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# RO-VIBRATIONAL ENERGIES AND WAVE FUNCTIONS OF IMPROVED TIETZ POTENTIAL

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## *Abstract*

***We have employed the techniques of exact quantization rule to obtain closed form expression for the bound state ro-vibrational energy eigenvalues of the improved Tietz potential. By considering the Morse potential as a special case of the improved Tietz potential, we have deduced closed form expression for the ro-vibrational energy of Morse potential from the results of improved Tietz potential. We have also solved the Riccati equation via ansatz solution and obtained closed form expressions for the unnormalized radial wave functions for the improved Tietz and Morse potentials. We have computed ro-vibrational energies for the improved Tietz and Morse potentials and obtained results for four diatomic molecules including HCl, LiH, $H_2$ and CO, our computed results are in near perfect agreement with available data of the diatomic molecules in the literature.***

**Keywords**: Improved Tietz potential, ro-vibrational energy, Riccati equation, Schrödinger equation, exact quantization rule

## 1. Introduction

The wave function is an important formulation in quantum mechanics because of the useful information they give regarding the quantum mechanical system under review [1-3]. Given a potential energy function, the Schrödinger or other wave equations must be solved, analytically or numerically to obtain eigenfunctions and eigenenergies of the system [2, 4]. The nature of the solution of the Schrödinger equation is characterized by the rotational quantum number $\ell$. Such a solution may be exact [5, 6] or approximate [7, 8].

For all values of $\ell$, the harmonic oscillator and Coulomb potentials are known to have exact solution with Schrödinger equation, other potential models also have, but with a restriction. Exact analytical solutions of the Schrödinger equation are also possible with most potential models for the special case $\ell = 0$ only, the solutions are known as s-wave solutions [9]. On the other hand, for nonzero rotational quantum numbers, only approximate numerical solutions [10, 11], or approximate analytical solutions [12-14] can be realized for the wave equations.

The first step to obtaining analytical solution of the Schrödinger equation is to model the centrifugal (or pseudo spin-orbit) term of the Schrödinger equation with an appropriate approximation scheme. The Pekeris approximation [15], Greene-Aldrich approximation [16] have been successful in eliminating the centrifugal term of the wave equation. other model of the Pekeris-type has also been used by researchers [17]. Various solution methods have been proposed for the wave equation, among the vast list include functional analysis (ansatz) method [18], generalized pseudospectral method (GPS) [7], exact quantization rule (EQR) [19-25] and path integral approach [26].

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The solution of Schrödinger equation has been obtained in the presence of different potential energy functions. The main focus of the present study is the improved Tietz potential. The potential has important applications in the atomic, molecular and chemical physics. In previous studies, solution of Schrödinger equation has been obtained in the presence of the improved Tietz potential [13, 26]. It is pertinent to point out that equations of bound state ro-vibrational energies, also known as energy eigenvalues of atomic oscillators and radial wave functions hold for nonzero values of deformation parameters ($q$) of the oscillator. However, if $q = 0$, the improved Tietz potential is finite, but the solution obtained in previous studies is infinite both for the eigenenergies and eigenfunctions.

In this paper, the concept of EQR and functional analysis methods are employed to obtain expressions of bound state ro-vibrational energies and radial wave functions of the Schrödinger equation. Cases in which $q \neq 0$ and $q = 0$ are specially considered, to the best of our knowledge, this approach has not been studied in the literature. Numerical data of bound state ro-vibrational energies obtained for the improved Tietz potential in this study are compared with available literature data for the potential where they exist.

## 2.0 Theoretical Formalism

### 2.1 Review of the concepts of exact quantization rule

Here we give a summary of the important concepts of exact quantization rule, the complete detail is given by Ma and Xu [19]. The exact quantization rule was proposed to solve the one-dimensional Schrödinger equation given as:

$$\psi''_{n\ell}(x) + k^2_{n\ell}(x)\psi_{n\ell}(x) = 0, \tag{1}$$

where prime denotes derivative with respect to the argument jn brackets, and the linear momentum of the system is given by

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

$\mu$ being the mass of the system, $E_{n\ell}$ is the energy eigenvalue, $V_{\text{eff}}(x)$ is the effective potential energy function which is a piecewise continuous real function of $x$. Eq. (1) can be reduced to the well-known Riccati nonlinear differential equation given by

$$\varphi'_{n\ell}(x) + k^2_{n\ell}(x) + \varphi^2_{n\ell}(x) = 0, \tag{3}$$

where $\phi_{n\ell}(x) = \psi'_{n\ell}(x) / \psi_{n\ell}(x)$ is the logarithmic derivative of the wavefunction $\psi_{n\ell}(x)$, it is also known as the phase angle. Due to Sturm-Liouville theorem, $\phi_{n\ell}(x)$ decreases monotonically with respect to $x$ between two turning points determined by the equation $E_{n\ell} \geq V_{\text{eff}}(x)$. Specifically, $x$ increases across a node of the wavefunction $\psi_{n\ell}(x)$, where $E_{n\ell} \geq V_{\text{eff}}(x)$, $\phi_{n\ell}(x)$ decreases to $-\infty$ and jumps to $+\infty$ and then decreases again. By carefully studying the one-dimensional Schrödinger equation, Ma and Xu [19] proposed an exact quantization rule given by:

$$\int_{x_{nA}}^{x_{nB}} \mathrm{k}_{n\ell}(x)\,\mathrm{d}x = N\pi + \int_{x_{nA}}^{x_{nB}} \varphi_{n\ell}(x)\left[\frac{\mathrm{d}\,\mathrm{k}_{n\ell}(x)}{\mathrm{d}x}\right]\left[\frac{\mathrm{d}\varphi_{n\ell}(x)}{\mathrm{d}x}\right]^{-1}\mathrm{d}x, \tag{4}$$

where $x_{n\mathrm{A}}$ and $x_{n\mathrm{B}}$ are two turning points determined by solving the equation $E_{n\ell} = V_{\text{eff}}(x)$ and $x_{n\mathrm{A}} < x_{n\mathrm{B}}$. $N$ is the number of nodes of $\phi_{n\ell}(x)$ in the neighborhood of $E_{n\ell} \geq V_{\text{eff}}(x)$ 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, $N\pi$, relates to the contribution from the nodes of the wave function, and the second term is referred to as the quantum correction. Ma and Xu [19] have found that the quantum correction is independent of the number of nodes for the exactly solvable systems, therefore, it can be evaluated for the ground state ($n = 0$), the second term in Eq. (4) can thus be represented by:

$$\mathrm{Q}_c = \int_{x_{nA}}^{x_{nB}} \varphi_{n\ell}(x)\left[\frac{\mathrm{d}\,\mathrm{k}_{n\ell}(x)}{\mathrm{d}x}\right]\left[\frac{\mathrm{d}\varphi_{n\ell}(x)}{\mathrm{d}x}\right]^{-1}\mathrm{d}x \equiv \int_{x_{0A}}^{x_{0B}} \varphi_{0\ell}(x)\left[\frac{\mathrm{d}\,\mathrm{k}_{0\ell}(x)}{\mathrm{d}x}\right]\left[\frac{\mathrm{d}\varphi_{0\ell}(x)}{\mathrm{d}x}\right]^{-1}\mathrm{d}x, \tag{5}$$

where $\mathrm{Q_c}$ is the quantum correction term. In three dimensional spherical coordinates, the exact quantization rule is given by:

$$\int_{r_{nA}}^{r_{nB}} \mathrm{k}_{n\ell}(r)\,\mathrm{d}r = N\pi + \int_{r_{nA}}^{r_{nB}} \varphi_{0\ell}(r)\left[\frac{\mathrm{d}k_{0\ell}(r)}{\mathrm{d}r}\right]\left[\frac{\mathrm{d}\varphi_{0\ell}(r)}{\mathrm{d}r}\right]^{-1}\mathrm{d}r. \tag{6}$$

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

$$\mathrm{I}_{n\ell} = N\pi + \mathrm{Q_c}, \tag{7}$$

where the momentum integral is given by

$$\mathrm{I}_{n\ell} = \int_{r_{nA}}^{r_{nB}} \mathrm{k}_{n\ell}(r)\,\mathrm{d}r, \tag{8}$$

and the quantum correction is:

$$\mathrm{Q_c} = \int_{r_{nA}}^{r_{nB}} \varphi_{0\ell}(r)\left[\frac{\mathrm{d}k_{0\ell}(r)}{\mathrm{d}r}\right]\left[\frac{\mathrm{d}\varphi_{0\ell}(r)}{\mathrm{d}r}\right]^{-1}\mathrm{d}r. \tag{9}$$

The Schrödinger equation in three dimensions for a spherically symmetric potential is given as [12]

$$\left\{-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+V_{\mathrm{eff}}(r)\right\}\mathrm{U}_{n\ell}(r)=E_{n\ell}\,\mathrm{U}_{n\ell}(r), \tag{10}$$

$\mathrm{U}_{n\ell}(r)$ being the radial wave function.

## 2.2 The effective improved Tietz potential

The effective improved Tietz rotating oscillator [13] is given by

$$V_{\mathrm{eff}}(r)=V(r)+V_{\ell}(r), \tag{11}$$

where $V(r)$ and $V_{\ell}(r)$ are respectively the improve Tietz potential and centrifugal term potential respectively, they are given by

$$V(r)=D_{\mathrm{e}}\left(1-\frac{b}{e^{\alpha r}+q}\right)^2, \tag{12}$$

where

$$b=\mathrm{e}^{\alpha r_{\mathrm{e}}}+q, \tag{13}$$

with $D_{\mathrm{e}}$ as the dissociation energy, $r_{\mathrm{e}}$ is the molecular bond length, $r$ is the internuclear separation, $\alpha$ and $q$ are respectively the potential screening and deformation parameters expressed as [13]

$$q=\left\{\frac{\alpha}{\omega_{\mathrm{e}}}\left(\frac{D_{\mathrm{e}}}{2\mu}\right)^{\frac{1}{2}}-1\right\}\mathrm{e}^{\alpha r_{\mathrm{e}}}, \tag{14}$$

$$\alpha=\omega_e\left(\frac{2\mu}{D_e}\right)^{\frac{1}{2}}-\frac{4\pi c\mu^2 r_e^3\alpha_e\omega_e}{3\hbar^2}-\frac{1}{r_e}, \tag{15}$$

where $\omega_{\mathrm{e}}$ and $\alpha_{\mathrm{e}}$ are the equilibrium harmonic vibrational frequency, and rotation-vibration coupling constant. The centrifugal term potential is given by [13, 20]

$$V_{\ell}(r)=\frac{\mathrm{L}\hbar^2}{2\mu r^2}, \tag{16}$$

where $\mathrm{L}=\ell(\ell+1)$. Oupon substituting Eq. (12) and Eq. (16) into Eq. (11), this translates to

$$V_{\mathrm{eff}}(r)=D_{\mathrm{e}}\left(1-\frac{b}{e^{\alpha r}+q}\right)^2+\frac{\mathrm{L}\hbar^2}{2\mu r^2}. \tag{17}$$

Eq. (10) when used with the effective potential of Eq. (17) has no exact solution except for the case of s-wave ($\ell=0$), to obtain analytical solution for all quantum states, one must use a suitable approximation scheme on the centrifugal term given by [13]

$$\frac{1}{r^2}\approx\frac{1}{r_{\mathrm{e}}^2}\left\{D_0+\frac{D_1}{\mathrm{e}^{\alpha r}+q}+\frac{D_2}{\left(\mathrm{e}^{\alpha r}+q\right)^2}\right\}, \tag{18}$$

where the adjustable parameters $D_0$, $D_1$ and $D_2$ read [13]

$$D_0=1-\frac{1}{\alpha^2 r_{\mathrm{e}}^2}\left(3-3\alpha r_{\mathrm{e}}+6q\mathrm{e}^{-\alpha r_{\mathrm{e}}}+3q^2\mathrm{e}^{-2\alpha r_{\mathrm{e}}}-2q\alpha r_{\mathrm{e}}\mathrm{e}^{-\alpha r_{\mathrm{e}}}+q^2\alpha r_{\mathrm{e}}\mathrm{e}^{-2\alpha r_{\mathrm{e}}}\right), \tag{19}$$

$$D_1=\frac{2}{\alpha^2 r_{\mathrm{e}}^2}\left(-9q+3q\alpha r_{\mathrm{e}}-3\mathrm{e}^{\alpha r_{\mathrm{e}}}+2\alpha r_{\mathrm{e}}\mathrm{e}^{\alpha r_{\mathrm{e}}}-9q^2\mathrm{e}^{-\alpha r_{\mathrm{e}}}-3q^3\mathrm{e}^{-2\alpha r_{\mathrm{e}}}-q^3\alpha r_{\mathrm{e}}\mathrm{e}^{-2\alpha r_{\mathrm{e}}}\right), \tag{20}$$

$$D_2=\frac{1}{\alpha^2 r_{\mathrm{e}}^2}\left(18q^2+12q\mathrm{e}^{\alpha r_{\mathrm{e}}}+3\mathrm{e}^{2\alpha r_{\mathrm{e}}}-2q\alpha r_{\mathrm{e}}\mathrm{e}^{\alpha r_{\mathrm{e}}}-\alpha r_{\mathrm{e}}\mathrm{e}^{-\alpha r_{\mathrm{e}}}+12q^3\mathrm{e}^{-\alpha r_{\mathrm{e}}}+3q^4\mathrm{e}^{-2\alpha r_{\mathrm{e}}}+2q^3\alpha r_{\mathrm{e}}\mathrm{e}^{-\alpha r_{\mathrm{e}}}+q^4\alpha r_{\mathrm{e}}\mathrm{e}^{-2\alpha r_{\mathrm{e}}}\right). \tag{21}$$

