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SPEED OF DIATOMIC MOLECULES IN SHIFTED TIETZ-WEI POTENTIAL

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Abstract

In this work, the shape invariant formalism of SUSYQM is employed in the derivation of approximate equation of bound state energy eigenvalues of the shifted Tietz-Wei potential (STWP). A Pekeris-type approximation model is used to eliminate the centrifugal term of the Schrödinger equation. The expression of bound state energy eigenvalues is used to obtain equation of speed of the system based on the Hellmann-Feynman theorem. Numerical data of bound state energy eigenvalues and speed of two diatomic molecules including O_2 ($X\ ^3\Sigma_g^-$) and NO ($X^2\ \Pi_f$) are obtained. The calculated energies are in excellent agreement with available literature data of the diatomic molecules. The results also show that the speed of the examined diatomic molecules increases with increase in vibrational quantum number and decreases with increasing rotational quantum number.

Keywords: Shifted Tietz-Wei potential, Tietz-Hua potential, SUSYQM, eigen energies, speed of diatomic molecules

1. Introduction

In the regime of relativistic and nonrelativistic quantum mechanics, it is natural to use the potential energy function to relate the interaction of a system with its environment [1, 2]. Information regarding the quantum system is obtained by solving a wave equation for the potential describing the system [3, 4].

One of the major obstacles encountered in this area of research is the absence of a universal potential model capable of explaining every atomic and molecular interactions [1, 2]. To surmount this problem, different potentials have been suggested to explaining observed atomic and molecular phenomena [5-8]. Some of the potentials include amongst others: Möbius squared potential [9, 10], Manning-Rosen potential [11-13], generalized Morse potential [14], Tietz potential [3, 15], Eckart potential [5] and Tietz-Hua potential [16-18].

A diatomic molecule potential energy function is required to fit the spectroscopic parameters of a prescribed diatomic molecule. The more number of parameters fitted by the potential, better the model [2, 19]. Unfortunately, many of the known potential models have failed to satisfy these restrictions, for this reason, improved versions of diatomic molecule potentials have been constructed [20-24].

Solution of Schrödinger equation have been used to study many physical properties of a system, such as oscillator strength [25, 26], spherical quantum dots [27], quantum information entropies [28, 29] and thermodynamics properties [30-32] among others. In the present work, the STWP is examined, it is given as [29, 32]

$$V(r)=D_{\mathrm{e}}\left\{\frac{2(c_{\mathrm{h}}-1)\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}-(c_{\mathrm{h}}^{2}-1)\mathrm{e}^{-2b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{\left[1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}\right]^{2}}\right\}, \tag{1}$$

where D_e is the dissociation energy, r_e is the equilibrium bond length, $b_h = \beta\,(1 - c_h)$, c_h is an optimization parameter, β is the Morse constant and r is the internuclear separation. The shifted Tietz-Wei potential has been used to study properties of

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Corresponding Author**:** Mark Z.K., Email: kwajimarkus6@gmail.com, Tel: +2348111811813, +2348036870057 (EES) diatomic molecules [33-35]. By employing the STWP to represent the internal vibration of diatomic molecules, analytical equation for the prediction of molar entropy of pure substances is derived, the equation has been successful in predicting the molar entropy of some diatomic molecules [29]. It is worth mentioning that in previous studies, the speed of diatomic molecules in the shifted Tietz-Wei potential has not been studied in the literature and worth investigating. The present work is aimed at obtaining speed of diatomic molecules in in the STWP. The paper is organized as follows: In section 2, bound state energy spectra of STWP is derived via supersymmetric quantum mechanics (SUSYQM) approach. Section 3 is devoted to derivation of normalized radial eigenfunctions of STWP. In section 4, expression for speed of diatomic molecules in STWP is derived in the context of Hellmann-Feynman theorem. Results obtained are discussed in section 5. A brief conclusion of the work is presented in section 6.

