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MEASUREMENT OF PHYSICAL OBSERVABLES OF A PARTICLE IN A MORSE POTENTIAL

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Abstract

In this paper we have solved the Schrödinger equation with Morse potential and obtained radial wave functions and energy eigenvalues. We have also obtained normalization constants, expectation values and uncertainty for both position and momentum and an estimate of the speed of the system, considered for four diatomic molecules: H_2, LiH, HCl and CO. Our computed energy eigenvalues are in perfect agreement with those in the literature and the results clearly demonstrates the usefulness of generalized Pekeris approximation in solving the Schrödinger equation for a given potential model.

Keywords: physical observables, Morse potential, Schrödinger equation, Pekeris approximation

1. Introduction

The solutions of wave equations are of paramount importance in quantum mechanics because of the valuable information they reveal about the quantum mechanical system under review [1-4]. Information such as: energy of the system, frequency, wavelength, phase shifts, speed and momentum can be readily obtained once the wave function is known [4]. The solution of wave equation largely depends on the potential energy function used to solve the Schrödinger equation, while some potential energy functions give exact analytical solutions for all quantum states, $n\lambda$[5-6] where n is the principal quantum number and λ is the principal angular momentum quantum number, on the other hand, few potential energy functions give exact analytical solution only for the special case of $\lambda = 0$ (s-wave solutions) [7]. Most of the known potential functions have no exact analytical solutions for all quantum states [8-10], therefore, for such potential models, the only means to obtain analytical solution is to employ approximate solution methods, various methods have been used by researchers to solve the Schrödinger equation, some of these methods include amongst others: power series solution methods [11-12], extended transformation method [13], J-matrix approach [14], asymptotic iteration method [15], factorization method [16-17], Nikiforov-Uvarov method [18-21], generalized pseudospectral method [22-23] and standard method [24-29]. The Morse potential has been regarded as very suitable for describing molecular vibrational spectra of diatomic and polyatomic molecules [30], and has been widely applied in many branches of physics such as molecular physics, solid state physics, chemical and particle physics [22]. The Morse potential is known to have exact solution for the case of s-wave, however, for the general case where $\lambda \neq 0$, only approximate analytical solutions are possible. Roy, [22] used the methods of generalized pseudospectral method to obtain accurate ro-vibrational spectroscopy of diatomic molecules in a Morse oscillator potential. The exact solutions for the vibrational levels of the Morse potential were obtained by Taseli [31] with the system confined in a spherical box of radius λ. Various approximation models have been proposed for the centrifugal term potential of the Schrödinger equation [32-35], however, these models are not only restricted to exponential-type potentials, but are restricted to short range potentials and/or short screening parameters. Recently a generalized Pekeris approximation [24] was proposed in which the centrifugal term potential of the Schrödinger equation was approximated by terms of a Taylor series expansion, this new approximation technique gives excellent result when used to solve the Schrödinger equation for many potential models [28]. In this paper, we will apply the generalized Pekeris approximation to solve the Schrödinger equation with Morse potential and compare results with those in the literature where they exist.

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2. Theoretical Approach

2.1 The Morse potential

The Morse potential can be used to represent the effective interaction in many-electron atoms, also, it has important applications in solid-state, nuclear and plasma physics as well as field theory [22]. The Morse potential [31] is given by:

$$V(r) = D_e\left\{e^{-2d(r-r_e)} - 2e^{-d(r-r_e)}\right\}. \quad (1)$$

where D_e is the potential strength, r is the internuclear separation of the atoms of the molecule, d is a positive constant and r_e is the equilibrium internuclear separation.

2.2 The Radial Schrödinger Equation

The radial Schrödinger equation given in [20] can be expressed as:

$$\frac{d^2R_{n\lambda}}{dr^2} + \frac{2\mu}{\eta^2}\left\{E_{n\lambda} - V(r) - \frac{\lambda(\lambda+1)\eta^2}{2\mu r_e^2}\left(\frac{r_e}{r}\right)^2\right\}R_{n\lambda} = 0. \quad (2)$$

where μ is the mass of the molecule, $E_{n\lambda}$ is the energy eigenvalue, $R_{n\lambda}$ is the radial wave function and n and λ are the principal quantum number and principal angular momentum quantum numbers respectively. If we substitute Eq. (1) into Eq. (2), we obtain:

$$\frac{d^2R_{n\lambda}}{dr^2} + \frac{2\mu}{\eta^2}\left\{E_{n\lambda} - D_e\left[e^{-2d(r-r_e)} - 2e^{-d(r-r_e)}\right] - \frac{\lambda(\lambda+1)\eta^2}{2\mu r_e^2}\left(\frac{r_e}{r}\right)^2\right\}R_{n\lambda} = 0. \quad (3)$$