Substituting Eq. (18) in Eq. (17), this leads to:

$$V_{\mathrm{eff}}(r)=D_{\mathrm{e}}\left(1-\frac{b}{\mathrm{e}^{\alpha r}+q}\right)^2+\frac{\mathrm{L}\hbar^2}{2\mu r_{\mathrm{e}}^2}\left\{D_0+\frac{D_1}{\mathrm{e}^{\alpha r}+q}+\frac{D_2}{\left(\mathrm{e}^{\alpha r}+q\right)^2}\right\}, \tag{22}$$

Using the following transformation equation,

$$y=\left(\mathrm{e}^{\alpha r}+q\right)^{-1}. \tag{23}$$

Eq. (22) transforms to:

$$V_{\mathrm{eff}}(y)=D_{\mathrm{e}}(1-by)^2+\frac{\mathrm{L}\hbar^2}{2\mu r_{\mathrm{e}}^2}\left(D_0+D_1 y+D_2 y^2\right). \tag{24}$$

Eq. (24) can be generalized as:

$$V_{\mathrm{eff}}(y)=\frac{\hbar^2}{2\mu r_{\mathrm{e}}^2}\left(LD_2+\frac{2\mu r_{\mathrm{e}}^2 D_{\mathrm{e}} b^2}{\hbar^2}\right)y^2+\frac{\hbar^2}{2\mu r_{\mathrm{e}}^2}\left(LD_2-\frac{4\mu r_{\mathrm{e}}^2 D_{\mathrm{e}} b}{\hbar^2}\right)y+\frac{\hbar^2}{2\mu r_{\mathrm{e}}^2}\left(LD_0+\frac{2\mu r_{\mathrm{e}}^2 D_{\mathrm{e}}}{\hbar^2}\right). \tag{25}$$

By defining the following constants

$$\eta^2 = L D_2 + \frac{2\mu r_e^2 D_e b^2}{\hbar^2}, \tag{26}$$

$$\kappa^2 = L D_1 - \frac{4\mu r_e^2 D_e b}{\hbar^2}, \tag{27}$$

$$\lambda^2 = L D_0 + \frac{2\mu r_e^2 D_e}{\hbar^2}. \tag{28}$$

Eq. (25) can be expressed in the more compact form as:

$$V_{\text{eff}}(y) = A y^2 + B y + C, \tag{29}$$

where

$$A = \frac{\hbar^2 \eta^2}{2\mu r_e^2}, \tag{30}$$

$$B = \frac{\hbar^2 \kappa^2}{2\mu r_e^2}, \tag{31}$$

$$C = \frac{\hbar^2 \lambda^2}{2\mu r_e^2}. \tag{32}$$

The turning points needed to solve Riccati equation are obtained by solving the following equation.

$$V_{\text{eff}}(y) = E_{n\ell}. \tag{33}$$

Putting Eq. (27) in Eq. (31), we have that

$$A y^2 + B y + C - E_{n\ell} = 0. \tag{34}$$

The turning points $y_{nA}$ and $y_{nB}$ (> $y_{nA}$) which are roots Eq. (34) are given by

$$y_{nA} = -\frac{B + \sqrt{B^2 - 4A\left(C - E_{n\ell}\right)}}{2A}, \tag{35}$$

and

$$y_{nB} = -\frac{B - \sqrt{B^2 - 4A\left(C - E_{n\ell}\right)}}{2A}. \tag{36}$$

From Eq. (35) and Eq. (36), it is obvious that

$$y_{nA} + y_{nB} = -\frac{B}{A}, \tag{37}$$

$$y_{nA}\, y_{nB} = \frac{C - E_{n\ell}}{A}. \tag{38}$$

For the ground (n = 0) state, Eq. (37) and Eq. (38) gives respectively

$$y_{0A} + y_{0B} = -\frac{B}{A}, \tag{39}$$

$$y_{0A}\, y_{0B} = \frac{C - E_{0\ell}}{A}. \tag{40}$$

The expression for the momentum is given by, following Eq. (2), this gives:

$$\mathrm{k}_{n\ell}(y) = \sqrt{\frac{2\mu}{\hbar^2}\left(E_{n\ell} - A y^2 - B y - C\right)}. \tag{41}$$

Eq. (41) can be written in terms of the turning points which will be required in what will follow, thus,

$$\mathrm{k}_{n\ell}(y) = \sqrt{\frac{2\mu A}{\hbar^2}\left(\frac{C - E_{n\ell}}{A} - y^2 - \frac{B}{A} y\right)}. \tag{42}$$

Using Eq. (37) and Eq. (38) in Eq. (42), this gives:

$$\mathrm{k}_{n\ell}(y) = \sqrt{\frac{2\mu A}{\hbar^2}\left(y - y_{nA}\right)\left(y_{nB} - y\right)}. \tag{43}$$

The derivative of Eq. (43) with respect to y is given by

$$\mathrm{k}'_{n\ell}(y) = -\frac{\sqrt{2\mu A}}{\hbar}\, \frac{y - \frac{1}{2}\left(y_{nA} + y_{nB}\right)}{\sqrt{\left(y - y_{nA}\right)\left(y_{nB} - y\right)}}. \tag{44}$$

Since the ground state derivative of the momentum is required for evaluating the quantum correction, Eq. (44) gives for the ground state (n = 0), and employing Eq. (39)

$$\mathrm{k}'_{0\ell}(y)=-\frac{\sqrt{2\mu A}}{\hbar}\frac{y+B/2A}{\sqrt{(y-y_{0A})(y_{0B}-y)}}\,. \qquad (45)$$

Using Eq. (2) and Eq. (3), the Riccati equation in three dimensional spherical coordinates [22] is

$$\varphi'_{n\ell}(r)+\frac{2\mu}{\hbar^2}\left\{E_{n\ell}-V_{\text{eff}}(r)\right\}+\varphi^2_{n\ell}(r)=0\,. \qquad (46)$$

To obtain the corresponding Riccati equation in terms of variable *y*, we substitute Eq. (23) in Eq. (46), this results in the following first order nonlinear differential equation given by

$$-\alpha\, y(1-q\,y)\varphi'_{n\ell}(y)+\frac{2\mu}{\hbar^2}\left(E_{n\ell}-Ay^2-B\,y-C\right)+\varphi^2_{n\ell}(y)=0\,\cdot \qquad (47)$$

where we have used Eq. (29) to eliminate $V_{n\ell}$ (y)
Eq. (47) gives for the ground state

$$-\alpha\, y(1-q\,y)\varphi'_{0\ell}(y)+\frac{2\mu}{\hbar^2}\left(E_{0\ell}-Ay^2-B\,y-C\right)+\varphi^2_{0\ell}(y)=0\,\cdot \qquad (48)$$

