum states, we must use a suitable approximation scheme to deal with the centrifugal or spin-orbit term, $1/r^2$ is approximated by a Pekeris-type approximation (Hamzavi *et al.*, 2012) given as:

$$\frac{1}{r^2} \approx \frac{1}{r_e^2} \left\{ c_0 + \frac{c_1}{e^{br} - H} + \frac{c_2}{(e^{br} - H)^2} \right\} \tag{21}$$

where c_0 , c_1 and c_2 are adjustable parameters given by:

$$c_0 = 1 + \frac{1}{br_e} (1 - h')(3 + h') - \frac{3}{b^2 r_e^2} (1 - h')^2 \tag{22}$$

$$c_1 = \frac{2e^{br_e}}{br_e} (1 - h')^2 (2 + h') - \frac{6e^{br_e}}{b^2 r_e^2} (1 - h')^3 \tag{23}$$

$$c_2 = -\frac{e^{2br_e}}{br_e}(1-h')^3(1+h') + \frac{3e^{2br_e}}{b^2r_e^2}(1-h')^4 \tag{24}$$

Substituting Eq. (21) in Eq. (20), this leads to:

$$V_{eff}(r) = D_e \left(1 - \frac{a}{e^{br} - H} \right)^2 + \frac{(\Lambda^2 - \frac{1}{4})\hbar^2}{2\mu r_e^2} \left\{ c_0 + \frac{c_1}{e^{br} - H} + \frac{c_2}{(e^{br} - H)^2} \right\} \tag{25}$$

the substitution:

$$x = (e^{br} - H)^{-1} \tag{26}$$

transforms Eq. (25) transforms to:

$$V_{eff}(x) = D_e (1 - ax)^2 + \frac{(\Lambda^2 - \frac{1}{4})\hbar^2}{2\mu r_e^2} (c_0 + c_1 x + c_2 x^2) \tag{27}$$

Eq. (27) can be expressed in polynomial form as:

$$V_{eff}(x) = \frac{\hbar^2}{2\mu r_e^2} \left\{ (\Lambda^2 - \frac{1}{4})c_2 + \frac{2\mu r_e^2 D_e a^2}{\hbar^2} \right\} x^2 + \frac{\hbar^2}{2\mu r_e^2} \left\{ (\Lambda^2 - \frac{1}{4})c_1 - \frac{4\mu r_e^2 D_e a}{\hbar^2} \right\} x + \frac{\hbar^2}{2\mu r_e^2} \left\{ (\Lambda^2 - \frac{1}{4})c_0 + \frac{2\mu r_e^2 D_e}{\hbar^2} \right\} \tag{28}$$

by defining the following parameters:

$$\varepsilon_1^2 = (\Lambda^2 - \frac{1}{4})c_2 + \frac{2\mu r_e^2 D_e a^2}{\hbar^2} \tag{29}$$

$$\varepsilon_2^2 = (\Lambda^2 - \frac{1}{4})c_1 - \frac{4\mu r_e^2 D_e a}{\hbar^2} \tag{30}$$

$$\varepsilon_3^2 = (\Lambda^2 - \frac{1}{4})c_0 + \frac{2\mu r_e^2 D_e}{\hbar^2} \tag{31}$$

$$\alpha = \frac{\hbar^2 \varepsilon_1^2}{2\mu r_e^2} \tag{32}$$

$$\beta = \frac{\hbar^2 \varepsilon_2^2}{2\mu r_e^2} \tag{33}$$

$$\gamma = \frac{\hbar^2 \varepsilon_3^2}{2\mu r_e^2} \tag{34}$$

in compact form, Eq. (28) can be expressed in the form:

$$V_{eff}(x) = \alpha x^2 + \beta x + \gamma \tag{35}$$

To enable determine the Riccati equation (Gu and Dong, 2011), first, we need to obtain two turning points x_{nA} and x_{nB} by solving the equation:

$$V_{eff}(x) = E_{n\ell} \tag{36}$$

Inserting Eq. (35) in Eq. (36), we have that:

$$\alpha x^2 + \beta x + \gamma - E_{n\ell} = 0 \tag{37}$$

x_{nA} and x_{nB} ($> x_{nA}$) being the roots Eq. (37) are given by:

$$x_{nA} = -\frac{\beta + \sqrt{\beta^2 - 4\alpha(\gamma - E_{n\ell})}}{2\alpha} \tag{38}$$

and

$$x_{nB} = -\frac{\beta - \sqrt{\beta^2 - 4\alpha(\gamma - E_{n\ell})}}{2\alpha} \tag{39}$$

using Eqs. (38) and (39), the sum and products of x_{nA} and x_{nB} which may be required later are given respectively by:

$$x_{nA} + x_{nB} = -\frac{\beta}{\alpha} \tag{40}$$

$$x_{nA} x_{nB} = \frac{\gamma - E_{n\ell}}{\alpha} \tag{41}$$

for the ground ($n = 0$) state, Eq. (40) and (41) gives respectively:

$$x_{0A} + x_{0B} = -\frac{\beta}{\alpha} \tag{42}$$

$$x_{0A} x_{0B} = \frac{\gamma - E_{0\ell}}{\alpha} \tag{43}$$

substituting Eq. (35) in the momentum relation given by Eq. (2), this gives:

$$k_{n\ell}(x) = \sqrt{\frac{2\mu}{\hbar^2}(E_{n\ell} - \alpha x^2 - \beta x - \gamma)} \tag{44}$$

an important result for the momentum is one which involves the turning points, thus, if we write Eq. (44) as in the following form:

$$k_{n\ell}(x) = \sqrt{\frac{2\mu\alpha}{\hbar^2}\left(\frac{E_{n\ell} - \gamma}{\alpha} - x^2 - \frac{\beta}{\alpha}x\right)} \tag{45}$$

inserting Eq. (32), (40) and (41), this gives:

$$k_{n\ell}(x) = \frac{\varepsilon_1}{r_e} \sqrt{(x - x_{nA})(x_{nB} - x)} \tag{46}$$

differentiating Eq. (46) with respect to x as this will be required in evaluating the quantum correction for the ground state, this gives:

$$k'_{n\ell}(x) = -\frac{\varepsilon_1}{r_e} \frac{x + \beta/2\alpha}{\sqrt{(x - x_{nA})(x_{nB} - x)}} \tag{47}$$

The Riccati equation given by Eq. (4), in three dimensional spherical coordinates is written as (Ikhdair and Sever, 2009):

$$\varphi'_{n\ell}(r) + \frac{2\mu}{\hbar^2}\{E_{n\ell} - V_{eff}(r)\} + \varphi_{n\ell}^2(r) = 0 \tag{48}$$

using Eq. (26) followed by Eq. (35) in Eq. (48), the Riccati equation in terms of variable x is therefore given by:

$$-bx(1 + Hx)\varphi'_{n\ell}(x) + \frac{2\mu}{\hbar^2}(E_{n\ell} - \alpha x^2 - \beta x - \gamma) + \varphi_{n\ell}^2(x) = 0 \tag{49}$$

which for the ground state ($n = 0$) gives;

$$-bx(1 + Hx)\varphi'_{0\ell}(x) + \frac{2\mu}{\hbar^2}(E_{0\ell} - \alpha x^2 - \beta x - \gamma) + \varphi_{0\ell}^2(x) = 0 \tag{50}$$

since $\varphi_{0\ell}(x)$ has one zero and no pole, we choose a linear polynomial as a trial solution, assume:

$$\varphi_{0\ell}(x) = -mx + c \tag{51}$$

where m and c are constants, substituting Eq. (51) in Eq. (50), get:

$$mb(x + Hx^2) + \frac{2\mu}{\hbar^2}(E_{0\ell} - \alpha x^2 - \beta x - \gamma) + m^2x^2 - 2cmx + c^2 = 0 \tag{52}$$

which simplifies to;

$$\left(mbH - \frac{2\mu\alpha}{\hbar^2} + m^2\right)x^2 + \left(mb - \frac{2\mu\beta}{\hbar^2} - 2cm\right)x + \frac{2\mu}{\hbar^2}(E_{0\ell} - \gamma) + c^2 = 0 \tag{53}$$

if we equate corresponding coefficients of x^2 , x and x^0 respectively on both sides of Eq. (53), we have the following set of equations:

$$m^2 + b H m = \frac{2 \mu \alpha}{\hbar^2} \equiv \frac{\varepsilon_1^2}{r_e^2} \tag{54}$$

$$b m - 2 c m = \frac{2 \mu \beta}{\hbar^2} \equiv \frac{\varepsilon_2^2}{r_e^2} \tag{55}$$

$$c^2 = \frac{2 \mu}{\hbar^2} (\gamma - E_{0\ell}) \tag{56}$$

from Eq. (54) we find:

$$m = -b H \lambda \tag{57}$$

where the parameter λ is given by:

$$\lambda = \frac{1}{2} \left\{ 1 + \left(1 + \frac{4 \varepsilon_1^2}{b^2 r_e^2 H^2} \right)^{\frac{1}{2}} \right\} \tag{58}$$

it is obvious that Eq. (58) leads to;

$$\varepsilon_1 = b r_e H (\lambda^2 - \lambda)^{\frac{1}{2}} \tag{59}$$

With m given by Eq. (57), Eq. (55) can be used to find the constant c , thus, our trial solution is well defined. The quantum correction can be evaluated using Eq. (10), which, when we use Eq. (26) to transform to variable x leads to:

$$Q_c = -\frac{1}{b} \int_{x_{0A}}^{x_{nB}} \frac{\varphi_{0\ell}(x)}{\varphi'_{0\ell}(x)} k'_{0\ell}(x) \frac{dx}{x(1+Hx)} \tag{60}$$

substituting Eq. (51) and Eq. (47) with $n = 0$ in Eq. (60), get:

$$Q_c = \frac{\varepsilon_1}{b r_e} \int_{x_{0A}}^{x_{nB}} \frac{(x-c/m)(x+\beta/2\alpha)}{x(1+Hx)} \frac{dx}{\sqrt{(x-x_{0A})(x_{0B}-x)}} \tag{61}$$