Let

$$z = e^{-d(r-r_e)}. \quad (4)$$

using Eq. (4), Eq. (3) transforms to:

$$z^2R''_{n\lambda}(z) + zR'_{n\lambda}(z) + \frac{2\mu}{d^2\eta^2}\left\{E_{n\lambda} - D_e\left(z^2 - 2z\right) - \frac{\lambda(\lambda+1)\eta^2}{2\mu r_e^2}\left(\frac{r_e}{r}\right)^2\right\}R_{n\lambda}(z) = 0. \quad (5)$$

Therefore,

$$z^2R''_{n\lambda}(z) + zR'_{n\lambda}(z) + \left\{\frac{2\mu E_{n\lambda}}{d^2\eta^2} - \frac{2\mu D_e}{d^2\eta^2}\left(z^2 - 2z\right) - \frac{\lambda(\lambda+1)}{d^2r_e^2}\left(\frac{r_e}{r}\right)^2\right\}R_{n\lambda}(z) = 0. \quad (6)$$

where prime denotes derivatives with respect to z. The factor $(r_e/r)^2$ occurring in Eq. (6) can be approximated by terms of a Taylor series expansion [24, 28]. In this work we have assumed that:

$$\left(\frac{r_e}{r}\right)^2 \approx c_0 + c_1\left(x - \alpha_{n\lambda}\right) + \tfrac{1}{2}c_2\left(x - \alpha_{n\lambda}\right)^2. \quad (7)$$

where $x(x)$ and its inverse, $x^{-1}(x)$ are appropriately chosen functions and $\alpha_{n\lambda}$, the energy determining parameter is an element in the domain of $x^{-1}(x)$. The coefficients $c_N\left(N = 0,1,2,\mathrm{K}\right)$ are defined by:

$$c_N = \left.\frac{d^N\varphi}{dx^N}\right|_{\varphi=\alpha}. \quad (8)$$

where the function, φ is given by [28]:

$$\varphi(x) \equiv \left(\frac{r_e}{r}\right)^m = \left[1 - \frac{x^{-1}(x)}{dr_e}\right]^{-m}. \quad (9)$$

where $m \in Z^+$ .In the present work we have chosen:

$$x = e^{\alpha_{n\lambda}r_e}z. \quad (10)$$

and

$$x^{-1} = \log_e x. \quad (11)$$

Using Eq. (8) and Eq. (9), and taking $m = 2$, we find:

$$c_0 = \frac{d^2r_e^2}{\left(dr_e - \log_e \alpha_{n\lambda}\right)^2}. \quad (12)$$

$$c_1 = \frac{2\,d^2 r_e^2}{\alpha\left(d\,r_e - \log_e \alpha_{n\lambda}\right)^3}. \tag{13}$$

and

$$c_2 = \frac{2\,d^2 r_e^2\left(3 - d\,r_e + \ln\alpha\right)}{\alpha^2\left(d\,r_e - \log_e \alpha_{n\lambda}\right)^4}. \tag{14}$$

where $\alpha \in [1,\infty)$. Substitute Eq. (7) in Eq. (6) and using Eq. (10) get:

$$z^2 R''_{n\lambda}(z) + z\,R'_{n\lambda}(z) + \left\{ \begin{array}{l} \frac{2\mu E_{n\lambda}}{d^2\eta^2} - \frac{2\mu D_e}{d^2\eta^2}\left(z^2 - 2z\right) + \\ \qquad -\frac{\lambda(\lambda+1)}{d^2 r_e^2}\left[c_0 - \alpha_{n\lambda} c_1 + \tfrac{1}{2}\alpha_{n\lambda}^2 c_2 + \left(c_1 - \alpha_{n\lambda} c_2\right) e^{\alpha_{n\lambda} r_e} z + \tfrac{1}{2} c_2\, e^{2\alpha_{n\lambda} r_e} z^2\right] \end{array} \right\} R_{n\lambda}(z) = 0 \tag{15}$$

By expanding out Eq. (15), we obtained:

$$z^2 R''_{n\lambda}(z) + z\,R'_{n\lambda}(z) + \left[-\varepsilon z^2 + \lambda z - \kappa\right] R_{n\lambda}(z) = 0. \tag{16}$$

where

$$\varepsilon = \frac{2\mu D_e}{d^2\eta^2} + \frac{\lambda(\lambda+1) e^{2\alpha_{n\lambda} r_e}}{2 d^2 r_e^2} c_2. \tag{17}$$

$$\lambda = \frac{4\mu D_e}{d^2\eta^2} - \frac{\lambda(\lambda+1) e^{\alpha_{n\lambda} r_e}}{d^2 r_e^2}\left(c_1 - \alpha\, c_2\right). \tag{18}$$

$$\kappa = -\frac{2\mu E_{n\lambda}}{d^2\eta^2} + \frac{\lambda(\lambda+1)}{2 d^2 r_e^2}\left(c_0 - \alpha_{n\lambda} c_1 + \tfrac{1}{2}\alpha_{n\lambda}^2 c_2\right). \tag{19}$$

To solve Eq. (15), we assume an ansatz [32] of the form:

$$R_{n\lambda}(z) = N_{n\lambda} e^{-\frac{1}{2}a z} z^{\frac{1}{2}b} F_{n\lambda}(z). \tag{20}$$

where $N_{n\lambda}$ is the normalization constant.

