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Approximate analytical solutions of Schrodinger equation for the Tiet-Hua potential

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***Abstract**: in this article we have employed the techniques of proper quantization rule and ansatz solution method to obtain closed form expressions for the rotational-vibrational eigensolutions of the Schrödinger equation for the Tiet-Hua potential. In dealing with the spin-orbit coupling potential of the effective potential energy function, we have employed the improved Pekeris type approximation scheme. Expressions for the bound states energy eigenvalues and normalized radial wave-functions were obtained in compact form. In addition, we have used our equations to compute bound state energy eigenvalues for some diatomic molecules viz : H_2 and O_2 most of the states are reported for the first state with exact outcome.*

***Keywords**: Tiet-Hua potential, proper quantization rule, ansatz solution, Schrodinger equations, Pekeris-type approximation.*

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I. Introduction

Extensive studies reveal 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, momentum, wavelength and speed are readily obtainable if the wave function of the system is known (Yabwa *et al*., 2020). Obtaining the wave function of a quantum mechanical system requires solving the Schrödinger equation for a given potential energy function (Yabwa *et al*., 2020). Exact solution of the Schrödinger equation is restricted to only few potential models such as the Coulombic potential and harmonic oscillator potential (Hitler *et al*., 2017; Tsaur and Wang, 2014) for all quantum states $n\ell$ where n is the principal quantum number and ℓ is the angular momentum 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. Researchers have developed and used various solution methods to solve the Schrödinger equation, amongst some of the methods include: ansatz method (Taskin and Kocal, 2010), Nikiforov-Uvarov method (Ikot *et al*., 2014; Yazarloo *et al*., 2012), factorization method (Pahlavani *et al*., 2013), asymptotic iteration method (Awoga and Ikot 2012), Fröbenius series solution method (Nyengeri *et al.,* 2018), proper quantization rule (Louis *et al*., 2019; Dong and Cruz-Irrison, 2012), path integral approach (Khodja *et al*., 2019) and exact quantization rule (Falaye *et al*., 2015; Ikhdair and Sever, 2009; Ma and Xu, 2005).

II. Theoretical Analysis

2.0.1 Tietz-Hua potential

In the present work, we have studied the Tit-Hua potential (Hamzavi *et al* 2012) (THP) given as:

$$V(r)=D_e\left(\frac{1-e^{-b\,h(r-r_e)}}{1-c_h e^{-b\,h(r-r_e)}}\right)^2 \tag{1}$$

where D_e is the dissociation energy r_e is the equilibrium bond length, r is the inter- nuclear separation, $b_h=\beta(1-c_h)$ and β the Morse constant while c_h is an optimization parameter obtained from *ab initio* or Rydber-Klein-Rees intramolecular potentials respectively.

The Tietz Hua potential is one of the very best analytical model potentials for the vibrational energy of diatomic molecules (Hamzavi, *et al* 2012) it has an exceptional fit within a broad range of internuclear distance with the RKR thus it is being regarded as more realistic than the molecular Morse oscillator (Tang *et al* 2014). Kunc and Gordillo-Vazquez (1997) derived analytical expression forms for the rotational-vibrational energy levels for the diatomic molecules of the Tietz-Hua rotating oscillator employing the Hamilton-Jacoby theory and Bohr-Somerfield quantization rule. Hamzavi *et al* (2012) employed the parametric Nikiforov-Uvarov method to obtain bound states solution of the Schrödinger equation with Tietz Hua potential and applied the results on some diatomic molecules. In another event, Amal Roy (2014) obtained the bound states solution of the Schrödinger equation with Tietz Hua potential using the generalized pseudo spectral method (GPS) and applied the results on six diatomic molecules.

From various literature studied on the solution methods on the Schrodinger equation the proper quantization rule has proved to be effective in giving near perfect results close to the numerical solutions when applied on other potentials (Hitler *et al* 2019 and Dong and Cruz-Irrison 2012)

In the present work, our main focus is to apply the proper quantization rule on the Tiet-Hua potential which to the best of our knowledge has not been used.

