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ℓ - WAVE ANALYTICAL SOLUTIONS OF SCHRÖDINGER EQUATION WITH TIETZ-HUA POTENTIAL

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Abstract

In this work we have solved the Schrödinger equation with the molecular Tietz-Hua potential by expanding the centrifugal term potential in Taylor series expansion, we have solved the resulting Gaussian hypergeometric ordinary differential equation by standard method. We have obtained normalization constant, normalized radial wave functions, energy eigenvalues and energy determining parameter for various low-lying quantum states considered for three diatomic molecules: H_2, HF and O_2. The result shows that the energy eigenvalues we obtained for the three diatomic molecule are in near perfect agreement with those in the literature to about six significant figures, the result we obtained also shows greater stability for the ro-vibrational states of the molecules.

1.0 Introduction

The relevance of the solutions of wave equation in the subject area of quantum mechanics cannot be over emphasized due to the information they hoist regarding the quantum mechanical system being investigated [1-3]. The Schrödinger wave equation is used to describe non-relativistic spinless particles, the Klein-Fuck-Gordon, Dirac, Duffin-Kemmer-Petiau equations are used to describe particles of spin zero, spin half and spin one respectively [4]. Exact solutions of the Schrödinger equation are possible only for some selected potentials for all quantum states $|n\ell\rangle$, where n is the principal quantum number and ℓ is the principal angular momentum quantum number [1,2]. And for some potentials, exact solutions are possible for all states with $\ell = 0$ (the s-wave state) [5-10]. Generally, for a majority of potential models, the Schrödinger equation has no exact solution for all quantum states [11-14], therefore, the only means to solving the wave equation is to adopt approximate solution method, which is usually numerical or analytical. Several methods have been used by researchers to solve the Schrödinger equation, some of these methods include, amongst others, the parametric Nikiforov-Uvarov method [15-17], standard method [18-19], supersymmetric quantum mechanics [20], factorization method [20-21], asymptotic iteration method [22], Laplace transform method [1], generalized pseudospectral method [23-24], exact and proper quantization rules [25]. Various potential models have been used to solve the Schrödinger equation; the bound state solutions of Schrödinger equation with modified Mobius square potential and its thermodynamic properties was obtained by [18]. Using parametric Nikiforov-Uvarov method. Also, the bound state solutions of the Schrödinger equation for the Kratzer potential plus screened Coulomb potential [11] was investigated for some selected diatomic molecules using the Nikiforov-Uvarov method. Fröbenius series solution of the Schrödinger equation with various types of symmetric potential in one dimension were obtained by [5]. Various approximation models for the centrifugal term potential have been proposed and used to solve the Schrödinger equation [7, 18], however, most of these models are limited to short screening parameters/short potential range and are limited for use with exponential-type potentials. Recently, researchers have proposed an approximation model termed [17,25] the generalized Pekeris approximation to the centrifugal term, these model gives excellent result when used to solve the Schrödinger equation with Hulthén, Manning-Rosen, Rosen-Morse, Eckart and Pöschl-Teller potentials, the model has not been used to solve the Schrödinger equation with Tietz-Hua potential [17]. It is against this background that we intend to solve the Schrödinger equation with the Tietz-Hua potential via the generalized Pekeris approximation model using standard methods.

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2.0 Theoretical Analysis

2.0.1 Tietz-Hua potential

The Tietz-Hua potential is widely used in various branches of physics such as molecular physics, solid state physics, particle physics and chemical physics, it can conveniently be used to describe molecular interactions and has been considered to be more realistic than the Morse potential for describing molecular vibrations. The Tietz-Hua potential is given by [26]:

$$V(r)=D_e\left[\frac{1-e^{-b_h(r-r_e)}}{1-c_h\,e^{-b_h(r-r_e)}}\right]^2. \tag{1}$$

where D_e is the depth of the potential well, r is the internuclear separation, r_e is the equilibrium internuclear separation and $b_h=\beta(1-c_h)$, with β as the Morse constant, and c_h, the chemical constant.