Since $\phi_{0\ell}$ (*y*) has one zero and no pole, it has to assume a linear form in *y*, for a trial solution, we assume

$$\phi_{0\ell}(y)=-c_1\,y+c_2\,\cdot \qquad (49)$$

$c_1$ and $c_2$ being constants, substituting Eq. (49) in Eq. (48), get

$$\alpha\, c_1\left(y-q\,y^2\right)+\frac{2\mu}{\hbar^2}\left(E_{0\ell}-C-A\,y^2-B\,y\right)+c_1^2\,y^2-2c_1\,c_2\,y+c_2^2=0\,\cdot \qquad (50)$$

Eq. (50) simplifies to

$$\left(-\alpha\,c_1\,q-\frac{2\mu A}{\hbar^2}+c_1^2\right)y^2+\left(\alpha\,c_1-\frac{2\mu B}{\hbar^2}-2c_1\,c_2\right)y+\frac{2\mu}{\hbar^2}\left(E_{0\ell}-C\right)+c_2^2=0\,\cdot \qquad (51)$$

By equating corresponding coefficients of $y^2$, *y* and $y^0$ respectively on both sides of Eq. (51), this results in the following relations

$$c_1^2-\alpha\,q\,c_1=\frac{2\mu A}{\hbar^2}\,, \qquad (52)$$

$$\alpha\,c_1-2c_1\,c_2=\frac{2\mu B}{\hbar^2}\,, \qquad (53)$$

$$c_2^2=\frac{2\mu}{\hbar^2}\left(C-E_{0\ell}\right)\cdot \qquad (54)$$

Therefore, solving for $c_1$ in Eq. (52), one obtains

$$c_1=\frac{\alpha\,q}{2}-\left(\frac{\alpha^2\,q^2}{4}+\frac{2\mu A}{\hbar^2}\right)^{\frac{1}{2}}\cdot \qquad (55)$$

We have chosen the negative square root in solving for $c_1$ in order to satisfy the monotonicity requirements.
It follows that by inserting Eq. (30) in Eq. (55), this yields

$$c_1=\frac{\alpha\,q}{2}\left\{1-\left(1+\frac{4\eta^2}{\alpha^2\,r_e^2\,q^2}\right)^{\frac{1}{2}}\right\}\cdot \qquad (56)$$

Letting

$$\omega=\tfrac{1}{2}\left\{1-\left(1+\frac{4\eta^2}{\alpha^2\,r_e^2\,q^2}\right)^{\frac{1}{2}}\right\}, \qquad (57)$$

Eq. (56) assumes the form

$$c_1=\alpha\,q\,\omega\,. \qquad (56)$$

Evidently, Eq. (57) leads to

$$\eta=\alpha\,r_e\,q\left(\omega^2-\omega\right)^{\frac{1}{2}}. \qquad (59)$$

Eq. (53) gives

$$c_2 = \frac{\alpha}{2} - \frac{\mu B}{c_1 \hbar^2}. \tag{60}$$

Having obtained $c_1$ and $c_2$, we are now in position to compute the various integrals appearing in Eq. (7), starting with the right hand side of this relation, Eq. (9) can be used to obtain the quantum correction, by employing the transformation relation given by Eq. (23) in Eq. (9), we have

$$\mathrm{Q_c} = -\frac{1}{\alpha}\int_{y_{0A}}^{y_{nB}} \frac{\varphi_{0\ell}(y)}{\varphi'_{0\ell}(y)} k'_{0\ell}(y) \frac{\mathrm{d}\,y}{y\,(1-q\,y)} \;. \tag{61}$$

Using Eq. (45) and Eq. (49) in Eq. (61), we have

$$\mathrm{Q_c} = \frac{\sqrt{2\mu A}}{\alpha\hbar}\int_{y_{0A}}^{y_{nB}} \frac{(y-c_2/c_1)(y+B/2A)}{y\,(1-q\,y)} \frac{\mathrm{d}\,y}{\sqrt{(y-y_{0A})(y_{0B}-y)}}\;. \tag{62}$$

After substituting Eq. (30) in Eq. (62) and dividing out the numerator by the denominator, we find

$$\mathrm{Q_c} = \frac{\eta}{\alpha r_e}\int_{y_{0A}}^{y_{nB}} \left\{ -\frac{1}{q} - \frac{c_2 B}{2c_1 A y} + \frac{(c_1 - q c_2)(2A + qB)}{2 q c_1 A (1-q\,y)} \right\} \frac{\mathrm{d}\,y}{\sqrt{(y-y_{0A})(y_{0B}-y)}}\;. \tag{63}$$

The integral in Eq. (63) can be evaluated by means of the following standard integral [24]

$$\int_{y_{nA}}^{y_{nB}} \frac{\mathrm{d}\,y}{(P+Q\,y)\sqrt{(y-y_{nA})(y_{nB}-y)}} = \frac{\pi}{\sqrt{(P+Q\,y_{nB})(P+Q\,y_{nA})}}\;. \tag{64}$$

Application of Eq. (64) in Eq. (63) results in the following

$$\mathrm{Q_c} = \frac{\pi\eta}{\alpha r_\mathrm{e}} \left\{ -\frac{1}{q} - \frac{c_2 B}{2c_1 A} I_1 + \frac{(c_1 - q c_2)(2A + qB)}{2 q c_1 A} I_2 \right\}, \tag{65}$$

where

$$I_1^{-2} = y_{0A}\, y_{0B} \equiv \frac{C - E_{0\ell}}{A}\;. \tag{66}$$

Thus, by putting Eq. (54) and Eq. (30) in Eq. (66), we find

$$I_1 = \frac{\eta}{c_2\, r_\mathrm{e}}\;. \tag{67}$$

Similarly, we have

$$I_2^{-2} = 1 - q\,(y_{0A} + y_{0B}) + q^2\, y_{0A}\, y_{0B}\,. \tag{68}$$

On substituting Eq. (35) and Eq. (36) in Eq. (64), this gives

$$I_2^{-2} = 1 + \frac{qB}{A} + \frac{q^2 (C - E_{0\ell})}{A}\,. \tag{69}$$

To further simplify Eq. (69), divide Eq. (53) and Eq. (54) each by Eq. (52), and the results substituted in Eq. (69), gives

$$I_2^{-2} = 1 + \frac{q\,(\alpha c_1 - 2c_1 c_2)}{c_1^2 - \alpha q c_1} + \frac{q^2 c_2^2}{c_1^2 - \alpha q c_1} \equiv \frac{(c_1 - q c_2)^2}{c_1^2 - \alpha q c_1}\,. \tag{70}$$