2.0.2 Overview of the proper quantization rule

A summary of the basic concepts of the PQR is given here as opposed to the complete details given in the literatures (Serrano *et al* 2010, Ma. Z.Q and Xu. B.W 2005). The PQR stems from the need to eliminate the complicated integrals encountered when using the exact quantization rule to obtain ro-vibrational energies. The EQR was initially proposed (Ma and Xu.2005) to solve the one-dimensional Schrödinger equation given by:

$$\frac{d^2\psi(x)}{dx^2}+k^2(x)\psi(x)=0 \tag{2}$$

where $\psi(x)$ is the radial wave function, $k(x)$ is the momentum of the system, it is defined as:

$$k(x)=\sqrt{\frac{2\mu}{\hbar^2}\{E-V_{eff}(x)\}} \tag{3}$$

in which μ is the reduced mass, E is the energy eigenvalue and $V_{eff}(x)$ is the effective potential energy of the system. It is usual to express Eq. (2) as a nonlinear Riccati equation (Serrano *et al* 2010) this takes the form:

$$\varphi'(x)+\varphi^2(x)+k^2(x)=0 \tag{4}$$

where prime denotes derivative with respect to the argument, x, the logarithmic derivative $\varphi(x)=\psi'(x)/\psi(x)$ of the wave function $\psi(x)$ is known as the phase angle. Yang explained that for the Sturm-Liouville problem (Serrano *et al* 2010) the phase angle must be monotonic with respect to the energy. From Eq. (4), $\varphi(x)$ decreases monotonically with respect to x between two turning points where $E\geq V_{eff}(x)$ specifically, as x increases across a node of the wave function $\psi(x)$, $\varphi(x)$ decreases to $-\infty$, jumps to $+\infty$, and then decreases again. After a careful study of the Schrödinger equation, the EQR was proposed (Ma and Xu.2005) as:

$$\int_{x_A}^{x_B}k(x)dx=N\pi+\int_{x_A}^{x_B}k'(x)\frac{\varphi(x)}{\varphi'(x)}dx \tag{5}$$

where x_A and x_B are two turning points determined by the equation $V_{eff}(x) = E$, $N = v + 1$ is the number of nodes of $\varphi(x)$ in the region $E \geq V_{eff}(x)$ and is larger by 1 than the number v of the nodes of the wave function $\psi(x)$ (Serrano *et al* 2010). The term $N\pi$ in Eq. (5) is the contribution from the nodes of the phase angle while the second term is the quantum correction and has the important property that it is independent of v for all exactly solvable quantum systems(Serrano *et al* 2010, Ma. Z.Q and Xu. B.W 2005), accordingly, it can be evaluated at the ground state ($n = 0$). For a spherically symmetric potential, Eqs. (2), (3) and (4) assume the following forms Falaye *et al* 2015):

$$H\psi_{vJ}(r) = E_{vJ}\psi_{vJ}(r) \tag{6}$$

$$k_{vJ}(r) = \sqrt{\frac{2\mu}{\hbar^2}\left\{E_{vJ} - V_{eff}(r)\right\}} \tag{7}$$

$$\varphi'_{vJ}(r) + k^2_{vJ}(r) + \varphi^2_{vJ}(r) = 0 \tag{8}$$

where

$$H = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{eff}(r) \tag{9}$$

$$V_{eff}(r) = V(r) + \frac{L\hbar^2}{2\mu r^2} \tag{10}$$

The EQR given by Eq. (5) can be expressed in spherical coordinates as:

$$I_{vJ} = N\pi + Q_c \tag{11}$$

where

$$I_{vJ} = \int_{r_{vA}}^{r_{vB}} k_{vJ}(r)\,dr \tag{12}$$

is the momentum integral and the quantum correctional term is:

$$Q_c = \int_{r_{vA}}^{r_{vB}} k'_{vJ}(r)\frac{\varphi_{vJ}(r)}{\varphi'_{vJ}(r)}\,dr \tag{13}$$

Letting $v = 0$ in Eq. (11) and eliminating Q_c between the resulting equation and Eq. (11), we have the expression for PQR (Serrano *et al* 2010) given by:

$$I_{vJ} = I_{0J} + v\pi \tag{14}$$

2.1 Ro-vibrational energy spectra of the THP

Substituting Eq. (1) in (10), the effective potential for the Tietz-Hua is given by

$$V_{eff}(r) = D_e\left(\frac{1 - e^{-bh(r-r_e)}}{1 - c_h e^{-bh(r-r_e)}}\right)^2 + \frac{L\hbar^2}{2\mu r^2} \tag{15}$$