2.0.2 Solution of Schrödinger Equation with Tietz-Hua Potential

The radial Schrödinger equation given in [4] can be expressed as:

$$\frac{d^2R_{n\ell}}{dr^2}+\frac{2\mu}{\hbar^2}\left[E_{n\ell}-V(r)-\frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}\left(\frac{r_e}{r}\right)^2\right]R_{n\ell}=0. \tag{2}$$

Using Eq. (1) in Eq. (2), we get:

$$\frac{d^2R_{n\ell}}{dr^2}+\frac{2\mu}{\hbar^2}\left\{E_{n\ell}-D_e\left[\frac{1-e^{-b_h(r-r_e)}}{1-c_h\,e^{-b_h(r-r_e)}}\right]^2-\frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}\left(\frac{r_e}{r}\right)^2\right\}R_{n\ell}=0. \tag{3}$$

Letting

$$z=b_h(r-r_e). \tag{4}$$

Eq. (3) becomes:

$$\frac{d^2R_{n\ell}}{dz^2}+\frac{2\mu}{b_h^2\hbar^2}\left[E_{n\ell}-D_e\left(\frac{1-e^{-z}}{1-c_h\,e^{-z}}\right)^2-\frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}\left(\frac{r_e}{r}\right)^2\right]R_{n\ell}=0. \tag{5}$$

Eq. (5) can also be written as:

$$\frac{d^2R_{n\ell}}{dz^2}+\frac{2\mu}{b_h^2\hbar^2}\left\{E_{n\ell}-D_e\left[1+2\sigma\frac{c_h\,e^{-z}}{1-c_h\,e^{-z}}+\sigma^2\left(\frac{c_h\,e^{-z}}{1-c_h\,e^{-z}}\right)^2\right]-\frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}\left(\frac{r_e}{r}\right)^2\right\}R_{n\ell}=0. \tag{6}$$

where

$$\sigma=1-\frac{1}{c_h}. \tag{7}$$

Eq. (6) can be solved analytically only by approximation method. The s-wave solution of this equation [14] was obtained using parametric Nikiforov-Uvarov method. The radial Schrödinger equation with the Tietz-Hua potential was solved by means of generalized pseudospectral method [23].In this communication, we will solve the Schrödinger equation with the Tietz-Hua potential, our procedure involves representing the centrifugal term in Eq. (6) by terms of a Taylor series expansion as proposed by [17,25], and using suitable ansatz, transform the resulting equation to a hypergeometric-type differential equation whose solution can be written in terms of a standard hypergeometric function. Following [17], we express $(r_e/r)^2$ that appears in Eq. (6)as:

$$\left(\frac{r_e}{r}\right)^2\approx c_0+c_1(y-\alpha)+\tfrac{1}{2}c_2(y-\alpha)^2. \tag{8}$$

where y and its inverse, $y^{=1}$ are appropriately chosen functions, and α is an element in the domain of $y^{=1}$. The coefficients, $c_j\,(j=0,1,2,\ldots)$ are given by:

$$c_j=\left.\frac{d^jF}{dy^j}\right|_{y=\alpha}. \tag{9}$$

with the function F given by [17]:

$$F(y)\equiv\left(\frac{r_e}{r}\right)^m=\left(1+\frac{2y^{-1}}{b_h\,r_e}\right)^{-m}. \tag{10}$$

In this work, we choose for y, the c_h-deformed hyperbolic function [3] given by:

$$y = \coth_{c_h} \tfrac{1}{2} b_h (r - r_e). \tag{11}$$

Thus,

$$y = \frac{1 + c_h e^{-z}}{1 - c_h e^{-z}} \equiv 1 + 2\frac{c_h e^{-z}}{1 - c_h e^{-z}} \cdot \tag{12}$$

and

$$y^{-1} = \coth_{c_h}^{-1} y \,. \tag{13}$$

Using Eq. (13), Eq. (10) and Eq. (9), and taking $m = 2$, we find:

$$c_0 = \frac{b_h^2 r_e^2}{\left(b_h r_e + 2\coth_{c_h}^{-1} \alpha\right)^2} \cdot \tag{14}$$

$$c_1 = -\frac{4 b_h^2 r_e^2}{\left(b_h r_e + 2\coth_{c_h}^{-1} \alpha\right)^3 \left(1 - \alpha^2\right)} \cdot \tag{15}$$