Eq. (61) can be expressed in partial fractions as:

$$Q_c = \frac{\varepsilon_1}{b r_e} \int_{x_{0A}}^{x_{nB}} \left\{ \frac{1}{H} - \frac{\beta c}{2\alpha m x} + \frac{(2\alpha - \beta H)(m + c H)}{2\alpha H m(1+Hx)} \right\} \frac{dx}{\sqrt{(x-x_{0A})(x_{0B}-x)}} \tag{62}$$

the following standard integral (Dong and Gu, 2011) given by:

$$\int_{x_{nA}}^{x_{nB}} \frac{dx}{(P+Qx)\sqrt{(x-x_{nA})(x_{nB}-x)}} = \frac{\pi}{\sqrt{(P+Qx_{nB})(P+Qx_{nA})}} \tag{63}$$

applied to Eq. (62) gives:

$$Q_c = \frac{\pi \varepsilon_1}{b r_e} \left\{ \frac{1}{H} - \frac{\beta c}{2\alpha m} I_1 - \frac{(2\alpha - \beta H)(m + c H)}{2\alpha H m} I_2 \right\} \tag{64}$$

where

$$I_1^{-2} = x_{0A} x_{0B} \equiv \frac{\gamma - E_{0\ell}}{\alpha} \tag{65}$$

Thus, by putting Eqs. (56) and (54) in Eq. (65), we find:

$$I_1 = \frac{\varepsilon_1}{c r_e} \tag{66}$$

similarly; we find:

$$I_2^{-2} = 1 + H(x_{0A} + x_{0B}) + H^2 x_{0A} x_{0B} \tag{67}$$

on substituting Eq. (42) and (43) in Eq. (67), this gives:

$$I_2^{-2} = 1 - \frac{\beta H}{\alpha} + \frac{H^2 (\gamma - E_{0\ell})}{\alpha} \tag{68}$$

by inserting Eqs. (54), (55) and (56) in (68) and simplifying, get:

$$I_2 = \frac{\varepsilon_1}{r_e (m + c H)} \tag{69}$$

substituting Eqs. (66) and (69) in (64) and employing (57) to eliminate m , we find:

$$Q_c = \frac{\pi \varepsilon_1}{b r_e} \left(\frac{1}{H} + \frac{\varepsilon_1}{b r_e H^2 \lambda} \right) \tag{70}$$

The momentum integral on the left hand side of Eq. (7) is given in terms of variable x as:

$$I = -\frac{1}{b} \int_{x_{nA}}^{x_{nB}} k_{n\ell}(x) \frac{dx}{x(1+Hx)} \tag{71}$$

using Eq. (46) to eliminate $k_{n\ell}(x)$ in Eq. (71), we have:

$$I = -\frac{\varepsilon_1}{b r_e} \int_{x_{nA}}^{x_{nB}} \frac{\sqrt{(x-x_{nA})(x_{nB}-x)}}{x(1+Hx)} dx \tag{72}$$

In order to evaluate the integral in Eq. (72) we use the following standard integral obtained from Falaye *et al.* (2015)

$$\int_{x_{nA}}^{x_{nB}} \frac{\sqrt{(x-x_{nA})(x_{nB}-x)}}{x(1+Qx)} dy = \pi \left\{ -\frac{1}{Q} - \sqrt{x_{nA}x_{nB}} + \frac{\sqrt{(Qx_{nA}+1)(Qx_{nB}+1)}}{Q} \right\} \tag{73}$$

this give:

$$I = \frac{\pi \varepsilon_1}{b r_e} \left\{ \frac{1}{H} + \sqrt{x_{nA}x_{nB}} - \sqrt{\frac{\sigma}{H} + x_{nA}x_{nB}} \right\} \tag{74}$$

where

$$\sigma = \frac{1}{H} - \frac{\beta}{\alpha} \equiv \frac{1}{H} - \frac{\varepsilon_2^2}{\varepsilon_1^2} \tag{75}$$

To find the rotational-vibrational energy eigenvalues of the effective improved Wei potential by EQR, we substitute Eq. (70) and (74) in Eq. (8) and replacing N by $n + 1$, this results to:

$$\sqrt{y_{nA}y_{nB}} - \sqrt{\frac{\sigma}{H} + y_{nA}y_{nB}} = \frac{N b r_e}{\varepsilon_1} + \frac{\varepsilon_1}{b r_e H^2 \lambda} \equiv \frac{b r_e (n + \lambda)}{\varepsilon_1} \tag{76}$$