2. Bound state energy spectra of the STWP

The energy spectrum $E_{\nu J}$ of a quantum mechanical system of reduced mass μ in a potential $V(r)$ is obtained by solving the Schrödinger equation for the system. In a three-dimensional coordinate system, the radial Schrödinger equation reads [18, 19]

$$\left\{\frac{\mathrm{p}^2}{2\mu}+V_{\mathrm{eff}}(r)\right\}\mathrm{u}_{\nu J}(r)=E_{\nu J}\,\mathrm{u}_{\nu J}(r), \tag{2}$$

where $\mathrm{u}_{\nu J}$ represent the radial eigenfunctions, $V_{\mathrm{eff}}(r)$ is the effective potential of the system expressed as

$$V_{\mathrm{eff}}(r)=V(r)+\frac{L\hbar^2}{2\mu r^2}\,. \tag{3}$$

the second term in (3) is the centrifugal, $L = J(J + 1)$ is the angular momentum of the system, J is the rotational quantum number term, ν denotes the vibrational quantum number and p is the momentum operator given by [6]

$$\mathrm{p}(r)=-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}r}\,. \tag{4}$$

Substituting equation (1) into (3) gives

$$V_{\mathrm{eff}}(r)=D_{\mathrm{e}}\left\{\frac{2(c_{\mathrm{h}}-1)\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}-(c_{\mathrm{h}}^2-1)\mathrm{e}^{-2b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{\left[1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}\right]^2}\right\}+\frac{L\hbar^2}{2\mu r^2}\,. \tag{5}$$

Due to the presence of the centrifugal term in (5), equation (2) has no exact analytical solution, except for the pure vibrational state ($J = 0$). However, approximate analytical solution is possible by means of a suitable approximation model. Here, like in previous works [33, 35], the Pekeris-like approximation model is used, it assumes the form [9]

$$\frac{L\hbar^2}{2\mu r^2}\approx\frac{L\hbar^2}{2\mu}\left\{c_0+\frac{c_1\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}+\frac{c_2\,\mathrm{e}^{-2\mathrm{b}_{\mathrm{h}}(r-\mathrm{r}_{\mathrm{e}})}}{\left[1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}\right]^2}\right\}, \tag{6}$$

where the constant coefficients c_{-1+j} (j = 1, 2, 3) are given in closed form as

$$c_{-1+j}=\frac{(2-j)(3-j)}{2r_{\mathrm{e}}^2}+\frac{(-1)^j\,2(4-j+c_{\mathrm{h}})(1-c_{\mathrm{h}})^j}{(-1+j)!(3-j)!b_{\mathrm{h}}\,r_{\mathrm{e}}^3}+\frac{(-1)^{-1+j}\,6(1-c_{\mathrm{h}})^{1+j}}{(-1+j)!(3-j)!b_{\mathrm{h}}^2\,r_{\mathrm{e}}^4}\,. \tag{7}$$

With the aid of equations (4)- (6), (2) gives

$$\frac{\mathrm{u}''_{\nu J}(r)}{\mathrm{u}_{\nu J}(r)}=-\lambda_{\nu J}-\frac{\lambda_1}{c_{\mathrm{h}}}\frac{\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}+\frac{\lambda_2}{\mathrm{c}_{\mathrm{h}}}\frac{\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{\left[1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}\right]^2}, \tag{8}$$

where prime denotes derivative with respect to the argument in parenthesis and parameters $\lambda_{\nu J}$, λ_1 and λ_2 are given by

$$\lambda_{\nu J}=\frac{2\mu E_{\nu J}}{\hbar^2}-Lc_0, \tag{9}$$

$$\lambda_1=-L(c_1c_{\mathrm{h}}-c_2)-\frac{2\mu D_{\mathrm{e}}}{\hbar^2}(c_{\mathrm{h}}^2-1), \tag{10}$$

$$\lambda_2=Lc_2+\frac{2\mu D_{\mathrm{e}}}{\hbar^2}(c_{\mathrm{h}}-1)^2\,. \tag{10}$$

Assuming supersymmetry (SUSY) as one in which $E_{0\mathrm{J}} = 0$, expression (8) is satisfied by

$$\mathrm{u}_{0J}(r)=N_{0J}\exp\left(-\int\varphi(r)\,\mathrm{d}r\right), \tag{11}$$

where $N_{0\mathrm{J}}$ is the normalization constant for the ground state wave function and φ is known as the superpotential [8, 13, 25]. Inserting equation (11) into (8) leads to the Riccati differential equation given by

$$\varphi^2-\varphi'\equiv-\lambda_{0J}-\frac{\lambda_1}{c_{\mathrm{h}}}\frac{\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}+\frac{\lambda_2}{c_{\mathrm{h}}}\frac{\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{\left[1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}\right]^2}\,. \tag{12}$$