Using Eq. (52) in Eq. (70) followed by Eq. (30), we find

$$I_2 = \frac{\eta}{r_\mathrm{e}\,(c_1 - q\,c_2)}\;. \tag{71}$$

Substituting Eq. (67) and Eq. (71) in Eq. (65) and eliminate $c_1$ from Eq. (58), we have for the quantum correction

$$Q_c = \frac{\pi\eta}{\alpha r_\mathrm{e}} \left( -\frac{1}{q} + \frac{\eta}{\alpha q^2 \omega r_\mathrm{e}} \right). \tag{72}$$

The other integral on the right hand side of Eq. (7) is obtained in terms of variable $y$ as

$$I = -\frac{1}{\alpha}\int_{y_{nA}}^{y_{nB}} \mathrm{k}_{n\ell}(y) \frac{\mathrm{d}y}{y\,(1-q\,y)} \qquad . \tag{73}$$

Putting Eq. (43) in Eq. (73) and using Eq. (30) to eliminate A in the result, this gives

$$I = -\frac{\eta}{\alpha r_\mathrm{e}}\int_{y_{nA}}^{y_{nB}} \frac{\sqrt{(y-y_{nA})(y_{nB}-y)}}{y\,(1-q\,y)}\,\mathrm{d}\,y\,. \tag{74}$$

In order to evaluate the integral in Eq. (74) we use the following standard integral [25]

$$\int_{y_{nA}}^{y_{nB}} \frac{\sqrt{(y-y_{nA})(y_{nB}-y)}}{y(1+Qy)}\,\mathrm{d}y = \pi\left\{-\frac{1}{Q}-\sqrt{y_{nA}y_{nB}}+\frac{\sqrt{(Qy_{nA}+1)(Qy_{nB}+1)}}{Q}\right\}. \tag{75}$$

Therefore, by using the definite integral of Eq. (75) we obtained,

$$I = \frac{\pi\eta}{\alpha r_{\mathrm{e}}}\left\{-\frac{1}{q}+\sqrt{y_{nA}\,y_{nB}}-\sqrt{\frac{1}{q^2}+\frac{B}{qA}+y_{nA}\,y_{nB}}\right\}. \tag{76}$$

Substitute Eq. (72) and Eq. (76) in Eq. (7) to get

$$\sqrt{y_{nA}\,y_{nB}}-\sqrt{\frac{1}{q^2}+\frac{B}{qA}+y_{nA}\,y_{nB}} = \frac{N\alpha r_{\mathrm{e}}}{\eta}+\frac{\eta}{\alpha r_{\mathrm{e}}\,\omega q^2}, \tag{77}$$

Eq. (77) can be solved for the ro-vibrational energy $E_{n\ell}$ of the improve Tietz potential, by substituting Eq. (59) on the right hand side of Eq. (77) and recalling that $N = n + 1$, this transforms to

$$\sqrt{y_{nA}\,y_{nB}}-\sqrt{\frac{1}{q^2}+\frac{B}{qA}+y_{nA}\,y_{nB}} = \frac{n+\omega}{q\sqrt{\omega^2-\omega}}, \tag{78}$$

Solving for $y_{nA}$ $y_{nB}$ and using Eq. (38), we find

$$E_{n\ell}\to E_{n\ell ITP} = \frac{\hbar^2\lambda^2}{2\mu r_e^2}-\frac{\hbar^2\alpha^2}{2\mu}\left\{\frac{q\tau\omega(\omega-1)}{2(n+\omega)}-\frac{n+\omega}{2}\right\}^2, \tag{79}$$

where $E_{n\ell\mathrm{ITP}}$ designates the ro-vibrational energy of the improved Tietz potential, and

$$\tau = \frac{1}{q}+\frac{\kappa^2}{\eta^2}. \tag{80}$$

If we replace the parameters; $\tau$, $\omega$, $\lambda$ and subsequently, $\eta$ and $\kappa$ in Eq. (79), the rotation-vibration energy levels of the improved Tietz potential, derived by Tang *et al*. [13] which was obtained using the approach of ansatz solution, is exactly reproduced. It must be emphasized that Eq. (79) is only valid for $q \neq 0$. However, if $q = 0$, the expression on the right hand side of Eq. (79) becomes infinite (this is immediately evident from Eq. (80) and also from Eq. (25) of ref. [13]. In the event of letting $q = 0$ in Eq. (12), the improved Tietz potential reduces to the well-known Morse oscillator [1, 7], *viz*.

$$V(r)\to V_M(r) = D_{\mathrm{e}}\left\{1-\mathrm{e}^{-\alpha(r-r_{\mathrm{e}})}\right\}^2, \tag{81}$$

where $V_{\mathrm{M}}(r)$ is the Morse potential, as a result, Eq. (14) gives

$$\alpha\to\alpha_M = \omega_{\mathrm{e}}\left(\frac{2\mu}{D_{\mathrm{e}}}\right)^{\frac{1}{2}}. \tag{82}$$

In all subsequent notations, when the subscript "M" is used, it refers to "Morse". In order to deduce the ro-vibrational energy eigenvalues of the Morse potential, we will re-evaluate the quantum correction $Q_{\mathrm{cM}}$ and the momentum integral $I_{\mathrm{M}}$ and re-write the exact quantization rule of Eq. (7) for the Morse potential as

$$\mathrm{I}_{\mathrm{M}} = N\pi+\mathrm{Q}_{\mathrm{cM}}. \tag{83}$$

First it must be noted that with q = 0, Eq. (52) gives, with $c_1$ replaced by $c_{1\mathrm{M}}$

$$c_{1\mathrm{M}} = \frac{\sqrt{2\mu A}}{\hbar}\equiv\frac{\eta}{r_{\mathrm{e}}}. \tag{84}$$

The quantum correction in Eq. (62) gives

$$\mathrm{Q}_{\mathrm{cM}} = \frac{\eta}{\alpha r_{\mathrm{e}}}\int_{y_{0A}}^{y_{nB}}\frac{(y-c_{2M}/c_{1M})(y+B/2A)}{y}\frac{\mathrm{d}y}{\sqrt{(y-y_{0A})(y_{0B}-y)}}. \tag{85}$$

Dividing out the integrand in Eq. (85) leads to

$$\mathrm{Q}_{\mathrm{cM}} = \frac{\eta}{\alpha r_{\mathrm{e}}}\int_{y_{0A}}^{y_{nB}}\left\{y+\frac{B}{2A}-\frac{c_{2\mathrm{M}}}{c_{1\mathrm{M}}}-\frac{c_{2\mathrm{M}}B}{2c_{1\mathrm{M}}Ay}\right\}\frac{\mathrm{d}y}{\sqrt{(y-y_{0A})(y_{0B}-y)}}. \tag{86}$$