From Eq. (20), we find:

$$R'_{n\lambda}(z) = \left[\frac{F'_{n\lambda}(z)}{F_{n\lambda}(z)} - \tfrac{1}{2}a + \tfrac{1}{2}\frac{b}{z}\right] R_{n\lambda}(z). \tag{21}$$

and

$$R''_{n\lambda}(z) = \left[\frac{F''_{n\lambda}(z)}{F_{n\lambda}(z)} + \left(-a + \frac{b}{z}\right)\frac{F'_{n\lambda}(z)}{F_{n\lambda}(z)} + \tfrac{1}{4}a^2 - \frac{\frac{1}{2}a\,b}{z} + \frac{\frac{1}{4}b^2}{z^2} - \frac{\frac{1}{2}b}{z^2}\right] R_{n\lambda}(z). \tag{22}$$

Substituting Eq. (21) and Eq. (22) in Eq. (16) and simplifying, we get:

:

$$z\,F''_{n\lambda}(z) + (b+1-a\,z) F'_{n\lambda}(z) + \left\{\lambda - \tfrac{1}{2}a\,b - \tfrac{1}{2}a + \left(\tfrac{1}{4}a^2 - \varepsilon\right)z + \frac{\frac{1}{4}b^2 - \kappa}{z}\right\} F_{n\lambda}(z) = 0. \tag{23}$$

Eq. (23) reduces to the hypergeometric-type (Laguerre) differential equation if the last-two terms of the coefficient of $F_{n\lambda}(z)$ separately varnish, this is true iff:

$$a = 2\varepsilon^{\frac{1}{2}}. \tag{24}$$

and

$$b = 2\kappa^{\frac{1}{2}}. \tag{25}$$

Therefore, by putting Eq. (24) and Eq. (25) in Eq. (23), the hypergeometric equation is:

$$u\,F''_{n\lambda}(u) + \left(2\kappa^{\frac{1}{2}} + 1 - u\right) F'_{n\lambda}(u) + \left(\frac{\lambda}{2\varepsilon^{\frac{1}{2}}} - \kappa^{\frac{1}{2}} - \tfrac{1}{2}\right) F_{n\lambda}(u) = 0. \tag{26}$$

where

$$u = a\,z \equiv a\,e^{-d\left(r - r_e\right)}. \tag{27}$$

so that:

$$R_{n\lambda}(u) = N_{n\lambda} a^{-\frac{1}{2}b} e^{-\frac{1}{2}u} u^{\frac{1}{2}b} F_{n\lambda}(u). \tag{28}$$

Eq. (26) has solution of the form:

$$F_{n\lambda}(u)={}_1F_1(-n,b+1;u)\cdot \tag{29}$$

where ${}_1F_1(-n,b+1;u)$ is the hypergeometric function

2.3 The Normalization Constant

Normalization of wave functions [4] requires that:

$$\int_0^{\infty}\left|R_{n\lambda}(r)\right|^2 dr=1\cdot \tag{30}$$

Putting Eq. (27) and Eq. (28) in Eq. (30) get:

$$N_{n\lambda}^2 a^{-b}\int_0^{u_0} u^{b-1}e^{-u}\left|F_{n\lambda}(u)\right|^2 du=d\cdot \tag{31}$$

where

$$u_0=a e^{d r_e}. \tag{32}$$

Eq. (31) gives the normalization constant as:

$$N_{n\lambda}=\left\{\frac{d\,a^b}{\int_0^{u_0} u^{b-1}e^{-u}\left|{}_1F_1(-n,b+1;u)\right|^2 du}\right\}^{\frac{1}{2}}\cdot \tag{33}$$

when Eq. (29) is used in Eq. (31).

2.4 Expectation and Uncertainty in Position

2.4.1 Expectation in Position

The expectation values in position [4] is given as:

$$\langle r_{n\lambda}\rangle=\langle R_{n\lambda}(r)|\, r\, R_{n\lambda}(r)\rangle. \tag{34}$$

Thus,

$$\langle r_{n\lambda}\rangle=\int_0^{\infty} r\left|R_{n\lambda}(r)\right|^2 dr\cdot \tag{35}$$

By substituting Eq. (27) and Eq. (28) in Eq. (35), we obtained:

$$\langle r_{n\lambda}\rangle=\frac{N_{n\lambda}^2}{d\,a^b}\int_0^{u_0} u^{b-1}\left\{r_e+\frac{1}{d}\log_e\left(\frac{a}{u}\right)\right\}e^{-u}\left|F_{n\lambda}(u)\right|^2 du\cdot \tag{36}$$