In order to solve equation (12), a trial solution of the following form is chosen

$$\varphi=-A\frac{\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}+B\,, \tag{13}$$

where A and B are constant. Upon substituting equation (13) into (12) and comparing coefficients gives

$$A=-\sigma\, b_{\mathrm{h}}\, c_{\mathrm{h}}\,, \tag{14}$$

$$B=\frac{\lambda_1}{2Ac_{\mathrm{h}}}-\frac{\mathrm{A}}{2c_{\mathrm{h}}}\,, \tag{15}$$

$$\lambda_{0J}=-\left(\frac{\lambda_1}{2Ac_{\mathrm{h}}}-\frac{\mathrm{A}}{2c_{\mathrm{h}}}\right)^2\cdot \tag{16}$$

where

$$\sigma=\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{\lambda_2}{b_{\mathrm{h}}^2\,c_{\mathrm{h}}^2}}\equiv\frac{1}{2}+\frac{1}{2}\sqrt{1+\frac{4Lc_2}{b_{\mathrm{h}}^2\,c_{\mathrm{h}}^2}+\frac{8\mu D_{\mathrm{e}}}{b_{\mathrm{h}}^2\,\hbar^2}\left(1-\frac{1}{c_{\mathrm{h}}}\right)^2}\cdot \tag{17}$$

Having obtained A and B, the next task in the SUSYQM method is to construct a pair of partner potentials given as [13, 23, 25]

$$V_-(r)\equiv\varphi^2-\varphi'=\left(\frac{\lambda_1}{2c_{\mathrm{h}}\,A}-\frac{\mathrm{A}}{2c_{\mathrm{h}}}\right)^2-\frac{\left(A^2/c_{\mathrm{h}}+2AB\right)\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}+\frac{\left(A^2/c_{\mathrm{h}}-Ab_{\mathrm{h}}\right)\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{\left[1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}\right]^2}\,, \tag{18}$$

$$V_+(r)\equiv\varphi^2+\varphi'=\left(\frac{\lambda_1}{2c_{\mathrm{h}}\,A}-\frac{A}{2c_{\mathrm{h}}}\right)^2-\frac{\left(A^2/c_{\mathrm{h}}+2AB\right)\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}+\frac{\left(A^2/c_{\mathrm{h}}+Ab_{\mathrm{h}}\right)\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}}{\left[1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}\right]^2}\,. \tag{19}$$

If shape invariant condition of SUSYQM holds [13, 23, 25], then equations (19) and (18) are related by

$$V_+(r,a_0)=V_-(r,a_1)+R(a_1)\,, \tag{20}$$

where a_1 is a new set of parameters determined from the old set $a_0\equiv A$ via the following relations $a_1 = a_0 - b_{\mathrm{h}}\, c_{\mathrm{h}}$, $a_2 = a_0 - 2\, b_{\mathrm{h}}\, c_{\mathrm{h}}$, …, $a_v = a_0 - \nu\, b_{\mathrm{h}}\, c_{\mathrm{h}}$. R ($a_1$) is the remainder and is independent of r, it follows that

$$R(a_1)=\left(\frac{\lambda_1}{2c_{\mathrm{h}}\,a_0}-\frac{a_0}{2c_{\mathrm{h}}}\right)^2-\left(\frac{\lambda_1}{2c_{\mathrm{h}}\,a_1}-\frac{a_1}{2c_{\mathrm{h}}}\right)^2, \tag{21}$$

or more generally,

$$R(a_k)=\left(\frac{\lambda_1}{2c_{\mathrm{h}}\,a_{k-1}}-\frac{a_{k-1}}{2c_{\mathrm{h}}}\right)^2-\left(\frac{\lambda_1}{2c_{\mathrm{h}}\,a_k}-\frac{a_k}{2c_{\mathrm{h}}}\right)^2, \tag{22}$$

Adapting procedures similar to those used in ref. [13, 23, 25], the energy eigenvalues are obtained as follows, define

$$\lambda_{\nu J}^{(-)}=\sum_{k=1}^{\nu}R(a_k)\cdot \tag{23}$$

Substituting equation (22) into (23) and expanding the summation, one obtains

$$\lambda_{\nu J}^{(-)}=\left(\frac{\lambda_1}{2c_{\mathrm{h}}\,a_0}-\frac{a_0}{2c_{\mathrm{h}}}\right)^2-\left(\frac{\lambda_1}{2c_{\mathrm{h}}\,a_\nu}-\frac{a_\nu}{2c_{\mathrm{h}}}\right)^2\equiv\left(\frac{\lambda_1}{2c_{\mathrm{h}}\,A}-\frac{A}{2c_{\mathrm{h}}}\right)^2-\left\{\frac{\lambda_1}{2c_{\mathrm{h}}\left(A-\nu b_{\mathrm{h}}\,c_{\mathrm{h}}\right)}-\frac{A-\nu b_{\mathrm{h}}\,c_{\mathrm{h}}}{2c_{\mathrm{h}}}\right\}^2. \tag{24}$$