Thus, by solving Eq. (41) and (76), the rotational-vibrational energy is given by:

$$E_{n\ell_IWP} = \frac{\hbar^2 \varepsilon_3^2}{2 \mu r_e^2} - \frac{\hbar^2 b^2}{2 \mu} \left\{ \frac{\sigma H \lambda (\lambda - 1)}{2(n + \lambda)} - \frac{n + \lambda}{2} \right\}^2 \tag{77}$$

where $E_{n\ell_IWP}$ designates the rotational-vibrational energy of the improved Wei potential. Upon substituting Eqs. (29), (31) and (58) in (77) and replacing H by $h' e^{br_e}$, this give:

$$E_{n\ell_IWP} = D_e + \frac{(\Lambda^2 - \frac{1}{4}) \hbar^2 c_0}{2 \mu r_e^2} - \frac{\hbar^2 b^2}{2 \mu} \left\{ \frac{\frac{2 \mu r_e^2 D_e}{\hbar^2} (1 - h'^2) e^{2br_e} + (\Lambda^2 - \frac{1}{4}) (c_2 - c_1 h' e^{br_e})}{2n + 1 + \sqrt{1 + \frac{(4 \Lambda^2 - 1) c_2}{b^2 r_e^2 h'^2 e^{2br_e}} + \frac{2 \mu r_e^2 D_e}{b^2 r_e^2 \hbar^2} \left(\frac{1}{h'} - 1 \right)^2}} \right. \\ \left. - \frac{2n + 1 + \sqrt{1 + \frac{(4 \Lambda^2 - 1) c_2}{b^2 r_e^2 h'^2 e^{2br_e}} + \frac{2 \mu r_e^2 D_e}{b^2 r_e^2 \hbar^2} \left(\frac{1}{h'} - 1 \right)^2}}{4} \right\}^2 \tag{78}$$

Evidently, Eq. (78) is only valid for $h' \neq 0$, however, in the event that $h' = 0$, $E_{n\ell_IWP} \rightarrow \infty$ which is not physically acceptable for a finite potential energy function. In order to deduce the rotational-vibrational energy eigenvalues of the

improved Wei potential for the case $h' = 0$, first we observe that by letting $h' = 0$ in Eq. (14), the improved Wei potential reduces to:

$$V_M(r) = D_e \left\{ 1 - e^{-b_M (r-r_e)} \right\}^2 \tag{79}$$

which is the well-known Morse potential (Roy, 2013; Hamzavi *et al.*, 2012), the subscript M in $V_M(r)$ and in b_M designates "Morse". In subsequent notations, whenever the subscript M appears, it represents the Morse counterpart of the subject of discussion. Inputting $h' = 0$ in Eq. (16) gives:

$$b_M = \pi c \omega_e \left(\frac{2\mu}{D_e} \right)^{\frac{1}{2}} \tag{80}$$

Next we will re-evaluate the quantum correction Q_{cM} and the momentum integral I_M and apply the EQR given by Eq. (8), with $h' = 0$ Eq. (61) gives:

$$Q_{cM} = \frac{\varepsilon_1}{br_e} \int_{x_{0A}}^{x_{nB}} \left(x + \frac{\beta}{2\alpha} - \frac{c_M}{m_M} - \frac{\beta c_M}{2\alpha m_M x} \right) \frac{dx}{\sqrt{(x-x_{0A})(x_{0B}-x)}} \tag{81}$$

Eq. (81) can be evaluated by means of the following standard integrals (Ikhdair and Sever, 2009)

$$\int_{x_{nA}}^{x_{nB}} \frac{x dx}{\sqrt{(x-x_{nA})(x_{nB}-x)}} = \frac{1}{2} \pi (x_{nA} + x_{nB}) \tag{82}$$

$$\int_{x_{nA}}^{x_{nB}} \frac{dx}{\sqrt{(x-x_{nA})(x_{nB}-x)}} = \pi \tag{83}$$

$$\int_{x_{nA}}^{x_{nB}} \frac{dx}{x \sqrt{(x-x_{nA})(x_{nB}-x)}} = \frac{\pi}{\sqrt{x_{nA} x_{nB}}} \tag{84}$$

$$\int_{x_{nA}}^{x_{nB}} \frac{\sqrt{(x-x_{nA})(x_{nB}-x)}}{x} dx = \pi \left\{ \frac{1}{2} (x_{nA} + x_{nB}) - \sqrt{x_{nA} x_{nB}} \right\} \tag{85}$$

by applying the integrals given by Eqs. (82)- (84) on Eq. (81), we obtained:

$$Q_{cM} = \frac{\pi \varepsilon_1}{br_e} \left\{ \frac{1}{2} (x_{0A} + x_{0B}) + \frac{\beta}{2\alpha} - \frac{c_M}{m_M} - \frac{\beta c_M}{2\alpha m_M} \frac{1}{\sqrt{x_{0A} x_{0B}}} \right\} \tag{86}$$

using Eqs. (54), (55) and (56) with $h' = 0$ while c and m are replaced with c_M and m_M respectively, get:

$$Q_{cM} = -\frac{\pi}{2} \tag{87}$$

similarly, the momentum integral of Eq. (72) with $h' = 0$ gives:

$$I_M = -\frac{\varepsilon_1}{br_e} \int_{x_{nA}}^{x_{nB}} \frac{\sqrt{(x-x_{nA})(x_{nB}-x)}}{x} dx \tag{88}$$

the standard integral of Eq. (85) applied to Eq. (88) gives,

$$I_M = -\frac{\pi \varepsilon_1}{br_e} \left(\frac{\varepsilon_2^2}{2\varepsilon_1^2} + \sqrt{x_{nA} x_{nB}} \right) \tag{89}$$