Following Eq. (35), we have:

$$\langle r_{n\lambda}^2\rangle=\int_0^{\infty} r^2\left|R_{n\lambda}(r)\right|^2 dr\cdot \tag{37}$$

Using Eq. (27) and Eq. (28) in Eq. (37), get:

$$\langle r_{n\lambda}^2\rangle=\frac{N_{n\lambda}^2}{d\,a^b}\int_0^{u_0} u^{b-1}\left\{r_e+\frac{1}{d}\log_e\left(\frac{a}{u}\right)\right\}^2 e^{-u}\left|F_{n\lambda}(u)\right|^2 du\cdot \tag{38}$$

2.4.2 Uncertainty in Position

The uncertainty in position [4] is given by:

$$\Delta r_{n\lambda}=\left\{\langle r_{n\lambda}^2\rangle-\langle r_{n\lambda}\rangle^2\right\}^{\frac{1}{2}}\cdot \tag{39}$$

2.5 Expectation and Uncertainty in Momentum

2.5.1 Expectation in momentum

The expectation values in momentum [4] is given as:

$$\langle p_{n\lambda}\rangle=\langle R_{n\lambda}(r)|\,\hat{p}\,R_{n\lambda}(r)\rangle. \tag{40}$$

where

$$\hat{p}_{n\lambda}=-i\eta\frac{d}{dr}\cdot \tag{41}$$

is the momentum operator.
Using Eq. (41) in Eq. (40) and the definition of scalar product [4], we have:

$$\langle p_{n\lambda}\rangle = -i\eta\int_0^{\infty} R_{n\lambda}(r)R'_{n\lambda}(r)dr\cdot \tag{42}$$

If we use Eq. (4) in Eq. (42), get;

$$\langle p_{n\lambda}\rangle = i\eta\int_0^{z_0} R_{n\lambda}(z)R'_{n\lambda}(z)dz\cdot \tag{43}$$

where

$$z_0 = e^{dr_e}. \tag{44}$$

Substituting Eq. (20) and Eq. (21) in Eq. (44) and simplifying, get:

$$\langle p_{n\lambda}\rangle = i\eta N_{n\lambda}^2\int_0^{z_0}\left\{F_{n\lambda}(z)F'_{n\lambda}(z)z^b - \tfrac{1}{2}\left(a-\frac{b}{z}\right)\left|F_{n\lambda}(z)\right|^2\right\}z^b e^{-az}dz\cdot \tag{45}$$

thus, on putting Eq. (27) in Eq. (45),we get:

$$\langle p_{n\lambda}\rangle = \frac{i\eta N_{n\lambda}^2}{a^{b+1}}\int_0^{u_0}\left\{F_{n\lambda}(u)F'_{n\lambda}(u) - \tfrac{1}{2}a\left(1-\frac{b}{u}\right)\left|F_{n\lambda}(u)\right|^2\right\}u^b e^{-u}du\cdot \tag{46}$$

Similarly,

$$\langle p_{n\lambda}^2\rangle = \langle R_{n\lambda}(r)|\,\hat{p}^2 R_{n\lambda}(r)\rangle\cdot \tag{47}$$

where

$$\hat{p}_{n\lambda}^2 = -\eta^2\frac{d^2}{dr^2}\cdot \tag{48}$$

Substituting Eq. (48) in Eq. (47) and following Eq. (42), we find:

$$\langle p_{n\lambda}^2\rangle = -d\eta^2\int_0^{z_0} R_{n\lambda}(z)\left\{zR''_{n\lambda}(z) + R'_{n\lambda}(z)\right\}dz\cdot \tag{49}$$

on using Eq. (21) and Eq. (22),Eq. (49) transforms to:

$$\langle p_{n\lambda}^2\rangle = -d\eta^2\int_0^{z_0}\left\{z\frac{F''_{n\lambda}(z)}{F_{n\lambda}(z)} + (b+1-az)\frac{F'_{n\lambda}(z)}{F_{n\lambda}(z)} + \tfrac{1}{4}a^2z - \tfrac{1}{2}a(b+1) + \tfrac{1}{4}\frac{b^2}{z}\right\}\left|R_{n\lambda}(z)\right|^2 dz\cdot \tag{50}$$

using Eq. (27) and Eq. (28) in Eq. (50) leads to:

$$\langle p_{n\lambda}^2\rangle = -\frac{d\eta^2 N_{n\lambda}^2}{a^{b+2}}\int_0^{u_0}\left\{uF''_{n\lambda}(u)F_{n\lambda}(u) + a(b+1-u)F'_{n\lambda}(u)F_{n\lambda}(u) + \left[\tfrac{1}{4}au - \tfrac{1}{2}a(b+1) + \tfrac{1}{4}\frac{ab^2}{u}\right]\left|F_{n\lambda}(u)\right|^2\right\}du \tag{51}$$