The expression for the ro-vibrational energy spectrum is determined from

$$\lambda_{\nu J}=\lambda_{0J}+\lambda_{\nu J}^{(-)}\,. \tag{25}$$

Using relations (9), (16) and (24) in (25) and with the help of equation (14), the energy spectrum is obtained as

$$E_{\nu J}=\frac{L\hbar^2c_0}{2\mu}-\frac{b_{\mathrm{h}}^2\,\hbar^2}{2\mu}\left(\frac{\eta}{\rho}-\frac{\rho}{2}\right)^2\cdot \tag{26}$$

where $\eta = \lambda_1 / (2\, b_{\mathrm{h}}\, c_{\mathrm{h}})^2$, $\rho = \nu + \sigma$

3. Radial eigenfunctions of the STWP

For the sake of completeness and to enable us obtain speed estimates of diatomic molecules in the STWP, attention is now focused on the normalized radial eigenfunctions of this potential model. With the help of the following coordinate transformation

$$z=c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}(r-r_{\mathrm{e}})}\,, \tag{27}$$

Equation (8) takes the form

$$\mathrm{z}(1-z)\mathrm{u}''_{\nu J}(z)+(1-z)\mathrm{u}'_{\nu J}(z)+\left(\frac{\lambda_1}{b_{\mathrm{h}}^2\,c_{\mathrm{h}}^2}-\frac{\lambda_{\nu J}}{b_{\mathrm{h}}^2}+\frac{\lambda_{\nu J}}{b_{\mathrm{h}}^2}\frac{1}{z}-\frac{\lambda_2}{b_{\mathrm{h}}^2\,c_{\mathrm{h}}^2}\frac{1}{1-z}\right)\mathrm{u}_{\nu J}(z)=0\cdot \tag{28}$$

Following ref. [9, 25], equation (28) has solution of the form

$$\mathrm{u}_{\nu J}\left(z\right)=N_{\nu J}\;z^{\delta}\left(1-z\right)^{\sigma}\;{}_{2}\mathrm{F}_{1}\left(-\nu,\;\nu+2\delta+2\sigma;2\delta+1;z\right), \tag{29}$$

where ${}_2\mathrm{F}_1$ $(-\nu,\ \nu + 2\delta + 2\sigma;\ 2\delta + 1;\ z)$ is the hypergeometric function, $N_{\nu J}$ is the normalization constant and the parameter δ is given by

$$\delta=\frac{1}{b_{\mathrm{h}}}\left(-\lambda_{\nu J}\right)^{\frac{1}{2}}\cdot \tag{30}$$

Normalization of wave functions requires that

$$\int_{0}^{\infty}\left|\mathrm{u}_{\nu J}\left(r\right)\right|^{2}\mathrm{d}\,r=1\cdot \tag{31}$$

Inserting equation (27) into (31) and employing equation (29) to eliminate $\mathrm{u}_{\nu J}$ (z) we obtain

$$\mathrm{N}_{\nu J}=\left(\frac{b_{\mathrm{h}}}{\mathrm{M}_{\nu J}}\right)^{\frac{1}{2}}, \tag{32}$$

where the upper bound limit of integration is $z_{0}=c_{\mathrm{h}}\,\mathrm{e}^{b_{\mathrm{h}}\,r_{\mathrm{e}}}$,

$$\mathrm{M}_{\nu J}=\int_{0}^{z_{0}}z^{2\delta-1}\left(1-z\right)^{2\sigma}\left|{}_{2}\mathrm{F}_{1}\left(-\nu,\;\nu+2\delta+2\sigma;2\delta+1;z\right)\right|^{2}\mathrm{d}\,z\;. \tag{33}$$

4. Speed estimates of diatomic molecules in shifted Tietz Wei potential

An estimate of the speed of diatomic molecules can be deduced from uncertainty in momentum $\Delta\ p$ of the system, it is given by [6]

$$\Delta\,p=\left\{\langle p^{2}\rangle-\langle p\rangle^{2}\right\}^{\frac{1}{2}}, \tag{34}$$

where $< x >$ defines the expectation or mean value of quantity x. In this work, we will assume that the momentum p ($= \mu$v, v being the estimated speed of the diatomic molecule) is of the order of Δp, that is μv ~ Δp, this leads to

$$\mathrm{v}\square\;\frac{1}{\mu}\left\{\langle p^{2}\rangle-\langle p\rangle^{2}\right\}^{\frac{1}{2}}, \tag{35}$$

