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Solutions of the Dirac and Schrödinger equations with shifted Tietz-Wei potential

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Abstract. We solved the Dirac equation using the modified factorization method with the shifted Tietz-Wei potential model. Relativistic and non-relativistic ro-vibrational energy spectra were obtained as well as numerical solutions for different diatomic molecules ($H_2(X^1\sum_g^+)$, $N_2(X^1\sum_g^+)$, and $O_2(X^3\sum_g^-)$). The eigenfunction for this potential has been obtained in terms of hypergeometric function. The energy variations were discussed graphically for different parameters of the shifted Tietz-Wei potential. Our results are in good agreement with the ones available in the literature.

1 Introduction

Researchers over the years have studied the relativistic and non-relativistic systems with various physical potentials [1–9]. Recently, this drive has led to the calculation of relativistic rotation-vibrational energy spectra for diatomic molecules and dimers. As such, various relativistic effects have been considered using quantum mechanical methods; this in turn has helped achieving accurate rotation-vibrational energy spectra [10]. Shui and Jia [11] noted that there exists a slight difference between the relativistic and the non-relativistic treatment, arising from the relativistic corrections of the rotation-vibrational energy. Such effects so far observed include a decrease in the vibrational energies for the $X^2\sum^+$ state of the CP molecule, the $X^1\sum^+$ state of the SiF$^+$ molecule, [12–15] etc.

Tietz diatomic molecule potential energy function was first proposed in 1963 [16] as

$$U_T = D_e + \frac{D_e(a+b)e^{-2\alpha r}}{(1+qe^{-\alpha r})^2}, \tag{1}$$

where D_e is the dissociation energy, a, b, q and α are spectroscopic parameters which can be determined.

Recently, a more convenient form of eq. (1) has been proposed [17]:

$$U_T = D_e\left[1 - \frac{e^{\alpha r_e}+q}{e^{\alpha r}+q}\right]^2, \tag{2}$$

where r_e is the equilibrium bond length, and q is a parameter.

Replacing q with 0, +1 and −1 in eq. (2) results in the Morse potential [18], Rosen-Morse potential [19] and Manning-Rosen potential [20]. Further research has shown that several other potentials are equivalent to the Tietz potential model [21–24].

In describing a suitable molecular potential for diatomic molecules, a modification for Tietz-Wei potential (called the shifted Tietz-Wei potential) was suggested as [25]

$$U_{sTWp}(r) = V_0\left(\frac{Ae^{-b_h(r-r_e)} - Be^{-2b_h(r-r_e)}}{(1 - c_he^{-b_h(r-r_e)})^2}\right), \tag{3}$$

where $A = 2(c_h - 1)$, $B = (c_h^2 - 1)$, $b_h = \gamma(1 - c_h)$, V_0 is the potential well depth, r_e is the molecular bond length, c_h is the optimization parameter, γ is the Morse constant, and r is the inter-nuclear distance. The Morse potential is a

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special case of the shifted Tietz-Wei potential, when $c_h \to 0$. The similarities between the shifted Tietz-Wei potential and the traditional Morse potential, and their relevance over the original Tietz-Wei potential was described in ref. [25].

To the best of our knowledge, a relativistic consideration has not been given to a shifted Tietz-Wei potential; hence our motivation to examine the relativistic correction of the rotation-vibrational energy spectra for the $X^1 \sum_g^+$, $X^1 \sum_g^+$ and $X^3 \sum_g^-$ states of hydrogen, nitrogen and oxygen molecules, respectively.

We seek to investigate the bound state solution of the Dirac equation with the shifted Tietz-Wei potential energy model within the framework of spin symmetry, using the modified factorization method analytically and numerically. We also explore the relativistic effects of the rotation-vibrational energy spectra for the diatomic molecules under consideration.

2 Bound state solutions of the Dirac equation

The Dirac equation with both scalar potential $S(r)$ and vector potential $V(r)$ can be written as

$$\left\{ c\vec{\alpha} \cdot \vec{p} + \beta \left[\mu c^2 + S(r) \right] \right\} \Psi(r,\theta,\varphi) = [E - V(r)]\Psi(r,\theta,\varphi), \tag{4}$$

$$\vec{p} = -i\hbar\nabla, \qquad \vec{\alpha} = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}, \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{5}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{6}$$

where $i = \sqrt{-1}$, $\hbar = \frac{h}{2\pi}$. In eq. (4) to eq. (6), E is the relativistic energy of the system, μ is the reduced mass of the system, c is the speed of light, h is the Planck constant, $\vec{p}$ is the momentum operator, $S(r)$ is the scalar potential, $V(r)$ is the vector potential, $\vec{\alpha}$ and β are the 4×4 Dirac matrices, I is the 2×2 unit matrix, and σ_1, σ_2, σ_3 are three-vector Pauli matrices.

Taking cognisance of the Dirac Hamiltonian commutation that exists between total angular momentum operator $\vec{J}$ and the spin-orbit coupling operator $K = -\beta(\vec{\sigma} \cdot \vec{L} + 1)$, where $\vec{L}$ is the orbital angular momentum, and the regularity conditions that are satisfied by the lower and upper spinor components under spin symmetry as documented in ref. [12], we adopt the following second-order Schrodinger-like equation:

$$\left(-\hbar^2 c^2 \frac{d^2}{dr^2} + \frac{\kappa(\kappa+1)\hbar^2 c^2}{r^2} + \left(\mu c^2 + E_{v\kappa} - C_s \right) \left(\frac{V(r)}{2} + \frac{S(r)}{2} \right) \right) F_{v\kappa}(r) = \left(E_{v\kappa}^2 - \mu^2 c^4 + C_s \left(\mu c^2 - E_{v\kappa} \right) \right) F_{v\kappa}(r), \tag{7}$$

where v is the vibrational quantum number, κ is the spin-orbit quantum number, C_s is a constant parameter. For unaligned spin ($j = J - \frac{1}{2}$), $\kappa = J > 0$; also for aligned spin ($j = J + \frac{1}{2}$), $\kappa = -(J + \frac{1}{2}) < 0$. Here, j and J denote total angular momentum quantum number and rotational quantum number for the dimers, respectively.