2.5.2 Uncertainty in Momentum

The uncertainty in momentum [4] is given by:

$$\Delta p_{n\lambda} = \left\{\langle p_{n\lambda}^2\rangle - \langle p_{n\lambda}\rangle^2\right\}^{\frac{1}{2}}\cdot \tag{52}$$

2.6 Estimation of the Speed of the System

Starting from the uncertainty principle [4], we have that:

$$\Delta r_{n\lambda}\Delta p_{n\lambda} \geq \eta/2\cdot \tag{53}$$

Therefore,

$$\Delta p_{n\lambda} \geq \frac{\eta}{2\Delta r_{n\lambda}}\cdot \tag{54}$$

In this work, we will assume that p_{nl} is of the order of $\Delta p_{n\lambda}$, that is:

$$\Delta p_{n\lambda} \sim p_{n\lambda}\cdot \tag{55}$$

Putting Eq. (55) in Eq. (54) we have:

$$p_{n\lambda} \geq \frac{\eta}{2\Delta r_{n\lambda}}\cdot \tag{56}$$

The momentum, p of the system [4] is given by:

$$p_{nl} = \mu v_{n\lambda}. \tag{57}$$

where $v_{n\lambda}$ is the speed of the system. Thus, using Eq. (57) in Eq. (56), the minimum speed of the system is given by choosing the equality sign in Eq. (56), namely:

$$v_{n\lambda} = \frac{\eta}{2\mu\Delta r_n}. \tag{58}$$

Eq. (58) will be used to compute the speed of the system

2.7Energy Eigenvalues

The polynomial condition [32] for Eq. (26) is given by:

$$\frac{\lambda}{2\varepsilon^{\frac{1}{2}}} - \kappa^{\frac{1}{2}} - \tfrac{1}{2} = n. \tag{59}$$

Using Eq. (17), Eq. (18) and Eq. (19) in Eq. (59), we find:

$$E_{n\lambda} = -\frac{d^2\eta^2}{2\mu}\left\{ n + \tfrac{1}{2} - \frac{\frac{4\mu D_e}{d^2\eta^2} - \frac{\lambda(\lambda+1)e^{\alpha_{n\lambda}r_e}}{d^2 r_e^2}\left(c_1 - \alpha_{n\lambda}c_2\right)}{2\left[\frac{2\mu D_e}{d^2\eta^2} + \frac{\lambda(\lambda+1)e^{2\alpha_{n\lambda}r_e}}{2d^2 r_e^2}c_2\right]^{\frac{1}{2}}}\right\}^2 + \frac{\lambda(\lambda+1)\eta^2}{4\mu r_e^2}\left(c_0 - \alpha_{n\lambda}c_1 + \tfrac{1}{2}\alpha_{n\lambda}^2 c_2\right). \tag{60}$$

3. Discussion

The data in Table 1 shows the input spectroscopic parameters [22] used in our computations, the analysis was carried out on four diatomic molecules: H_2, LiH, HCl and CO to enable us compare result with those in the literature, the work was carried out on low lying states, $n, \lambda = 0, 1, 2$. First, we considered the special case of s-wave ($\lambda = 0$). Eq. (60) reduces to:

$$E_{n0} = -\frac{d^2\eta^2}{2\mu}\left\{ n + \tfrac{1}{2} - \left(\frac{2\mu D_e}{d^2\eta^2}\right)^{\frac{1}{2}}\right\}^2. \tag{61}$$

It is clear that Eq. (61) is independent of $\alpha_{n\lambda}$ and only vary with n.Tables 2 and 3 shows result of computed energy eigenvalues, for all the diatomic molecules considered, our results agrees perfectly with existing results, except in few isolated cases of s-wave where our result is slightly lower than those obtained in the literature [22]. Also shown in the Tables are normalization constants, expectation values for both position and momentum. We have also obtained estimates for the speeds of the ro-vibrational molecules, the estimated speeds are quite feasible within the contest of non-relativistic cases ,however, for LiH (with relatively large values of $\alpha_{n\lambda}$),the speed and uncertainty inmomentum are not physically feasible for states 10 and 20 and so also for HCl for states 20,21 and 22

Figures 1 and 2 show plots of normalized radial wave functions for each of the four molecules, for the states: 01, 11 and 21. Plots of the variation of $E_{n\lambda}(\alpha_{n\lambda})$ with $\alpha_{n\lambda}$ are shown in Figures 3 and 4 where $E_{n\lambda}(\alpha_{n\lambda})$ is constant and independents of α as indicated in Figures 3(a) and 4(a) (s-wave). However, in Figures 3(b) and 4(b), where $\lambda \neq 0$, $E_{n\lambda}(\alpha_{n\lambda})$ varies slowly with $\alpha_{n\lambda}$ and then rapidly decreases.