with Eq. (89) and (87), the EQR of Eq. (8) gives:

$$E_{n\ell-M} = \frac{\hbar^2 \varepsilon_3^2}{2\mu r_e^2} - \frac{\hbar^2 b^2}{2\mu} \left(n + \frac{1}{2} + \frac{\varepsilon_2^2}{2br_e \varepsilon_1} \right)^2 \tag{90}$$

which upon substituting Eq. (29) and (30) in Eq. (90) gives the rotational-vibrational energies of Morse potential *viz.*

$$E_{n\ell_M} = D_e + \frac{(\Lambda^2 - \frac{1}{4})\hbar^2 c_0}{2\mu r_e^2} - \frac{\hbar^2 b^2}{2\mu} \left\{ n + \frac{1}{2} + \frac{(\Lambda^2 - \frac{1}{4})c_1 - \frac{4\mu r_e^2 D_e e^{br_e}}{\hbar^2}}{2br_e \sqrt{(\Lambda^2 - \frac{1}{4})c_2 + \frac{2\mu r_e^2 D_e e^{2br_e}}{\hbar^2}}} \right\}^2 \tag{91}$$

The radial eigenfunctions of the improved Wei potential

To obtain the radial wave function corresponding to the rotational-vibrational energies of the improved Wei potential, we need to solve the Riccati equation given by Eq. (49), using the definition of the phase angle and the following transformation equation:

$$z = 1 + Hx \tag{92}$$

Eq. (49) transforms to:

$$z(1-z)\psi''_{n\ell}(z) + (1-2z)\psi'_{n\ell}(z) + \left(\varepsilon_4 - \frac{\varepsilon_5}{z} - \frac{\varepsilon_6}{1-z} \right) \psi_{n\ell}(z) = 0 \tag{93}$$

where

$$\varepsilon_4 = \frac{2\mu\alpha}{b^2\hbar^2 H^2} \tag{94}$$

$$\varepsilon_5 = \frac{2\mu}{b^2\hbar^2} \left(\frac{\alpha}{H^2} - \frac{\beta}{H} + D_e - E_{n\ell} \right) \tag{95}$$

$$\varepsilon_6 = \frac{2\mu}{b^2\hbar^2} (D_e - E_{n\ell}) \tag{96}$$

in order to solve Eq. (96) we assume the following ansatz:

$$\psi_{n\ell}(z) = N_{n\ell} z^\tau (1-z)^\nu {}_2F_1(-n, n+2\tau+2\nu+1; 2\tau+1; z) \tag{97}$$

where $N_{n\ell}$ is the normalization constant, τ and ν are constants and ${}_2F_1$ is the hypergeometric function. Inserting Eq. (97) in (93), the resulting equation is Gaussian-hypergeometric if the following constraints are imposed:

$$\tau = \varepsilon_5^{\frac{1}{2}} \tag{98}$$

$$\nu = \varepsilon_6^{\frac{1}{2}} \tag{99}$$

If $h' = 0$, the constants ε_5 and ε_6 becomes infinite, thus, making the wave function infinite which is not physically acceptable for a finite potential energy function. To obtain a physically acceptable wave function corresponding to $h' = 0$, Riccati Eq. (49) give for $h' = 0$:

$$x^2 \psi''_{n\ell}(x) + x\psi'_{n\ell}(x) + (-\varepsilon_7 x^2 + \varepsilon_8 x - \varepsilon_9) \psi_{n\ell}(x) = 0 \tag{100}$$

where

$$\varepsilon_7 = \frac{2\mu\alpha}{b^2\hbar^2} \tag{101}$$

$$\varepsilon_8 = -\frac{2\mu\beta}{b^2\hbar^2} \tag{102}$$

$$\varepsilon_9 = -\frac{2\mu}{b^2\hbar^2} (D_e - E_{n\ell}) \tag{103}$$

where we have used the definition of the phase angle $\varphi_{n\ell}(x)$ to recover the wave function $\psi_{n\ell}(x)$. Following Eyube *et al.* (2019a), Eq. (101) has solution of the form:

$$\psi_{n\ell M}(x) = N_{n\ell M} e^{-\frac{1}{2}\xi x} x^{\frac{1}{2}\zeta} {}_1F_1(-n, \zeta + 1; \xi x) \tag{104}$$

where the constants ζ and ξ are respectively given by:

$$\xi = 2\varepsilon_7^{\frac{1}{2}} \tag{105}$$

$$\zeta = 2\varepsilon_9^{\frac{1}{2}} \tag{106}$$

RESULTS AND DISCUSSION

Table 1 shows model parameters of three diatomic molecules studied in the present work, viz: CO, LiH and H₂. The data for α_e for all the three molecules were adopted from NIST data base. Data for μ, D_e, r_e and ω_e for CO were obtained from Yanar *et al.* (2020) and that of LiH and H₂ were extracted from Ikhdair (2009)