and

$$c_2 = \frac{8 b_h^2 r_e^2 \left(3 - \alpha b_h r_e - 2\alpha \coth_{c_h}^{-1} \alpha\right)}{\left(b_h r_e + 2\coth_{c_h}^{-1} \alpha\right)^4 \left(1 - \alpha^2\right)^2} \cdot \tag{16}$$

where $\alpha \in (-\infty, -1) \cup (1, \infty)$ if $c_h > 0$ and $\alpha \in (-1, 1)$ if $c_h < 0$. Substituting Eq. (12) in Eq. (8), one gets:

$$\left(\frac{r_e}{r}\right)^2 \approx c_0 + c_1 - \alpha c_1 + \tfrac{1}{2} c_2 - \alpha c_2 + \tfrac{1}{2}\alpha^2 c_2 + \left(2c_1 + 2c_2 - 2\alpha c_2\right)\frac{c_h e^{-z}}{1 - c_h e^{-z}} + 2c_2\left(\frac{c_h e^{-z}}{1 - c_h e^{-z}}\right)^2 \cdot \tag{17}$$

Putting Eq. (17) in Eq. (6), we find:

$$\frac{d^2 R_{n\ell}}{d z^2} + \left[-\varsigma\left(\frac{c_h e^{-z}}{1 - c_h e^{-z}}\right)^2 - \xi\frac{c_h e^{-z}}{1 - c_h e^{-z}} - \zeta\right] R_{n\ell} = 0 \cdot \tag{18}$$

where

$$\varsigma = \frac{2\mu\sigma^2 D_e}{b_h^2 \hbar^2} + \frac{2\ell(\ell+1)}{b_h^2 r_e^2} c_2 \cdot \tag{19}$$

$$\xi = \frac{4\mu\sigma D_e}{b_h^2 \hbar^2} + \frac{\ell(\ell+1)}{b_h^2 r_e^2}\left(2c_1 + 2c_2 - 2\alpha c_2\right) \cdot \tag{20}$$

$$\zeta = \frac{2\mu}{b_h^2 \hbar^2}\left(D_e - E_{n\ell}\right) + \frac{\ell(\ell+1)}{b_h^2 r_e^2}\left(c_0 + c_1 - \alpha c_1 + \tfrac{1}{2} c_2 - \alpha c_2 + \tfrac{1}{2}\alpha^2 c_2\right) \cdot \tag{21}$$

Letting

$$u = c_h e^{-z} \,. \tag{22}$$

Eq. (18) gives;

$$u^2 \frac{R''_{n\ell}(u)}{R_{n\ell}(u)} + u\frac{R'_{n\ell}(u)}{R_{n\ell}(u)} - \varsigma\frac{u^2}{(1-u)^2} - \xi\frac{u}{1-u} - \zeta = 0 \cdot \tag{23}$$

where prime denote derivative. Now, let us analyze the asymptotic behavior of Eq. (18). When $z \to 0$, Eq. (22) gives $u \to c_h$ and when $z \to \infty$, $u \to 0$, thus, we assume solution for Eq. (23) of the form:

$$R_{n\ell}(u) = N_{n\ell} u^{\delta} (1-u)^{\nu+1} F_{n\ell}(u) \,. \tag{24}$$

where $N_{n\ell}$ are the normalization constants to be determined from normalization condition, δ and ν are constants to be determined when Eq. (24) is satisfied by Eq. (23). Eq. (24) gives:

$$\frac{R'_{n\ell}(u)}{R_{n\ell}(u)} = \frac{F'_{n\ell}(u)}{F_{n\ell}(u)} + \frac{\delta}{u} + \frac{\nu+1}{1-u} \cdot \tag{25}$$

and

$$\frac{R'_{n\ell}(u)}{R_{n\ell}(u)}=\frac{F''_{n\ell}(u)}{F_{n\ell}(u)}+\left(\frac{2\delta}{u}-\frac{2\nu+2}{1-u}\right)\frac{F'_{n\ell}(u)}{F_{n\ell}(u)}-\frac{2\delta(\nu+1)}{u(1-u)}+\frac{\nu(\nu+1)}{(1-u)^2}+\frac{\delta^2-\delta}{u^2}. \quad (26)$$