4. Conclusion

In this paper we have solved the radial Schrödinger equation with Morse oscillator potential and obtained closed form expressions for normalized radial wave functions, energy eigenvalues, normalization constant, expectation values and uncertainty in position and momentum, we have also applied our results no four diatomic molecules *viz* H_2, LiH, HCl and CO and compared result with those in the literature. This work can be extended to include high lying states, the method used in this work can also be tried on other potential models

Table 1 Input spectroscopic parameters of selected molecules used in the present work

Molecule	$D_e(eV)$ [22]	$r_e(nm)$ [22]	$\mu(amu)$ [22]	$d(nm^{-1})$ [22]
H_2	6	0.07416	0.50391	14.40558
LiH	287	0.15956	0.8801221	17.998368
HCl	107	0.12746	0.9801045	23.8057
CO	256	0.11283	0.8606719	25.9441

Table 2 Energy Determining Parameters, Energy Eigen Values (in eV), Normalization Constants, Expectation and Uncertainty Values and Speeds (in SI Units) for H_2 and LiH

H_2											
$n\lambda$	$\alpha_{n\lambda}$	$-E_{n\lambda}$	$-E_{n\lambda}$ [22]	$N_{n\lambda}$	$\langle r_{n\lambda}\rangle$	$\langle r_{n\lambda}^2\rangle$	$\Delta r_{n\lambda}$	$-i\langle p_{n\lambda}\rangle$	$-\langle p_{n\lambda}^2\rangle$	$\Delta p_{n\lambda}$	$v_{n\lambda}$
00	…	4.544666447615	4.47601312	3.08E+15	7.65E-11	5.95E-21	1.02E-11	-7.32E-41	1.53E-102	7.32E-41	6205
01	1.469635893836	4.461228520000	4.46122852	3.77E+15	7.73E-11	6.08E-21	1.02E-11	6.58E-40	2.58E-102	6.58E-40	6197
02	1.177115787735	4.431799750003	4.43179975	4.04E+15	7.78E-11	6.16E-21	1.02E-11	-9.81E-41	5.86E-102	9.81E-41	6183
10	…	4.157710391100	3.96231534	1.96E+16	8.11E-11	6.90E-21	1.79E-11	3.41E-40	1.42E-97	3.41E-40	3524
11	1.751828886090	3.948116470000	3.94811647	3.17E+16	8.25E-11	7.12E-21	1.79E-11	-6.46E-40	1.08E-97	6.46E-40	3528
12	1.462205451636	3.919864230000	3.91986423	3.34E+16	8.36E-11	7.30E-21	1.80E-11	7.64E-40	6.70E-97	7.64E-40	3509
20	…	3.787969065594	3.47991882	8.11E+16	8.60E-11	7.95E-21	2.34E-11	1.23E-39	9.31E-93	1.23E-39	2690
21	1.859533098177	3.466338750004	3.46633875	1.66E+17	8.76E-11	8.21E-21	2.33E-11	-1.01E-39	2.34E-93	1.01E-39	2703
22	1.587964618394	3.439328390000	3.43932836	1.71E+17	8.91E-11	8.49E-21	2.35E-11	-3.00E-40	3.46E-92	3.00E-40	2682
LiH											
$n\lambda$	$\alpha_{n\lambda}$	$-E_{n\lambda}$	$-E_{n\lambda}$ [22]	$N_{n\lambda}$	$\langle r_{n\lambda}\rangle$	$\langle r_{n\lambda}^2\rangle$	$\Delta r_{n\lambda}$	$-i\langle p_{n\lambda}\rangle$	$-\langle p_{n\lambda}^2\rangle$	$\Delta p_{n\lambda}$	$v_{n\lambda}$
00	…	2.378107059143	2.42886321	1.46E+13	1.62E-10	2.63E-20	8.72E-12	-1.45E-40	7.89E-84	1.45E-40	4139
01	12.394182236109	2.427022100088	2.42702210	1.30E+13	1.52E-10	2.31E-20	7.90E-12	-3.95E-40	5.09E-95	3.95E-40	4565
02	11.250966308041	2.423342440013	2.42334244	1.31E+13	1.52E-10	2.31E-20	7.89E-12	-1.96E-40	3.12E-95	1.96E-40	4572
10	…	2.115286428924	2.26054805	7.94E+13	1.67E-10	2.81E-20	1.61E-11	-1.77E-40	4.82E-77	…	4139
11	12.990527879036	2.258755590364	2.25875559	6.39E+13	1.48E-10	2.21E-20	1.36E-11	2.04E-40	3.73E-98	2.04E-40	2648
12	11.922694819222	2.255173240005	2.25517324	6.49E+13	1.48E-10	2.20E-20	1.36E-11	-3.87E-40	1.83E-98	3.87E-40	2653
20	…	1.867851467365	2.09827611	2.75E+14	1.72E-10	3.01E-20	2.13E-11	3.56E-41	1.91E-70	…	1690
21	13.278900961347	2.096533040004	2.09653304	2.35E+14	1.46E-10	2.15E-20	1.71E-11	5.87E-40	8.95E-100	5.87E-40	2109
22	12.252259084750	2.093049500070	2.09304950	2.40E+14	1.45E-10	2.14E-20	1.71E-11	9.36E-40	3.88E-100	9.36E-40	2114