The integral of Eq. (86) can be evaluated by means of the following standard integral [22]

$$\int_{y_{nA}}^{y_{nb}}\frac{y\,\mathrm{d}y}{\sqrt{(y-y_{nA})(y_{nB}-y)}} = \tfrac{1}{2}\pi(y_{nA}+y_{nB}), \tag{87}$$

$$\int_{y_{nA}}^{y_{nb}} \frac{\mathrm{d}\,y}{\sqrt{\left(y-y_{nA}\right)\left(y_{nB}-y\right)}} = \pi \,, \tag{88}$$

$$\int_{y_{nA}}^{y_{nb}} \frac{\mathrm{d}\,y}{y\sqrt{\left(y-y_{nA}\right)\left(y_{nB}-y\right)}} = \frac{\pi}{\sqrt{y_{nA}\,y_{nB}}} \,, \tag{89}$$

$$\int_{y_{nA}}^{y_{nb}} \frac{\sqrt{\left(y-y_{nA}\right)\left(y_{nB}-y\right)}}{y}\mathrm{d}\,y = \pi\left\{ \tfrac{1}{2}\left(y_{nA}+y_{nB}\right) - \sqrt{y_{nA}\,y_{nB}} \;\right\} \cdot \tag{90}$$

By applying the integrals defined in Eq. (87)-Eq. (89) on Eq. (86), we obtained

$$\mathrm{Q}_{\mathrm{cM}} = \frac{\pi\eta}{\alpha\, r_{\mathrm{e}}}\left\{ \tfrac{1}{2}\left(y_{0A}+y_{0B}\right) + \frac{B}{2A} - \frac{c_{2\mathrm{M}}}{c_{1\mathrm{M}}} - \frac{c_{2\mathrm{M}}\,B}{2\,c_{1\mathrm{M}}A}\frac{1}{\sqrt{y_{0A}y_{0B}}} \right\} \cdot \tag{91}$$

Using Eq. (53) and Eq. (54) with $q$ = 0 while $c_1$, and $c_2$ are replaced by $c_{1\mathrm{M}}$ and $c_{2\mathrm{M}}$ respectively, get

$$\mathrm{Q}_{\mathrm{cM}} = -\frac{\pi}{2} \,, \tag{92}$$

similarly, the momentum integral of Eq. (74) with $q$ = 0, gives

$$\mathrm{I}_{\mathrm{M}} = -\frac{\eta}{\alpha\, r_{\mathrm{e}}} \int_{y_{nA}}^{y_{nB}} \frac{\sqrt{\left(y-y_{nA}\right)\left(y_{nB}-y\right)}}{y}\mathrm{d}\,y \cdot \tag{93}$$

Using the standard integral of Eq. (70) on Eq. (93), get

$$\mathrm{I}_{\mathrm{M}} = -\frac{\pi\eta}{\alpha\, r_{\mathrm{e}}}\left( \frac{\kappa^2}{2\eta^2} + \sqrt{y_{nA}\,y_{nB}} \right) \cdot \tag{94}$$

Inserting the results in Eq. (92) and Eq. (94) in Eq. (83) and remembering that $N = n + 1$, we find the ro-vibrational energy eigenvalues of the Morse potential as

$$E_{n\ell\mathrm{M}} = \frac{\lambda^2\hbar^2}{2\mu r_{\mathrm{e}}^2} - \frac{\alpha^2\hbar^2}{2\mu}\left( n + \tfrac{1}{2} + \frac{\kappa^2}{2\eta\alpha\, r_{\mathrm{e}}} \right)^2 , \tag{95}$$

where $\alpha$ is given by Eq. (82).

### 2.3 The radial wave functions of the improved Tietz potential

We can obtain the radial wave functions corresponding to the energy eigenvalues of the improved Tietz potential by solving the Riccati equation, therefore, in Eq. (47), therefore, if we let

$$z = 1 - q\,y \,, \tag{96}$$

and use the logarithmic definition of the phase angle, $\phi_{n\ell}$ ($y$) to recover the wave function $\mathrm{U}_{n\ell}$ ($y$) in terms of the variable $z$, we have

$$z\left(1-z\right)\mathrm{U}''_{n\ell}\left(z\right) + \left(1-2z\right)\mathrm{U}'_{n\ell}\left(z\right) + \left( \varepsilon_1 - \frac{\varepsilon_1-\varepsilon_2+\varepsilon_3}{z} - \frac{\varepsilon_3}{1-z} \right)\mathrm{U}_{n\ell}\left(z\right) = 0 \,, \tag{97}$$

where the constants $\varepsilon_1$, $\varepsilon_2$ and $\varepsilon_3$ are given by

$$\varepsilon_1 = \frac{2\mu A}{\alpha^2\hbar^2 q^2} \,, \tag{98}$$

$$\varepsilon_2 = \frac{2\mu B}{\alpha^2\hbar^2 q} \,, \tag{99}$$

$$\varepsilon_3 = \frac{2\mu}{\alpha^2\hbar^2}\left(C - E_{n\ell}^{\mathrm{ITP}}\right) \cdot \tag{100}$$

Eq. (97) is satisfied by the following ansatz [9] solution

$$\mathrm{U}_{n\ell}\left(z\right) = N_{n\ell}\, z^{\sigma}\left(1-z\right)^{\upsilon}\Omega_{n\ell}\left(z\right) , \tag{101}$$

where the constants $\sigma$, $\upsilon$ and the function $\Omega_{n\ell}$ (z) are chosen such that

$$\sigma = \left(\varepsilon_1 - \varepsilon_2 + \varepsilon_3\right)^{\frac{1}{2}} , \tag{102}$$

$$\upsilon = \varepsilon_3^{\frac{1}{2}} , \tag{103}$$

and

$$\Omega_{n\ell}\left(z\right) = {}_2F_1\left(-n, n+2\sigma+2\upsilon+1; 2\sigma+1; z\right) . \tag{104}$$

$N_{n\ell}$ being the normalization constant and ${}_2F_1$ is the hypergeometric function. In the event that $q = 0$, both $\varepsilon_1$ and $\varepsilon_2$ are infinite, thus, making $U_{n\ell}$ (z) infinite, which is unphysical for a wave function. In order to have a physically acceptable wave functions we insert $q = 0$ in Eq. (47), using Eq. (23) and the logarithmic definition of the phase angle, we find

$$y^2 \mathrm{u}''_{n\ell}(y) + y\,\mathrm{u}'_{n\ell}(y) + \left(-\varepsilon_4 y^2 + \varepsilon_5 y - \varepsilon_6\right)\mathrm{u}_{n\ell}(y) = 0\,, \tag{105}$$

where

$$\varepsilon_4 = \frac{2\mu A}{\alpha^2\hbar^2}\cdot \tag{106}$$

$$\varepsilon_5 = -\frac{2\mu B}{\alpha^2\hbar^2}\,, \tag{107}$$

$$\varepsilon_6 = \frac{2\mu}{\alpha^2\hbar^2}\left(C - E_{n\ell\mathrm{M}}\right)\cdot \tag{108}$$

In order to solve Eq. (105), following [1, 15], we assume ansatz of the form

$$\mathrm{u}_{n\ell\mathrm{M}}(y) = N_{n\ell M}\,\mathrm{e}^{-\frac{1}{2}\beta y}\,y^{\frac{1}{2}\nu}\,\Omega_{n\ell\mathrm{M}}(y)\,. \tag{109}$$

Eq. (109) is a solution of Eq. (105) if constants $\beta$, $\nu$ and the function $\Omega_{n\ell M}$ (y) are chosen so that

$$\beta = 2\,\varepsilon_4^{\frac{1}{2}}\,, \tag{110}$$

$$\nu = 2\,\varepsilon_6^{\frac{1}{2}}\,, \tag{111}$$

and

$$\Omega_{n\ell\mathrm{M}}(y) = {}_1\mathrm{F}_1\left(-n, \nu+1; \beta y\right), \tag{112}$$

where ${}_1F_1$ is the hypergeometric function and $N_{n\ell M}$ is the normalization constant.