Using Eq. (25) and Eq. (26) in Eq. (23) and simplifying, we obtained:

$$u(1-u)F''_{n\ell}(u)+\{2\delta+1-(2\delta+2\nu+3)u\}F'_{n\ell}(u) -\left\{(2\delta+1)(\nu+1)+\xi-\frac{\nu(\nu+1)-\varsigma}{1-u}u-\frac{(\delta^2-\zeta)(1-u)}{u}\right\}F_{n\ell}(u). \quad (27)$$

Eq. (27) is of the hypergeometric-type differential equation if the last-two terms of the coefficient of $F_{n\ell}(u)$ separately varnish, this is true iff:

$$\nu(\nu+1)=\varsigma. \quad (28)$$

and also.

$$\delta^2=\zeta. \quad (29)$$

Eq. (28) gives:

$$\nu=-\tfrac{1}{2}+\left(\frac{2\mu\sigma^2 D_e}{b_h^2\hbar^2}+\frac{2\ell(\ell+1)}{b_h^2 r_e^2}c_2+\tfrac{1}{4}\right)^{\frac{1}{2}}. \quad (30)$$

Putting Eq. (28) and Eq. (29) in Eq. (27), we obtain the Gaussian hypergeometric-type differential equation:

$$u(1-u)F''_{n\ell}(u)+\{2\delta+1-(2\delta+2\nu+3)u\}F'_{n\ell}(u)-\{(2\delta+1)(\nu+1)+\xi\}F_{n\ell}(u). \quad (31)$$

whose solution is the hypergeometric function given by:

$$F_{n\ell}(u)={}_2F_1(a,b;c;u). \quad (32)$$

where

$$a=\delta+\nu+1-\sqrt{\delta^2+\nu^2+\nu-\xi}. \quad (33)$$

$$b=\delta+\nu+1+\sqrt{\delta^2+\nu^2+\nu-\xi}. \quad (34)$$

$$c=2\delta+1. \quad (35)$$

Considering the finiteness of the solution, the quantum condition requires either a or b to be an integer, therefore, we can have:

$$\delta+\nu+1-\sqrt{\delta^2+\nu^2+\nu-\xi}=-n. \quad (36)$$

where $n=0,1,2,\ldots,$

Using Eq. (32), the polynomial solution of the Gaussian hypergeometric-type differential equation given by Eq. (31) is:

$$F_{n\ell}(u)={}_2F_1(-n,\ n+2\delta+2\nu+2;\ 2\delta+1;\ u). \quad (37)$$

2.0.2.1 Normalization Constant

The normalization requirement for the radial wave function is given as:

$$\int_0^{\infty}\left|R_{n\ell}(r)\right|^2 dr=1. \quad (38)$$

Using Eq. (4) and Eq. (22), Eq. (38) can be expressed in terms of variable u as:

$$\int_0^{u_0}u^{-1}\left|R_{n\ell}(u)\right|^2 du=b_h. \quad (39)$$

where

$$u_0=c_h e^{b_h r_e}. \quad (40)$$

Substitute Eq. (24) in Eq. (39) to obtain:

$$N_{n\ell}^2\int_0^{u_0}u^{2\delta-1}(1-u)^{2\nu+2}\left|F_{n\ell}(u)\right|^2 du=b_h. \quad (41)$$

From Eq. (41) we obtain the normalization constants as:

$$N_{n\ell}=\left\{\frac{b_h}{\int_0^{u_0}u^{2\delta-1}(1-u)^{2\nu+2}\left|{}_2F_1(-n,\,n+2\delta+2\nu+2;\,2\delta+1;\,u)\right|^2du}\right\}^{\frac{1}{2}}. \tag{42}$$

when Eq. (37) is used in Eq. (41).