Note that Eq. (6) has no exact solution with the effective THP, except for the pure vibrational state. Thus, to obtain approximate analytical solution, we apply the Pekeris-type approximation (Serrano *et al* 2010 and Mustafa. O. 2015), on the second term of Eq. (15) *viz*:

$$\frac{L\hbar^2}{2\mu r^2} \approx \frac{L\hbar^2}{2\mu}\left\{c_0 + c_1 x + c_2 x^2\right\} \tag{16}$$

where the constant coefficients $c_{j-1}\ (j = 1,2,3)$ (Serrano *et al* 2010) are given in compact form as:

$$c_{-1+j} = \tfrac{1}{2}(2-j)(3-j) + \frac{(-1)^j\, e^{b_h(r-r_e)(-1+j)}}{(-1+j)!(3-j)!(r-r_e)}\left(4 - j + c_h e^{-b_h(r-r_e)}\right)\left(1 - c_h e^{-2b_h(r-r_e)}\right)^j + \frac{3(-1)^{-1+j}\, e^{b_h(r-r_e)(-1+j)}}{(-1+j)!(3-j)!\,b_h\,(r-r_e)^2}\left(1 - c_h\, e^{-b_h(r-r_e)}\right)^{1+j}$$

(17)

substituting Eq. (16) in (15) and introducing the following coordinate transformation:

$$x = \left(e^{b_h(r-r_e)} - c_h\right)^{-1} \qquad\qquad x \in \left(\left(1-c_h\right)^{-1}, 0\right) \tag{18}$$

this results in:

$$V_{eff}\left(x\right) = \frac{\hbar^2}{2\mu}\sum_{j=0}^{2}\varepsilon_j^2\, x^{2-j} \tag{19}$$

where

$$\varepsilon_j^2 = L\, c_{2-j} + \frac{\left(-1\right)^{2-j}}{\left(j\right)!\left(2-j\right)!}\frac{4\,\mu\, D_e}{\hbar^2}\left(c_h - 1\right)^{2-j} \tag{20}$$

In order to solve the Riccati equation given by (8), we need to obtain the turning points $r_{\nu A} = 2^{-1}\ln\left(x_{\nu A}^{-1} + c_h\right)$ and $r_{\nu B} = 2^{-1}\ln\left(x_{\nu B}^{-1} + c_h\right)$, these turning points are just the roots of the equation $V_{eff}\left(x\right) = E_{\nu J}$, solving this equation, we find:

$$\sum_{j=0}^{2}\varepsilon_j^2\, x^{2-j} = \frac{2\,\mu\, E_{\nu J}}{\hbar^2} \equiv \varepsilon_{\nu J}^2 \tag{21}$$

from Eq. (21) we obtain:

$$x_{\nu A} + x_{\nu B} = -\frac{\varepsilon_1^2}{\varepsilon_0^2} \tag{22}$$

$$x_{\nu A}\, x_{\nu B} = \frac{\varepsilon_2^2 - \varepsilon_{\nu J}^2}{\varepsilon_0^2} \tag{23}$$

The momentum $k_{\nu J}\left(x\right)$ given by Eq. (3) is expressed as:

$$k_{\nu J}\left(x\right) = \sqrt{\varepsilon_{\nu J}^2 - \varepsilon_0^2\, x^2 - \varepsilon_1^2\, x - \varepsilon_2^2} \tag{24}$$

which in terms of the turning points $x_{\nu A}$ and $x_{\nu B}$ gives:

$$k_{\nu J}\left(x\right) = \varepsilon_0\sqrt{\left(x - x_{\nu A}\right)\left(x_{\nu B} - x\right)} \tag{25}$$

Using Eq. (18) in (8), Riccati equation in terms of coordinate x reads:

$$-b_h\, x\left(1 + c_h x\right)\varphi_{\nu J}'\left(x\right) + \varphi_{\nu J}^2\left(x\right) + \varepsilon_{\nu J}^2 - \sum_{j=0}^{2}\varepsilon_j^2\, x^{2-j} = 0 \tag{26}$$

due to Sturm-Liouville theorem, for the ground state wave functions we choose a trial wave function as:

$$\varphi_{0J}\left(x\right) = -c_1 x + c_2 \tag{27}$$

where $c_1\left(<0\right)$ and c_2 are constants. Setting $\nu = 0$ in (26) and putting Eq. (27) in the resulting expression, we obtained:

$$\left(c_1^{\,2} + b_h c_h c_1 - \varepsilon_0^2\right)x^2 + \left(b_h c_1 - 2c_1 c_2 - \varepsilon_1^2\right)x + \varepsilon_{0J}^2 - \varepsilon_2^2 + c_2^{\,2} = 0 \tag{28}$$