To obtain $\langle p^{2}\rangle$, the Hellmann-Feynman theorem (HFT) [9, 25], will be used. The HFT states that if the Hamiltonian H (ζ) of a quantum system is a function of some parameter, ζ, then H (r, ζ), $E_{\nu J}$ (ζ) and $\mathrm{u}_{\nu J}$ (r, ζ) are mathematically related by

$$\frac{\partial E_{\nu J}\left(\zeta\right)}{\partial\zeta}=\left\langle\mathrm{R}_{\nu J}\left(r,\;\zeta\right)\left|\frac{\partial\mathrm{H}\left(r,\;\zeta\right)}{\partial\zeta}\right|\mathrm{R}_{\nu J}\left(r,\;\zeta\right)\right\rangle\cdot \tag{36}$$

The Hamiltonian of the system is given by the expression in curly brackets in equation (2). Substituting equation (5) into (2), the Hamiltonian is written as

$$\mathrm{H}=\frac{\mathrm{p}^{2}}{2\mu}+D_{\mathrm{e}}\left\{\frac{2\left(c_{\mathrm{h}}-1\right)\mathrm{e}^{-b_{\mathrm{h}}\left(r-r_{\mathrm{e}}\right)}-\left(c_{\mathrm{h}}^{2}-1\right)\mathrm{e}^{-2b_{\mathrm{h}}\left(r-r_{\mathrm{e}}\right)}}{\left[1-c_{\mathrm{h}}\,\mathrm{e}^{-b_{\mathrm{h}}\left(r-r_{\mathrm{e}}\right)}\right]^{2}}\right\}+\frac{L\hbar^{2}}{2\mu r^{2}}\cdot \tag{37}$$

At this stage, equations (26) and (37) will be used to obtain the expression for the speed of diatomic molecules in the oscillator. Differentiating (37) and (26) with respect to L, we have

$$\frac{\partial\mathrm{H}}{\partial L}=\frac{\hbar^{2}}{2\mu r^{2}}, \tag{38}$$

$$\frac{\partial E_{\mathrm{vJ}}}{\partial L}=\frac{\hbar^{2}c_{0}}{2\mu}-\frac{\Omega^{\frac{1}{2}}}{\mu}\left\{\frac{c_{1}c_{\mathrm{h}}-c_{2}}{2\rho}-\frac{c_{2}}{\gamma\left(2\sigma-1\right)}\right\}, \tag{39}$$

where, for compactness, we have employed the following notations

$$\Omega=\left(\frac{\eta}{\rho}-\frac{\rho}{2}\right)^{2}, \tag{40}$$

$$\gamma^{-1}=\frac{\eta}{\rho^{2}}+\frac{1}{2}\cdot \tag{41}$$

Substituting equations (39) and (38) in (36) taking $\zeta = L$, we have the expectation value of the inverse separation squared as given by

$$\left\langle r^{-2}\right\rangle=c_{0}+\frac{\Omega^{\frac{1}{2}}}{c_{\mathrm{h}}^{2}}\left\{\frac{2c_{2}}{\gamma\left(2\sigma-1\right)}+\frac{c_{1}c_{\mathrm{h}}-c_{2}}{\rho}\right\}\cdot \tag{42}$$

Also, differentiating equation (37) with respect to μ and replacing the result in (36), we have

$$\left\langle \mathrm{p}^2 \right\rangle = -2\mu^2 \frac{\partial E_{\nu \mathrm{J}}}{\partial \mu} - L\hbar^2 \left\langle r^{-2} \right\rangle \cdot \tag{43}$$

From equation (26) we obtain

$$\frac{\partial E_{\nu \mathrm{J}}}{\partial \mu} = -\frac{L\hbar^2 c_0}{2\mu^2} + \frac{b_{\mathrm{h}}^2 \hbar^2 \Omega}{2\mu^2} + \frac{D_{\mathrm{e}} \Omega^{\frac{1}{2}}}{\mu} \left\{ \frac{1}{\rho}\left(1 - \frac{1}{c_{\mathrm{h}}^2}\right) - \frac{2}{\gamma(2\sigma - 1)}\left(1 - \frac{1}{c_{\mathrm{h}}}\right)^2 \right\} \cdot \tag{44}$$