2.0.2.2Energy Eigenvalues

From Eq. (28), Eq. (29)and Eq. (36), we find:

$$\zeta=\tfrac{1}{4}\left(n+1+\nu+\frac{\xi-\varsigma}{n+1+\nu}\right)^2. \tag{43}$$

The energy eigenvalue $E_{n\ell}$ can be found by substituting Eq. (19), Eq. (20), Eq. (21) and Eq. (30) in Eq. (43), this gives:

$$E_{n\ell}=D_e-\frac{b_h^2\hbar^2}{8\mu}\left\{n+\tfrac{1}{2}+\left(\frac{2\mu\sigma^2D_e}{b_h^2\hbar^2}+\frac{2\ell(\ell+1)}{b_h^2r_e^2}c_2+\tfrac{1}{4}\right)^{\frac{1}{2}}+\frac{\frac{2\mu\sigma D_e}{b_h^2\hbar^2}(2-\sigma)+\frac{\ell(\ell+1)}{b_h^2r_e^2}(2c_1-2\alpha c_2)}{n+\tfrac{1}{2}+\left(\frac{2\mu\sigma^2D_e}{b_h^2\hbar^2}+\frac{2\ell(\ell+1)}{b_h^2r_e^2}c_2+\tfrac{1}{4}\right)^{\frac{1}{2}}}\right\}^2 \tag{44}$$

$$+\frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}\left\{c_0+(1-\alpha)c_1+\tfrac{1}{2}(1-\alpha)^2c_2\right\}$$

2.1 Input spectroscopic parameters

Table 1 shows the spectroscopic parameters, taken from [23], used in our numerical computation

Table 1 shows the spectroscopic parameters [23] of the molecules used in our computations

Molecule	c_h	$\mu/10^{-23}(g)$	$b_h(nm)^{-1}$	$r_e(nm)$	$\beta(nm)^{-1}$	$D_e(cm)^{-1}$
H_2	0.170066	0.084	16.1890	0.0741	19.506	38318
HF	0.127772	0.160	19.4207	0.0917	22.266	49382
O_2	0.027262	1.377	25.9103	0.1207	26.636	42041

3.0 Discussion

We consider the special case of s-wave ($\ell=0$), Eq. (44) reduces to:

$$E_{n0}=D_e-\frac{b_h^2\hbar^2}{8\mu}\left\{n+\tfrac{1}{2}+\left(\frac{2\mu\sigma^2D_e}{b_h^2\hbar^2}+\tfrac{1}{4}\right)^{\frac{1}{2}}+\frac{\frac{2\mu\sigma D_e}{b_h^2\hbar^2}(2-\sigma)}{n+\tfrac{1}{2}+\left(\frac{2\mu\sigma^2D_e}{b_h^2\hbar^2}+\tfrac{1}{4}\right)^{\frac{1}{2}}}\right\}^2 \tag{45}$$

It is clear that Eq. (45) is independent of $c_j\,(j=0,1,2,\ldots)$ and therefore, independent of energy determining parameter, α. Shown in Table 2 are computed energy eigenvalues (relative to the well depth, $-(E_{n\ell}-D_e)$) and corresponding normalization constants for some low lying quantum states $n\ell$, we have also computed the energy determining parameter, α for quantum states with $\ell\neq0$, the analysis was carried out for three diatomic molecules: H_2, HF and O_2. For the diatomic molecules considered, our results for the energy eigenvalues are in near perfect agreement (to about 6 significant figures) with those of [23] and shows better stabilization for the molecules. Figures 1, 2 and 3 shows plots of normalized wave functions for states 2s, 3s and 5s for H_2, HF and O_2 respectively.

4.0 Conclusion

We have obtained the ℓ - wave analytical solutions of Schrödinger equation with Tietz-Hua potential using standard methods, we have also obtained normalization constant, energy eigenvalues, energy determining parameters and normalized radial wave functions, special case of s-wave was also derived from the result.

Table 2. Energy Determining Parameter (α), Normalization Constant ($N_{n\ell}$) and Energy Eigenvalues of H_2, HF and O_2