Eq. (28) is valid if the coefficients of x^2, x and x^0 are each equal to zero, leading to:

$$c_1^{\,2} + b_h c_h c_1 = \varepsilon_0^2 \tag{29}$$

$$b_h c_1 - 2\,c_1\, c_2 = \varepsilon_1^2 \tag{30}$$

$$c_2^{\,2} = \varepsilon_2^2 - \varepsilon_{0J}^2 \tag{31}$$

Eq. (29) yields:

$$c_1 = -b_h c_h \sigma \tag{32}$$

where

$$\sigma = \frac{1}{2} + \left(\frac{1}{4} + \frac{2\mu D_e}{b_h^2\hbar^2}\left(1 - \frac{1}{c_h}\right)^2 + \frac{Lc_2}{b_h c_h}\right)^{\frac{1}{2}} \tag{33a}$$

Let $\Lambda = \left(1 - \dfrac{1}{c_h}\right)$ (33b)

With c1 given by (32) and c_2 by (31), Eq. (27) is completely defined, the momentum integral of Eq. (12) in terms of coordinate *x* is:

$$I_{\nu J} = -\frac{\varepsilon_0}{b_h} \int_{x_{\nu A}}^{x_{\nu B}} \frac{\sqrt{\left(x - x_{\nu A}\right)\left(x_{\nu B} - x\right)}}{x\left(1 + c_h x\right)} dx \tag{34}$$

where the definite integral in (34) can be evaluated using the following standard integral adopted from Ref. (Falaye *et al* 2015):

$$\int_{x_{\nu A}}^{x_{\nu B}} \frac{\sqrt{\left(x - x_{\nu A}\right)\left(x_{\nu B} - x\right)}}{x\left(1 + q x\right)} dx = \pi \left\{ -\frac{1}{q} - \sqrt{x_{\nu A}\, x_{\nu B}} + \frac{\sqrt{\left(1 + q x_{\nu A}\right)\left(1 + q x_{\nu B}\right)}}{q} \right\} \tag{35}$$

Thus, application of (35) to Eq. (34) yields:

$$I_{\nu J} = \frac{\pi}{b_h} \left\{ \frac{\varepsilon_0}{c_h} + \sqrt{\varepsilon_2^2 - \varepsilon_{\nu J}^2} - \frac{1}{c_h} \sqrt{\varepsilon_0^2 - c_h\, \varepsilon_1^2 + c_h{}^2 \left(\varepsilon_2^2 - \varepsilon_{\nu J}^2\right)} \right\} \tag{36}$$

Now Eq. (36) corresponding to the ground state (ν = 0) reduces to:

$$I_{0J} = \frac{\pi}{b_h} \left\{ \frac{\varepsilon_0}{c_h} + \sqrt{\varepsilon_2^2 - \varepsilon_{0J}^2} - \sqrt{\frac{\varepsilon_0^2 - c_h\, \varepsilon_1^2}{c_h^2} + \left(\varepsilon_2^2 - \varepsilon_{0J}^2\right)} \right\} \tag{37}$$

Substituting Eqs. (29), (30) and (31) in Eq. (37), we get:

$$I_{0J} = \frac{\pi}{b_h} \left(\frac{\varepsilon_0}{c_h} + b_h\, \sigma \right) \tag{38}$$

Replacing Eqs. (36) and (38) in the expression for PQR given by (14) and eliminating ε_j^2 and σ, we find the ro-vibrational energy of the THP as:

$$E_{\nu J}^{(\mathrm{THP})} = D_e + \frac{L \hbar^2 c_0}{2\mu} - \frac{b_h^2 \hbar^2}{2\mu} \left\{ \frac{\frac{\mu D_e}{b_h^2 \hbar^2} \Lambda + \frac{L}{2 b_h^2 c_h^2} \left(c_1 c_h - c_2\right)}{\nu + \sigma} + \frac{\nu + \sigma}{2} \right\}^2 \tag{39}$$

2.2 The radial Eigen functions of the Tiet-Hua potential

By choosing $V\left(r\right)$ to be the Tiet-Hua potential ((Hamzavi *et al* 2012)):
The radial wave function is given by inserting *Q* = 0 in Eq. (26), gives:

$$-2\alpha x \varphi_{\nu J M}'\left(x\right) + \varphi_{\nu J}^2\left(x\right) + \varepsilon_{\nu J M}^2 - \sum_{j=1}^{3} \varepsilon_{jM}^2\, x^{3-j} = 0 \tag{40}$$