Equations (42) and (44) inserted into (43) gives

$$\left\langle \mathrm{p}^2 \right\rangle = -b_{\mathrm{h}}^2 \hbar^2 \Omega - 2\mu D_{\mathrm{e}} \Omega^{\frac{1}{2}} \left\{ \frac{2(1 - 1/c_{\mathrm{h}})^2}{\gamma(2\sigma - 1)} - \frac{1}{\rho}\left(1 - \frac{1}{c_{\mathrm{h}}^2}\right) \right\} - \frac{L\hbar^2 \Omega^{\frac{1}{2}}}{c_{\mathrm{h}}^2} \left\{ \frac{c_2}{\gamma(2\sigma - 1)} + \frac{c_1 c_{\mathrm{h}} - c_2}{2\rho} \right\} \tag{45}$$

Having obtained the expression for $\left\langle p^2 \right\rangle$, equation for $\left\langle p \right\rangle$ is deduced as follows. Following Chen et al. [6], the expectation value of momentum is given by

$$\langle p \rangle = \int_0^{\infty} \mathrm{u}_{\nu J}^{*}(r)\, \hat{\mathrm{p}}(r)\, \mathrm{u}_{\nu J}(r)\, \mathrm{d}r , \tag{46}$$

where $\mathrm{u}_{\nu J}^{*}$ is the complex conjugate of $\mathrm{u}_{\nu J}$. Substituting equation (4) into (46) and using equation (27) to transform to coordinate *z*, one obtains

$$\langle p \rangle = i\hbar \int_0^{z_0} \mathrm{u}_{\nu J}^{*}(z)\, \mathrm{u}_{\nu J}'(z)\, \mathrm{d}z \cdot \tag{47}$$

Upon replacing equation (29) in (47) and simplifying, we obtained

$$\langle p \rangle = i\hbar\, \mathrm{N}_{\nu J}^2\, \mathrm{S}_{\nu J} , \tag{48}$$

where

$$S_{\nu J} = \int_0^{z_0} z^{2\delta} (1 - z)^{2\sigma} \left\{ {}_2\mathrm{F}_1'\, {}_2\mathrm{F}_1 + (\delta - \delta z - \sigma z) \left| {}_2\mathrm{F}_1 \right|^2 \right\} \mathrm{d}z \cdot \tag{49}$$

Equations (45) and (48) inserted in (35) gives

$$\mathrm{v}_{\nu J} = \frac{1}{\mu} \left\{ N_{\nu J}^4 \hbar^2 \mathrm{S}_{\nu J}^2 - b_{\mathrm{h}}^2 \hbar^2 \Omega - 2\mu D_{\mathrm{e}} \Omega^{\frac{1}{2}} \left[\frac{2(1 - 1/c_{\mathrm{h}})^2}{\gamma(2\sigma - 1)} - \frac{1}{\rho}\left(1 - \frac{1}{c_{\mathrm{h}}^2}\right) \right] - \frac{L\hbar^2 \Omega^{\frac{1}{2}}}{c_{\mathrm{h}}^2} \left[\frac{c_2}{\gamma(2\sigma - 1)} + \frac{c_1 c_{\mathrm{h}} - c_2}{2\rho} \right] \right\}^{\frac{1}{2}} \cdot \tag{50}$$

5. Results and discussion

Evidently, the mapping $L \rightarrow (\mathrm{D} + 2\ell - 3)(\mathrm{D} + 2\ell - 1)/4$ and $r_{\mathrm{e}}^2 c_{-1+j} \rightarrow \mathrm{D}_{-1+j}$ transforms expression (26) to the energy spectrum of shifted Tietz-Wei oscillator in D-dimensions [33]. On the other hand, subjecting relation (26) to the transformations $E_{\nu J} \rightarrow E_{\nu J} - D_{\mathrm{e}}$ and $r_{\mathrm{e}}^2 c_{-1+j} \rightarrow c_{-1+j}$ recovers the energy eigenvalues of the Tietz-Hua potential [1]. This shows that equation (26) is a valid expression for the bound state ro-vibrational energies of the STWP.

The data in Table 1 shows model parameters of two diatomic molecules used in the present research, the data are obtained from literature [16, 35]. With the aid of Table 1, equation (26) is used to compute bound state ro-vibrational energies for the two diatomic molecules. Also included in the table are literature data for binding energies, $E_{\mathrm{bind}} = E_{\nu J} - D_{\mathrm{e}}$ of Tietz-Hua potential [36]. Evidently, the energies obtained are in favorable agreement with binding energies of Tietz-Hua potential, this shows that the STWP and the Tietz-Hua potential only differ in the position of their equilibrium minima but are equivalent models for the diatomic molecules. Figure 1 is the graphical representation of the variation of bound state energy eigenvalues as a function of vibrational quantum number, the plot shows that as ν is gradually increased from zero, the energy eigenvalues increases to a peak for each of the diatomic molecules, then decreases afterwards as ν is further increased.