## 3.0 Results and Discussion

Table 1 shows the input spectroscopic model parameters of diatomic molecules used in the present work.

**Table 1: Spectroscopic model parameters of diatomic molecules used in the present work**

| **property** | **Molecule** | | | |
|---|---|---|---|---|
| | HCl | LiH | CO | $H_2$ |
| $\mu$ (amu) [7] | 0.9801045 | 0.8801221 | 6.8606719 | 0.50391 |
| $D_e$ (eV) [7] | 4.61907 | 2.515287 | 11.2256 | 4.7446 |
| $r_e$ (Å) [7] | 1.2746 | 1.5956 | 1.1283 | 0.7416 |
| $\omega_e$ ($cm^{-1}$) [27] | 2990.9 | 1405.5 | 2169.8 | 4401.2 |
| $\alpha_e$ ($cm^{-1}$) [27] | 0.3069985 | 0.2163911 | 0.01750513 | 3.0622 |

The data in Table 2 shows computed values of $q$ and $\alpha$ obtained from Eq. (14) and Eq. (15) respectively applied to four diatomic molecules *viz*: HCl, LiH, CO and $H_2$, also shown in the table are, corresponding to $q = 0$, the values of $\alpha$ calculated from Eq. (15) and from the literature. The result shows that our computed values of $\alpha$ at $q = 0$ are in close agreement with those in the literature.

**Table 2: Computed values of potential parameters**

| Molecules | $q \neq 0$ | | $q = 0$ | |
|---|---|---|---|---|
| | | | $\alpha$ ($Å^{-1}$) | |
| | $q$ | $\alpha$ ($Å^{-1}$) | PR | [7] |
| HCl | 0.01141643 | 1.87014967 | 1.86818303 | 2.238057 |
| LiH | -0.29507995 | 1.06671325 | 1.12736073 | 1.7998368 |
| CO | -0.26900708 | 2.25129679 | 2.30008783 | 2.59441 |
| $H_2$ | -0.40887291 | 1.72339457 | 1.94492460 | 1.440558 |

To further ascertain the validity of our results, Table 3 shows computed bound states ro-vibrational energies in the form of - ($E_{n\ell} - D_e$) of the improved Tietz potential calculated using Eq. (79) and Eq. (80), where $q \neq 0$ and $q = 0$ respectively, the computation was carried out for four diatomic molecules *viz*. HCl, LiH, CO, and $H_2$. To enable us compare results with available data, we have included columns for the results of - ($E_{n\ell} - D_e$) adopted from the literature corresponding to $q = 0$ which was obtained by generalized pseudospectral (GPS) method [17] for Morse potential, the results show an excellent agreement between the present result (PR) and the literature data. It is also worthy to note the peculiar results of HCl, here, $q$ (0.01141643) is numerically small, thus, the ro-vibrational energy eigenvalues corresponding to $q \neq 0$ quite agree with those of $q = 0$ for all quantum states, however, this remarkable trend does not hold for $H_2$, LiH and CO since $|\,q\,|$ for this molecules is relatively large. Figures 1-3 shows graphical representation of unnormalized wave functions of the HCl molecule for 2s, 3p and 4d quantum states, except for the different scales used for the plots, the shapes of the unnormalized wave functions for the improved Tietz and Morse potentials are quite identical.