Following procedures similar to that used to obtain $\psi_{\nu J}\left(z\right)$, we have that:

$$\psi_{\nu J M}\left(x\right) = N_{\nu J M}\, e^{-\frac{1}{2} u x}\, x^{\frac{1}{2} \upsilon}\, {}_1F_1\left(-\nu, \upsilon + 1 : u x\right) \tag{41}$$

where $N_{\nu J M}$ is the normalization constant, ${}_1F_1\left(-\nu, \upsilon + 1 : u x\right)$ is the Laguerre polynomial and the parameters *u* and *υ* are given by:

$$u = \frac{\varepsilon_{1M}}{\alpha_M} \tag{42}$$

$$\upsilon = \frac{\left(\varepsilon_{3M} - \varepsilon_{\nu J M}\right)^{\frac{1}{2}}}{\alpha_M} \tag{43}$$

2.3 Input spectroscopic parameters

Table 1 shows the spectroscopic parameters taken from (Hamzavi *et al* 2012)

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

III. Discussion

We consider special case of s-wave (ℓ =0).Eq. (39) reduces to

$$E_{0J}^{(\mathrm{THP})}=D_e-\frac{b_h^2\hbar^2}{8\mu}\left\{\frac{\frac{2\mu D_e}{b_h^2\hbar^2}\Lambda}{\nu+\frac{1}{2}+\left(\frac{2\mu D_e}{b_h^2\hbar^2}\Lambda^2+\frac{1}{4}\right)^{\frac{1}{2}}}+\nu+\frac{1}{2}+\left(\frac{2\mu D_e}{b_h^2\hbar^2}\Lambda^2+\frac{1}{4}\right)^{\frac{1}{2}}\right\}^2 \tag{44}$$

It is clear that Eq.(44) is independent of c_j (j = 0,1,2,...) and therefore independent of energy determining parameter Λ .Shown in Table 2 are computed energy eigenvalues corresponding to quantum states with $\ell \neq 0$,the analysis was carried out for two diatomic molecules:O_2 and H_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 literature and shows better stabilization for the molecules.

IV. Conclusion

We have obtained the ℓ wave analytical solutions of Schrodinger equation with the Tietz-Hua potential using the proper quantization rule, we have also obtained the energy eigenvalues and normalized radial wavefunctions, special case of s-wave was also derived from our results. The results obtained in this work might be useful in areas of molecular physics, chemical physics, analytic chemistry, atomic physics and solid-state physics.

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Table 2: The bound state energies E_{nl} (in eV) for H_2 and O_2

	H_2				O_2	
n	L	PRESENT	ROY (2014)	HAMZAVI *et al* (2012)	PRESENT	ROY(2014)
0	0	4.4815764961	4.4815797825	4.4815718267	5.1149025433	5.1163223113
0	1	4.4669750676	4.4669801579	…	5.1145484174	5.1159784440
0	2	4.4379034238	4.4379154622	…	5.1138401797	5.1152907228
0	5	4.2670413527	…	4.2658220403	5.1095911497	…
0	10	3.7374063844	…	3.7336304360	5.0954326220	…
3	0	3.0595150913	3.0595425362	…	4.5497017063	4.5590745476
3	1	3.0472595186	3.0474413866	…	4.5493609717	4.5587436240
3	2	3.0228546847	3.0233638406	…	4.5486795166	4.5580817907
3	5	2.8793161800	…	…	4.5445911837	…
3	10	2.4331751852	…	…	4.5309683249	…
5	0	2.2815541870	2.2815913849	2.6696509300	4.1917403884	4.2058686976
5	1	2.2706974784	2.2710928924	…	4.1914085485	4.2055464879
5	2	2.2490759990	2.2502130058	…	4.1907448831	4.2049020823
5	5	2.1218464564	…	2.1070072990	4.1867632880	…
5	10	1.7256796852	…	1.7105026080	4.1734962302	…
7	0	1.6300221428	…	…	3.8487952908	…
7	1	1.6204521791	…	1.6130911000	3.8484723195	…

7	2	1.6013913135	…	…	3.8478263913	…
7	5	1.4891748857	…	1.4722799590	3.8439512202	…
7	10	1.1391123074	…	1.1225356530	3.8310389169	…

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