In figure 2, we have plotted bound state energy eigenvalues of the STWP versus rotational quantum number, as can be seen from the plot, it is observed that as J is increased from zero, the energy eigenvalues increases monotonically. Normalized radial wave functions of some selected quantum states are shown in figure 3, the plot is a demonstration that equation (30) is a physically realizable wave function of the STWP.

Equation (50) is used to calculate the speed of the two diatomic molecules, the results are shown by the entries under the columns for $\mathrm{v}_{\nu J}$ in Table2. The plot in Figure 4 is the variation of speed as a function of vibrational quantum number for the O_2 and NO diatomic molecules in shifted Tietz-Wei oscillator. The result shows that for small increases in vibrational quantum number, the speed increases slowly to attain a threshold value after which it decreases as the vibrational quantum number is further raised. On the other hand, in Figure 5, the speed is plotted as a function of rotational quantum number, here, it is clear that the classical root-mean-square speed decreases with increasing rotational quantum number.

6. Conclusion

In this paper, expressions for bound state energy eigenvalues and normalized radial wave functions of the STWP were analytically derived using the ideas of supersymmetric quantum mechanics and ansatz solution approach respectively. A

Pekeris-like approximation scheme is used to model the centrifugal term of the Schrödinger equation. With the help of the equation for bound state energy eigenvalues, speed of the system in STWP in derived. Bound state energy eigenvalues and speed were computed for O_2 (X $^3\Sigma_g^-$) and NO (X^2 Π_f) diatomic molecules. Our computed bound state energy eigenvalues for the STWP are in total agreement with existing literature results for binding energies of the O_2 (X $^3\Sigma_g^-$) and NO (X^2 Π_f) diatomic molecules in the Tietz-Hua potential. Furthermore, studies have shown that for the two diatomic molecules considered, the speed increases with increase in vibrational quantum number. On the other hand, the speed decreases as the rotational quantum number is gradually raised.

List of Tables

Table 1. Model parameters of the diatomic molecules studied in this work

Molecule	Molecular state	Parameter				
		D_e (cm^{-1})	$\mu/10^{-23}$ (g)	b_h (Å^{-1})	r_e (Å)	c_h
O_2	X $^3\Sigma_g^-$	42041	1.337	2.59103	1.207	0.027262
NO	X $^2\Pi_f$	53341	1.249	2.71559	1.151	0.013727

Table 2. Bound state energy eigenvalues and classical speed of diatomic molecules in STWP along with literature data of binding energy of Tietz-Hua potential

state		O_2 (X $^3\Sigma_g^-$)			NO (X^2 Π_f)		
ν	J	$-E_{\nu J}$ (eV)	$-E_{\text{bind}}$ (eV) [36]	$v_{\nu J}$ (kms^{-1})	$-E_{\nu J}$ (eV)	$-E_{\text{bind}}$ (eV) [36]	$v_{\nu J}$ (kms^{-1})
0	0	5.1149025433	5.1163223113	1.08	6.4959366828	6.4959334209	1.22
	1	5.1145484174	5.1159784440	1.08	6.4955196618	6.4955164040	1.23
	2	5.1138401797	5.1152907228	1.09	6.4946856358	6.4946823862	1.24
	5	5.1095911497	…	1.13	6.4896819248	…	1.29
	10	5.0954326220	…	1.27	6.4730084017	…	1.44
3	0	4.5497017063	4.5590745476	2.77	5.8133435356	5.8133374461	3.15
	1	4.5493609717	4.5587436240	2.77	5.8129413385	5.8129354009	3.16
	2	4.5486795166	4.5580817907	2.78	5.8121369601	5.8121313267	3.16
	5	4.5445911837	…	2.79	5.8073111362	…	3.18
	10	4.5309683249	…	2.85	5.7912305821	…	3.24
5	0	4.1917403884	4.2058686976	3.48	5.3795904024	5.3795826206	3.99
	1	4.1914085485	4.2055464879	3.48	5.3791980702	5.3791906688	3.99
	2	4.1907448831	4.2049020823	3.49	5.3784134218	5.3784067819	3.99
	5	4.1867632880	…	3.49	5.3737059783	…	4.00
	10	4.1734962302	…	3.52	5.3580200336	…	4.03
7	0	3.8487952908	…	4.98	4.9628548944	…	5.65
	1	3.8484723195	…	4.98	4.9624724131	…	5.65
	2	3.8478263913	…	4.99	4.9617074665	…	5.65
	5	3.8439512202	…	5.01	4.9571182348	…	5.59
	10	3.8310389169	…	5.08	4.9418263373	…	5.79