Table 3 Energy Determining Parameters, Energy Eigen Values (in eV), Normalization Constants, Expectation and Uncertainty Values and Speeds (in SI Units) for HCl and CO

HCl											
$n\lambda$	$\alpha_{n\lambda}$	$-E_{n\lambda}$	$-E_{n\lambda}$ [22]	$N_{n\lambda}$	$\langle r_{n\lambda}\rangle$	$\langle r_{n\lambda}^2\rangle$	$\Delta r_{n\lambda}$	$-i\langle p_{n\lambda}\rangle$	$-\langle p_{n\lambda}^2\rangle$	$\Delta p_{n\lambda}$	$v_{n\lambda}$
00	…	4.385824021659	4.43556394	7.44E+13	1.29E-10	1.67E-20	6.21E-12	2.51E-40	5.65E-88	2.51E-40	5214
01	0.031499185705	4.432977530007	4.43297753	6.75E+13	1.29E-10	1.66E-20	6.20E-12	5.09E-41	2.67E-88	5.09E-41	5227
02	0.065209459848	4.427806300010	4.42780630	6.83E+13	1.29E-10	1.66E-20	6.20E-12	-3.49E-40	2.88E-88	3.49E-40	5226
10	…	3.937459812337	4.07971006	4.24E+14	1.33E-10	1.77E-20	1.16E-11	9.67E-40	6.21E-81	9.64E-40	2792
11	0.016163980075	4.077201439997	4.07720144	3.27E+14	1.31E-10	1.73E-20	1.15E-11	3.54E-40	5.92E-82	3.53E-40	2815
12	0.031801947172	4.072185790001	4.07218579	3.30E+14	1.31E-10	1.73E-20	1.15E-11	-6.65E-40	6.39E-82	6.65E-40	2814
20	…	3.513265932831	3.73873384	1.55E+15	1.36E-10	1.88E-20	1.54E-11	5.97E-40	4.41E-74	…	…
21	0.012001357805	3.736303829992	3.73630383	1.07E+15	1.34E-10	1.81E-20	1.52E-11	-1.69E-39	8.27E-76	…	…
22	0.023355837494	3.731445389996	3.73144539	1.08E+15	1.34E-10	1.81E-20	1.52E-11	7.15E-40	8.95E-76	…	…
CO											
$n\lambda$	$\alpha_{n\lambda}$	$-E_{n\lambda}$	$-E_{n\lambda}$ [22]	$N_{n\lambda}$	$\langle r_{n\lambda}\rangle$	$\langle r_{n\lambda}^2\rangle$	$\Delta r_{n\lambda}$	$-i\langle p_{n\lambda}\rangle$	$-\langle p_{n\lambda}^2\rangle$	$\Delta p_{n\lambda}$	$v_{n\lambda}$
00	…	10.801329183390	11.09153532	6.52E+16	1.14E-10	1.30E-20	4.76E-12	3.14E-39	9.23E-110	3.14E-39	7744
01	0.013211493054	11.091058749995	11.09105875	4.68E+16	1.13E-10	1.28E-20	4.74E-12	-4.78E-40	6.11E-111	4.78E-40	7791
02	0.025482294090	11.090105650005	11.09010565	4.69E+16	1.13E-10	1.28E-20	4.74E-12	-5.64E-40	6.13E-111	5.64E-40	7791
10	…	9.977306050656	10.82582206	4.41E+17	1.16E-10	1.36E-20	9.06E-12	1.19E-39	1.98E-102	1.19E-39	4074
11	0.007050366330	10.825349590096	10.82534959	1.75E+17	1.13E-10	1.29E-20	8.88E-12	1.82E-40	5.30E-106	1.82E-40	4154
12	0.013513592772	10.824404650011	10.82440465	1.76E+17	1.13E-10	1.29E-20	8.88E-12	-8.02E-40	5.33E-106	8.02E-40	4154
20	…	9.185974251903	10.56333028	1.96E+18	1.19E-10	1.42E-20	1.20E-11	-1.19E-40	2.79E-95	1.19E-40	3071
21	0.005335117545	10.562861899813	10.56286190	4.77E+17	1.13E-10	1.30E-20	1.16E-11	-1.69E-39	2.75E-101	1.69E-39	3175
22	0.010199106939	10.561925159903	10.56192516	4.77E+17	1.13E-10	1.30E-20	1.16E-11	4.84E-41	2.77E-101	4.84E-41	3175