$n\ell$		H_2				HF				O_2			
		α	$N_{n\ell}(nm)^{-\frac{1}{2}}$	$-(E_{n\ell}-D_e)eV$ present	$-(E_{n\ell}-D_e)eV$ [23]	α	$N_{n\ell}(nm)^{-\frac{1}{2}}$	$-(E_{n\ell}-D_e)eV$ present	$-(E_{n\ell}-D_e)eV$ [23]	α	$N_{n\ell}(nm)^{-\frac{1}{2}}$	$-(E_{n\ell}-D_e)eV$ present	$-(E_{n\ell}-D_e)eV$ [23]
00			…	6.167E+24	4.4815764961	4.4815797825	…	8.656E+35	5.8687261066	5.8687195228	…	6.657E+110	5.1163227377	5.1163223113
30			…	8.300E+23	3.0595150931	3.0595425362	…	9.685E+34	4.4737838016	4.4737571516	…	4.092E+108	4.5590651926	4.5590745476
50			…	5.176E+22	2.2815541870	2.2815913849	…	8.656E+35	3.6602104422	3.6601740988	…	4.725E+106	4.2058534805	4.2058686976
01			1.292209	6.351E+24	4.4669143761	4.4669801579	-1.186954	6.251E+33	5.8635834521	5.8636625262	-5.26	6.297E+110	5.1159779903	5.1159784440
31			1.296307	8.390E+23	3.0474364161	3.0474413866	-1.142993	7.534E+35	4.4693389177	4.4692935886	-6.18	3.879E+108	4.5587425353	4.5587436240
51			1.298356	5.164E+22	2.2710826188	2.2710928924	-1.130063	7.743E+34	3.6585698346	3.6560952745	-6.60	4.484E+106	4.2055461301	4.2055464879
02			1.293029	6.729E+24	4.4379462892	4.4379154622	-1.186954	4.760E+33	5.8534805541	5.8535547327	-5.26	5.635E+110	5.1152907824	5.1152907228
32			1.297537	8.558E+23	3.0233297498	3.0233638406	-1.142993	4.491E+34	4.4608354737	4.4603723647	-6.22	3.488E+108	4.5580768039	4.5580817907
52	1.299586	5.132E+22	2.2501750838	2.2502130058	-1.130063	2.754E+33	3.6557991066	3.6479433575	-6.64	4.039E+106		4.2049069057	4.2049020823	

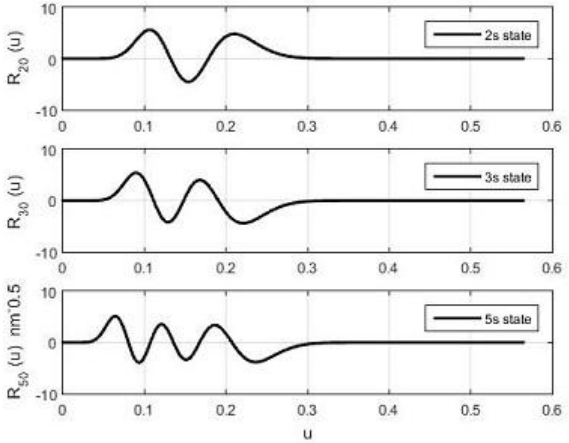
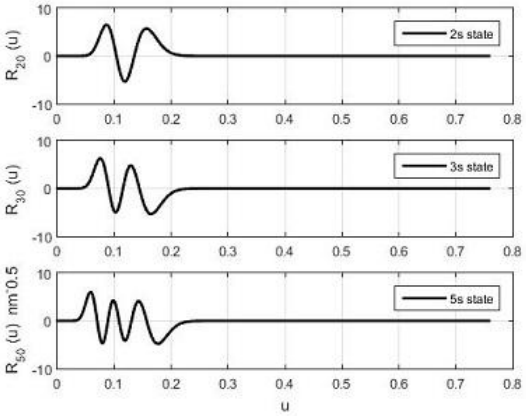


Fig. 1 Normalized Wave Functions for H_2



2 Normalized Wave Functions for HF

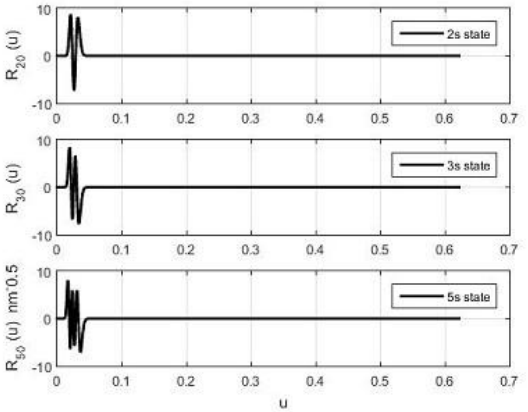


Fig. 3 Normalized Wave Functions for O_2

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