**Table 3 Bound states energy eigenvalues – ($E_{n\ell} - D_e$) (in eV) of improved Tietz potential**

| State | | HCl | | | LiH | | | CO | | | $H_2$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | $q \neq 0$ | $q = 0$ | | $q \neq 0$ | $q = 0$ | | $q \neq 0$ | $q = 0$ | | $q \neq 0$ | $q = 0$ | |
| $n$ | $\ell$ | | PR | [7] | | PR | [7] | | PR | [7] | | PR | [7] |
| 0 | 0 | 4.43551688 | 4.43551688 | 4.43556394 | 2.60317357 | 2.42891174 | 2.42886321 | 11.36051089 | 11.09149515 | 11.09153532 | 5.02141451 | 4.47568270 | 4.47601313 |
| | 1 | 4.43292800 | 4.43293039 | 4.43297753 | 2.60139954 | 2.42707057 | 2.42702210 | 11.36003817 | 11.09101858 | 11.09105875 | 5.00866166 | 4.46089838 | 4.46122852 |
| | 2 | 4.42775180 | 4.42775896 | 4.42780630 | 2.59785406 | 2.42339075 | 2.42334244 | 11.35909276 | 11.09006547 | 11.09010565 | 4.98329734 | 4.43146360 | 4.43179975 |
| | 5 | 4.39673856 | 4.39677438 | … | 2.57665351 | 2.40138265 | … | 11.35342078 | 11.08434731 | … | 4.83494763 | 4.25847387 | … |
| | 10 | 4.29390333 | 4.29403464 | 4.29440924 | 2.50686824 | 2.32888569 | 2.3288546 | 11.33452050 | 11.06529309 | 11.0653333 | 4.38306134 | 3.72153731 | 3.7247470 |
| 1 | 0 | 4.07955996 | 4.07957467 | 4.07971006 | 2.78383063 | 2.26068851 | 2.26054805 | 11.63282097 | 10.82570300 | 10.82582206 | 5.60284482 | 3.96138272 | 3.96231534 |
| | 1 | 4.07704796 | 4.07706518 | 4.07720144 | 2.78200252 | 2.25889518 | 2.25875559 | 11.63234403 | 10.82523051 | 10.82534959 | 5.58930757 | 3.94715064 | 3.94811647 |
| | 2 | 4.07202550 | 4.07204776 | 4.07218579 | 2.77834895 | 2.25531102 | 2.25517324 | 11.63139018 | 10.82428554 | 10.82440465 | 5.56238326 | 3.91881415 | 3.91986423 |
| | 5 | 4.04193429 | 4.04198674 | … | 2.75650150 | 2.23387547 | … | 11.62566758 | 10.81861628 | … | 5.40491329 | 3.75224506 | … |
| | 10 | 3.94216718 | 3.94232023 | … | 2.68458017 | 2.16327014 | … | 11.60659855 | 10.79972503 | … | 4.92529748 | 3.23482034 | … |
| 2 | 0 | 3.73847558 | 3.73851783 | 3.73873384 | 2.97092289 | 2.09850164 | 2.09827611 | 11.90842813 | 10.56313425 | 10.56333028 | 6.22081378 | 3.47846220 | 3.47991882 |
| | 1 | 3.73604046 | 3.73608534 | 3.73630382 | 2.96904027 | 2.09675617 | 2.09653304 | 11.90794697 | 10.56266584 | 10.56286190 | 6.20646352 | 3.46478238 | 3.46633875 |
| | 2 | 3.73117177 | 3.73122192 | 3.73144539 | 2.96527774 | 2.09326766 | 2.09304950 | 11.90698467 | 10.56172903 | 10.56192516 | 6.17792241 | 3.43754417 | 3.43932836 |
| | 5 | 3.70200272 | 3.70208446 | … | 2.94277819 | 2.07240466 | … | 11.90121140 | 10.55610866 | … | 6.01100221 | 3.27739571 | … |
| | 10 | 3.60530418 | 3.60549119 | … | 2.86870371 | 2.00369097 | … | 11.88197351 | 10.53738039 | … | 5.50267667 | 2.77948283 | … |
| 3 | 0 | 3.41226561 | 3.41234635 | … | 3.16448853 | 1.94235114 | … | 12.18733495 | 10.30378892 | … | 6.87613872 | 3.02692115 | … |
| | 1 | 3.40990740 | 3.40999087 | … | 3.16255095 | 1.94065353 | … | 12.18684956 | 10.30332458 | … | 6.86094517 | 3.01379358 | … |
| | 2 | 3.40519249 | 3.40528145 | … | 3.15867858 | 1.93726068 | … | 12.18587881 | 10.30239591 | … | 6.83072716 | 2.98765366 | … |
| | 5 | 3.37694573 | 3.37706756 | … | 3.13552165 | 1.91697022 | … | 12.18005484 | 10.29682445 | … | 6.65400764 | 2.83392584 | … |
| | 10 | 3.28331621 | 3.28354752 | … | 3.05927661 | 1.85014817 | … | 12.16064792 | 10.27825915 | … | 6.11593562 | 2.35552479 | … |
| 5 | 0 | 2.80447648 | 2.80465948 | … | 3.57119448 | 1.64815927 | … | 12.75505784 | 9.79476847 | … | 8.30226528 | 2.21797747 | … |
| | 1 | 2.80227210 | 2.80245802 | … | 3.56914564 | 1.64655735 | … | 12.75456399 | 9.79431228 | … | 8.28528729 | 2.20595441 | … |
| | 2 | 2.79786484 | 2.79805660 | … | 3.56505084 | 1.64335581 | … | 12.75357632 | 9.79339991 | … | 8.25152109 | 2.18201106 | … |
| | 5 | 2.77146306 | 2.77168984 | … | 3.54056286 | 1.62421046 | … | 12.74765080 | 9.78792624 | … | 8.05407414 | 2.04112450 | … |
| | 10 | 2.68397288 | 2.68431627 | … | 3.45992321 | 1.56117167 | … | 12.72790544 | 9.76968691 | … | 7.45315832 | 1.60174713 | … |
| 7 | 0 | 2.25620765 | 2.25651408 | … | 4.00426120 | 1.37811287 | … | 13.33601026 | 9.29864165 | … | 9.88833728 | 1.53455167 | … |
| | 1 | 2.25415715 | 2.25446664 | … | 4.00209921 | 1.37660666 | … | 13.33550794 | 9.29819361 | … | 9.86943160 | 1.52363311 | … |
| | 2 | 2.25005762 | 2.25037321 | … | 3.99777825 | 1.37359643 | … | 13.33450332 | 9.29729755 | … | 9.83183274 | 1.50188633 | … |
| | 5 | 2.22550134 | 2.22585358 | … | 3.97193682 | 1.35559618 | … | 13.32847609 | 9.29192167 | … | 9.61200670 | 1.37384105 | … |
| | 10 | 2.14415224 | 2.14462648 | … | 3.88682900 | 1.29634066 | … | 13.30839173 | 9.27400829 | … | 8.94334700 | 0.97348735 | … |

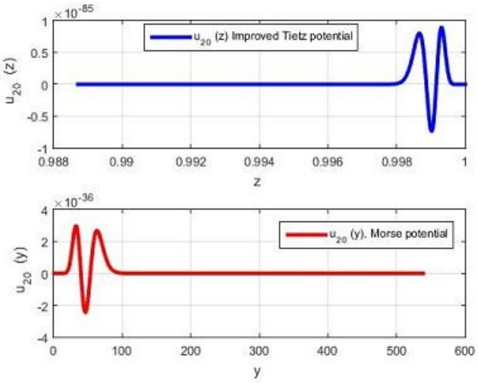

**Figure 1: Unnormalized radial wave function of the HCl molecule for 2s state**

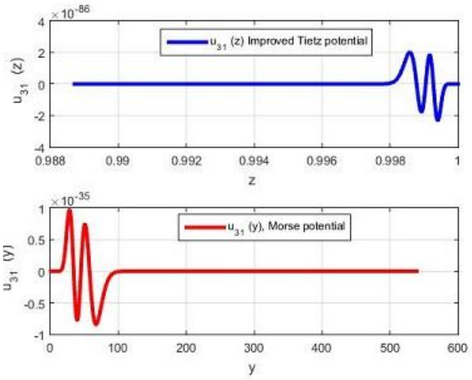

**Figure 2: Unnormalized radial wave function of the HCl molecule for 3p state**

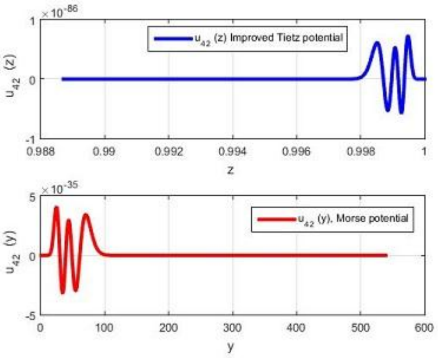

**Figure 3: Unnormalized radial wave function of the HCl molecule for 4d state[**

## 4.0 Conclusion

We have applied exact quantization rule and ansatz solution method to obtain bound state ro-vibrational energy eigenvalues and unnormalized radial wave functions of the improved Tietz potential, by considering the special case of q = 0, we have also deduced the energy eigenvalues of the molecular Morse potential and also its radial wave function. The results of this work might be useful in areas of solid state, molecular or chemical physics.

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