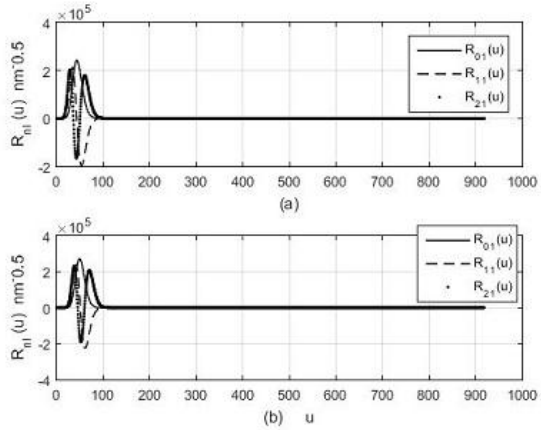

Fig.1 Plot of Radial wave function for (a) H_2 (b) LiH

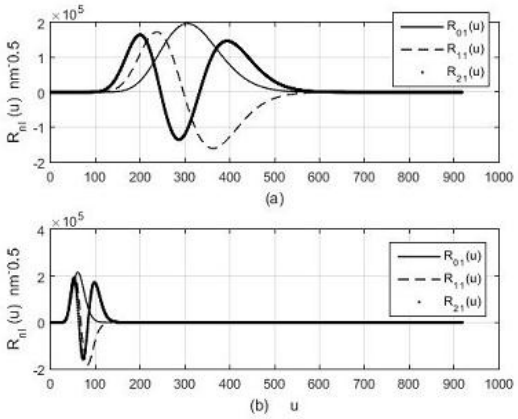

Fig. 2 Plot of Radial Wave Function for (a) HCL (b) CO

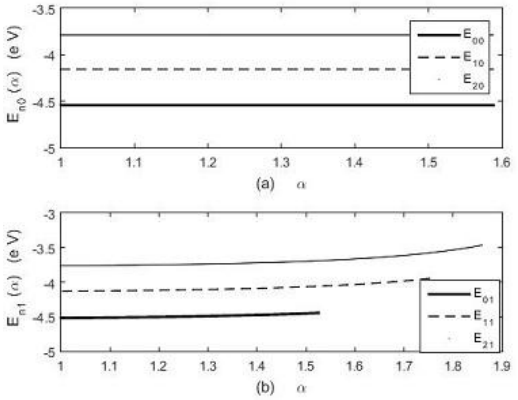

Fig. 3 Energy Eigenvalues of H_2

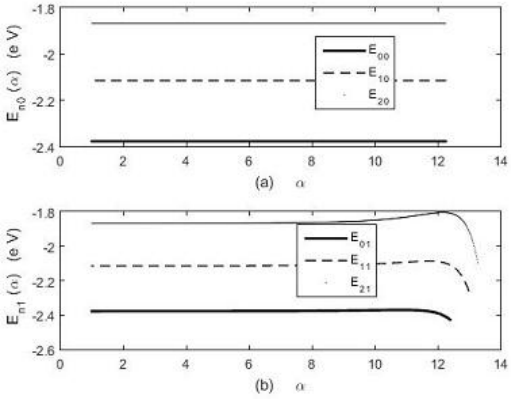

Fig. 4 Energy Eigenvalues of LiH

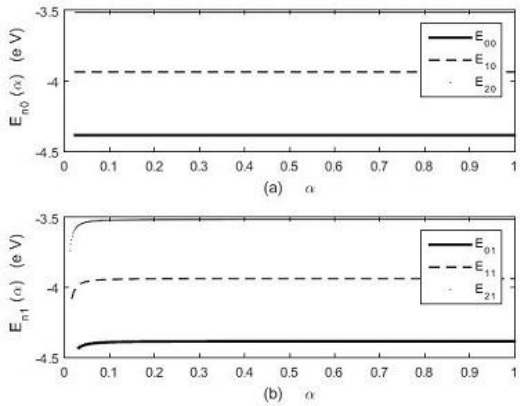

Fig. 5 Energy Eigenvalues of HCl

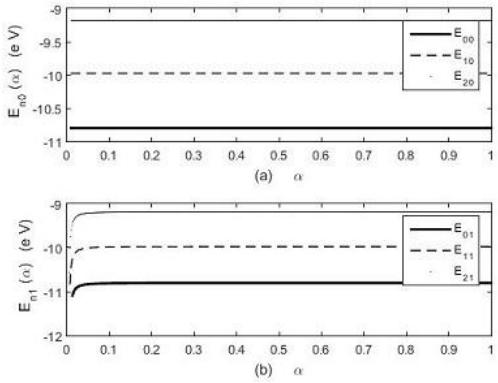

Fig. 6 Energy Eigenvalues of CO

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