Table 1: model parameters of diatomic molecules in the present study

parameter	molecule		
	LiH	CO	H ₂
μ (amu)	0.8801221	6.85620871	0.50391
D _e (cm ⁻¹)	20287	90670	38266
r _e (Å)	1.5956	1.12832320	0.7416
ω _e (cm ⁻¹)	1405.5	2169.8129	4401.2
α _e (cm ⁻¹)	0.2163911	0.01750513	3.0622

Firstly, using Eqs. (16), (19) and (80), we have computed the values of the parameters h', b and b_M respectively for each of the diatomic molecule as indicated in Table 2. Also shown in Table 1 are the literature values of b_M corresponding to h' = 0. For all the three diatomic molecules, our present result (PR) of b_M is almost indistinguishable from those of Ikhdair (2009) and differ significantly from the values used by Roy (2013) owing to the fact that some of the molecular parameters (μ and D_e) used by Roy (2013) are not in accord with Eq. (15). CO molecule has a relatively smaller h' (0.04) and b ≈ b_M, therefore, the molecular properties of CO can approximately be described by Morse potential (see Figure 1), there is no need for a larger parameter potential such as the improved Wei or improved Tietz potential, LiH almost has the same trend as CO. However, for H₂, the trend is different (see Figure 2)

Table 2: computed values of parameters h', b and b_M and corresponding literature values

molecule	h' ≠ 0		b _M (Å ⁻¹), h' = 0		
	b (Å ⁻¹)	h'	PR	(Ikhdair, 2009)	(Roy, 2013)
CO	2.207914	0.040096	2.300141	2.2994	2.59441
LiH	1.066724	0.053791	1.127367	1.1280	1.7998368
H ₂	1.722896	0.114178	1.944969	1.9426	1.440558

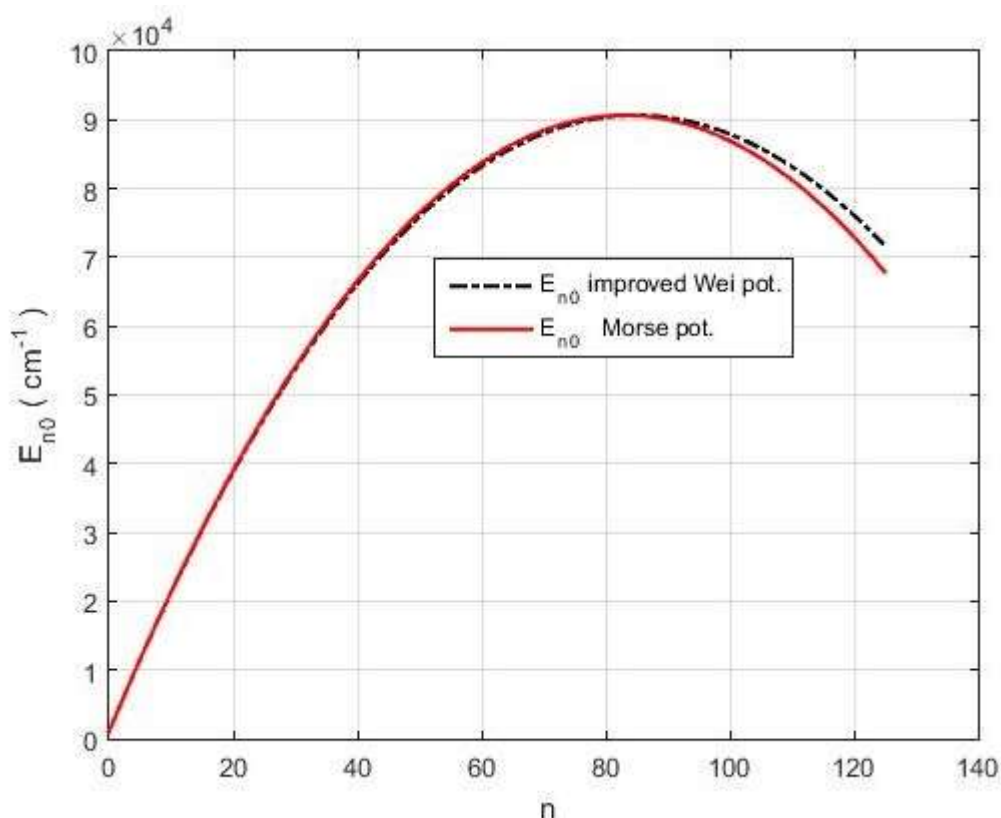


Figure 1 plot of pure vibrational energy of improved Wei potential for h' ≠ 0 and for h' = 0 as a function of n for CO molecule