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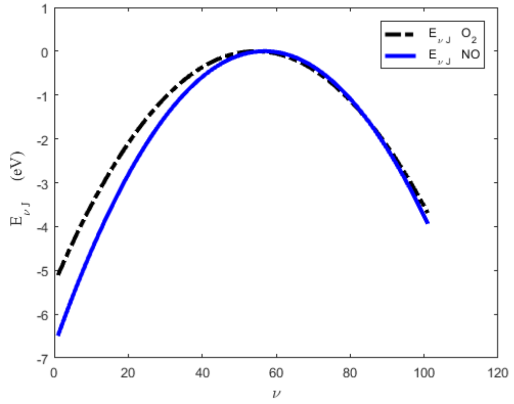

Figure 1. Variation of energy eigenvalues as a function of vibrational quantum number

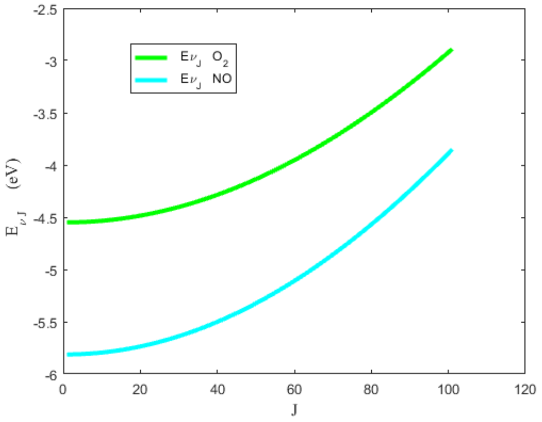

Figure 2. Variation of energy eigenvalues as a function of rotational quantum number

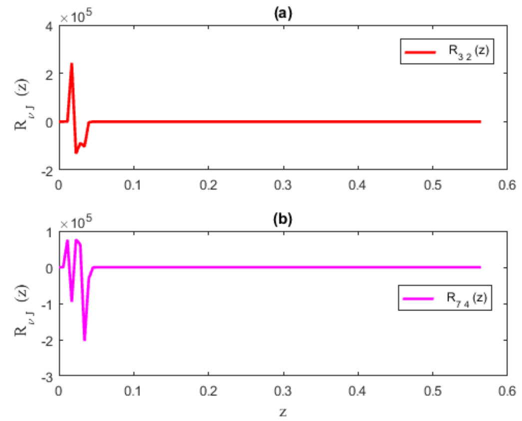

Figure 3. Normalized radial eigenfunctions of the STWP

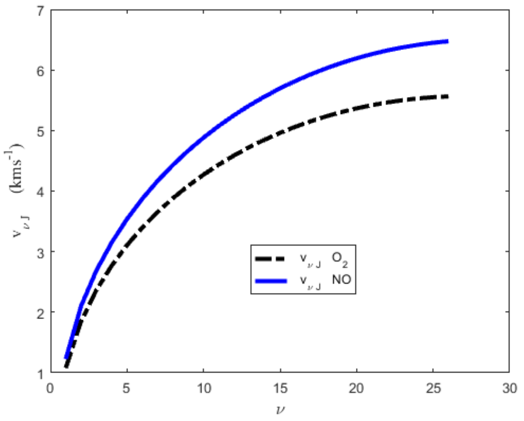

Figure 4. Graphical representation of the variation of root-mean-square speed versus vibrational quantum number

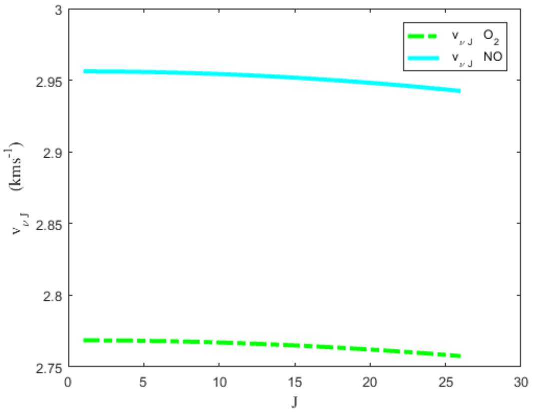

Figure 5. Graphical representation of the variation of root-mean-square speed versus rotational quantum number.

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