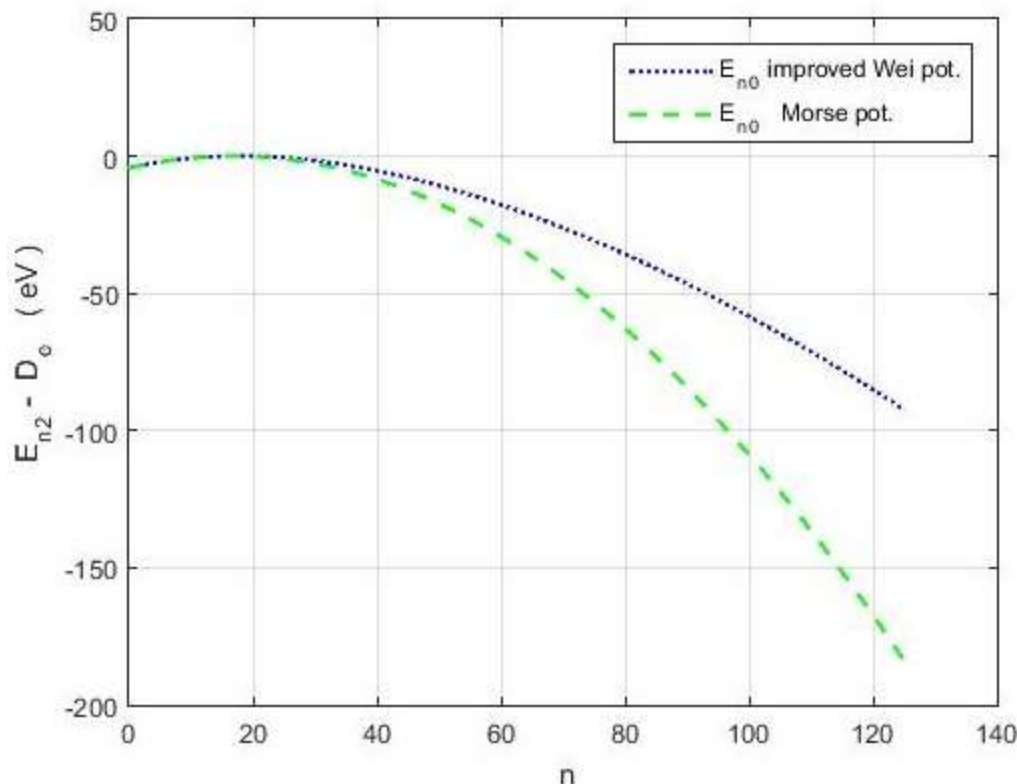


Figure 2 plot of d-state rotational-vibrational energy of improved Wei potential for $h' \neq 0$ and for $h' = 0$ as a function of n for H_2 molecule

In their work, Tang *et al.* (2014) have demonstrated how the improved Tietz potential fits the experimental Rydberg-Klein-Rees (RKR) data for two species of the Na_2 diatomic molecules. Since the improved Wei potential is known to be an equivalent of the of the improved Tietz potential (Jia *et al.*, 2012), it is quite logical to infer that the improved Wei potential can equally fits the RKR data, therefore, using Eqs. (78) and (91), we have computed pure vibrational state energies ($\ell = 0$) of the CO molecule for $h' \neq 0$ represented by E_{n0_IWP} and for $h' = 0$ represented by E_{n0_M} respectively, to enable comparison, we have carried out our computation in three dimensions ($D = 3$), the computed results are shown in Table 3. Also reported in the table are corresponding energies of the CO molecule adopted in the literature for the RKR data herein, represented by E_{RKR} and that computed by Yanar *et al.* (2020) for the improved Tietz potential represented by E_{n0_ITP} . To confirm the accuracy of our result we have calculated the mean absolute percentage deviation deviations (σ_{mean}) defined as (Yanar *et al.*, 2020; Tang *et al.*, 2014):

$$\sigma_{mean} = \frac{100}{N_p} \sum_{n=0}^N \left| \frac{E_{RKR} - E_{n0}}{E_{RKR}} \right| \tag{107}$$

where N_p is the number of experimental data points. Eq. (107) applied to the data of Table 3 give: 0.2862%, 0.2896% and 0.0662% for improved Wei potential, improved Tietz potential and Morse potential respectively, the calculated mean absolute percentage deviations are each less than 1% as required by Lippincott criterion (Tang *et al.*, 2014), these results show that the Morse potential can best fit the RKR CO data followed by improved Wei potential, then the improved Tietz potential, this is further evident from the result of our calculated value of $h' (\approx 0.04)$ which is relatively small, thus reducing the improved Wei potential to Morse potential. To further affirm the validity of our results, we have used Eqs. (78) and (91) to compute bound state energy of H_2 and LiH for arbitrary values of n and ℓ , to enable comparison with literature data, we have computed the differences $E_{n\ell} - D_e$ both for $h' \neq 0$ and $h' = 0$, the results, along with corresponding literature results are presented in Table 4. For both H_2 and LiH , energies for improved Wei potential is in good agreement with those of Morse potential (obtained from Wei potential with $h' = 0$) and with literature results, however, this agreement is more emphasized in LiH which has relatively smaller h' (0.054) than H_2 with relatively larger h' (0.114).

Table 3: pure vibrational energies (in cm^{-1}) of CO molecule of improved Wei (for $h' \neq 0$ and for $h' = 0$) potential, improved Tietz potential and Rydberg-Klein-Rees data

n	E_{RRR}	E_{n0_IWP}	E_{n0_ITP}	E_{n0_M}
0	1081.7791	1081.6494	1081.6555	1081.6547
1	3225.0522	3224.4172	3224.4230	3225.4922
2	5341.8437	5340.1933	5340.1864	5343.3673
3	7432.2200	7429.0182	7428.9867	7435.2799
4	9496.2494	9490.9324	9490.8649	9501.2301
5	11534.0013	11525.9762	11525.8618	11541.2178
6	13545.5470	13534.1898	13534.0180	13555.2431
7	15530.9592	15515.6133	15515.3743	15543.3059
8	17490.3124	17470.2868	17469.9711	17505.4062
9	19423.6825	19398.2502	19397.8488	19441.5441
10	21331.1469	21299.5433	21299.0477	21351.7195
11	23212.7846	23174.2059	23173.6081	23235.9325
12	25068.6758	25022.2776	25021.5700	25094.1830
13	26898.9019	26843.7980	26842.9736	26926.4711
14	28703.5456	28638.8066	28637.8587	28732.7967
15	30482.6901	30407.3427	30406.2651	30513.1598
16	32236.4197	32149.4455	32148.2326	32267.5605
17	33964.8189	33865.1543	33863.8009	33995.9987
18	35667.9725	35554.5081	35553.0094	35698.4745
19	37345.9652	37217.5459	37215.8976	37374.9878
20	38998.8817	38854.3066	38852.5049	39025.5386
21	40626.8057	40464.8291	40462.8704	40650.1270
22	42229.8199	42049.1520	42047.0335	42248.7529
23	43808.0060	43607.3139	43605.0331	43821.4164
24	45361.4437	45139.3534	45136.9082	45368.1174
25	46890.2106	46645.3088	46642.6976	46888.8560
26	48394.3817	48125.2187	48122.4403	48383.6321
27	49874.0291	49579.1211	49576.1747	49852.4458
28	51329.2212	51007.0542	51003.9397	51295.2970
29	52760.0226	52409.0562	52405.7736	52712.1857
30	54166.4932	53785.1650	53781.7148	54103.1120

Table 4: Bound state energy eigenvalues (eV) for H₂ and LiH of the improved Wei potential for h' ≠ 0 represented by E_{nℓ_{IWP}} and for h' = 0 represented by E_{nℓ_M} along with literature values, for arbitrary quantum states

state		H ₂				LiH			
n	ℓ	E _{nℓ_{IWP}} - D _e	E _{nℓ_M} - D _e	Roy (2013)	Ikhdair (2009)	E _{nℓ_{IWP}} - D _e	E _{nℓ_M} - D _e	Roy (2013)	Ikhdair (2009)
0	0	4.47551366	4.47546399	4.47601313	4.47601	2.42889514	2.42889300	2.42886321	2.42886
	1	4.41692266	4.42130175	4.46122852	...	2.42204173	2.42225366	2.42702210	...
	2	4.30109884	4.31416214	4.43179975	...	2.40835920	2.40899771	2.42334244	...
	5	3.64054831	3.70142462	...	4.25880	2.32693340	2.33008763	...	2.40133
0	7	2.98090728	3.08685599	2.23997887	2.24577709
	0	3.48838786	3.47824783	3.47991882	...	2.09941796	2.09848258	2.26054805	...
	1	3.43433615	3.42757966	3.46633875	...	2.09283548	2.09208249	2.25875559	...
	2	3.32742668	3.32732139	3.43932836	...	2.07969341	2.07930391	2.25517324	...
	5	2.71618313	2.75311471	2.00147156	2.00322761
2	7	2.10309849	2.17565220	1.91791494	1.92192947
	0	3.04548267	3.02671113	1.94412680	1.94233203
	1	2.99358880	2.97778999	1.93767791	1.93605155
	2	2.89091795	2.88097239	1.92480234	1.92351165
	5	2.30314419	2.32603114	1.84816046	1.84885224
3	7	1.71226020	1.76712168	1.76627961	1.76906032
	0	2.25750611	2.21778048	...	2.22052	1.65225713	1.64814021	...	1.64771
	1	2.20972534	2.17235341	1.64607183	1.64209897
	2	2.11513579	2.08241714	1.63372209	1.63003645
	5	1.57215718	1.56600675	...	2.04355	1.56019781	1.55821082	...	1.62377
5	7	1.02372251	1.04420339	1.48162401	1.48143131
	0	1.59558520	1.53437350	...	1.53744	1.38509861	1.37809413	...	1.37756
	1	1.55167317	1.49244051	1.37917229	1.37229212
	2	1.46468732	1.40938557	1.36733920	1.36070697
	5	0.96391735	0.93150602	...	1.37658	1.29687836	1.29171512	...	1.35505
7	7	0.45557842	0.44680878	1.22155462	1.21794802

CONCLUSION

In this research work, we have applied the ideas of exact quantization rule and ansatz solution method to obtain closed form expressions for the bound state rotational-vibrational eigenfunctions of the D-dimensional Schrödinger equation for the improved Wei potential, cases of $h' \neq 0$ as well as $h' = 0$ were considered. We have computed rotational-vibrational energies for three diatomic molecules viz: CO, LiH and H₂ and compared our result with existing results in the literature. The results obtained in this work might be useful in areas of molecular physics, chemical physics, atomic physics and solid state physics.

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