For bound state solutions, the scalar potential is equated to the shifted Tietz-Wei potential (i.e. $S(T) = U_{sTWp}(r)$) and the vector potential $V(r) = C_s + S(r) = C_s + U_{sTWp}(r)$. Invoking this condition and substituting eq. (3) into eq. (7), we obtain the following equation:

$$\left\{ -\hbar^2 c^2 \frac{d^2}{dr^2} + \left(\mu c^2 + E_{v\kappa} - C_s \right) \left(\frac{C_s}{2} + V_0 \left(\frac{Ae^{-b_h(r-r_e)} - Be^{-2b_h(r-r_e)}}{(1 - c_h e^{-b_h(r-r_e)})^2} \right) \right) + \frac{\kappa(\kappa+1)\hbar^2 c^2}{r^2} \right\} F_{v\kappa}(r) =$$
$$\left(E_{v\kappa}^2 - \mu^2 c^4 + C_s \left(\mu c^2 - E_{v\kappa} \right) \right) F_{v\kappa}(r). \tag{8}$$

Exact solution of eq. (8) is only possible for $J = 0$, $\kappa = -1$ (s-wave). For l-wave ($J \neq 0$), we apply a Pekeris-approximation scheme [26] to take care of the centrifugal term as

$$\frac{1}{r^2} \approx \frac{1}{r_e^2} \left(D_0 + \frac{D_1 e^{-\alpha x}}{1 - c_h e^{-\alpha x}} + \frac{D_2 e^{-2\alpha x}}{(1 - c_h e^{-\alpha x})^2} \right), \tag{9}$$

where $\alpha = b_h r_e$, $x = \frac{r-r_e}{r_e}$. D_i is the parameter of the coefficients ($i = 0, 1, 2$) and α is the screening parameter. With proper expansion of eq. (9) up to the x^2 term and rearranging the terms, we obtain [9]

$$D_0 = 1 + \frac{1 - c_h}{\alpha} \left[\frac{3}{\alpha}(1 - c_h) - (3 + c_h) \right], \tag{10}$$

$$D_1 = \frac{2}{\alpha}(1 - c_h)^2 \left[(2 + c_h) - \frac{3}{\alpha}(1 - c_h) \right], \tag{11}$$

$$D_2 = \frac{(1 - c_h)^3}{\alpha} \left[\frac{3}{\alpha}(1 - c_h) - (1 + c_h) \right]. \tag{12}$$

Substituting eq. (9) into eq. (8) gives

$$
\left\{ -\hbar^2 c^2 \frac{\mathrm{d}^2}{\mathrm{d}r^2} + \left(\mu c^2 + E_{v\kappa} - C_s \right) \left(\frac{C_s}{2} + V_0 \left(\frac{A e^{-b_h(r-r_e)} - B e^{-2b_h(r-r_e)}}{(1 - c_h e^{-b_h(r-r_e)})^2} \right) \right) \right.
$$
$$
\left. + \frac{\kappa(\kappa+1)\hbar^2 c^2}{r_e^2} \left(D_0 + \frac{D_1 e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} + \frac{D_2 e^{-2b_h(r-r_e)}}{(1 - c_h e^{-b_h(r-r_e)})^2} \right) \right\} F_{v\kappa}(r) = \left(E_{v\kappa}^2 - \mu^2 c^4 + C_s \left(\mu c^2 - E_{v\kappa} \right) \right) F_{v\kappa}(r). \quad (13)
$$

Equation (13) can be rewritten as

$$
\frac{\mathrm{d}^2 F_{v\kappa}(r)}{\mathrm{d}r^2} + \left[\frac{\xi_1 e^{-2b_h(r-r_e)}}{\left(1 - c_h e^{-b_h(r-r_h)} \right)^2} + \frac{\xi_2 e^{-b_h(r-r_e)}}{\left(1 - c_h e^{-b_h(r-r_h)} \right)^2} + \frac{\xi_3 e^{-b_h(r-r_e)}}{\left(1 - c_h e^{-b_h(r-r_h)} \right)} \right] F_{v\kappa}(r) = \tilde{E}_{v\kappa} F_{v\kappa}(r), \quad (14)
$$

where ξ_1, ξ_2, ξ_3, and $\tilde{E}$ are defined as

$$
\xi_1 = \frac{1}{\hbar^2 c^2} \left[\left(\mu c^2 + E_{v\kappa} - C_s \right) V_0 B - \frac{\kappa(\kappa+1)\hbar^2 c^2 D_2}{r_e^2} \right], \quad (15)
$$

$$
\xi_2 = -\frac{1}{\hbar^2 c^2} \left[\left(\mu c^2 + E_{v\kappa} - C_s \right) V_0 A \right], \quad (16)
$$

$$
\xi_3 = -\frac{1}{\hbar^2 c^2} \left[\frac{\kappa(\kappa+1)\hbar^2 c^2 D_1}{r_e^2} \right], \quad (17)
$$

$$
\tilde{E}_{v\kappa} = -\frac{1}{\hbar^2 c^2} \left\{ \left[E_{v\kappa}^2 - \mu^2 c^4 + C_s \left(\mu c^2 - E_{v\kappa} \right) \right] - \left(\mu c^2 + E_{v\kappa} - C_s \right) \frac{C_s}{2} - \frac{\kappa(\kappa+1)\hbar^2 c^2 D_0}{r_e^2} \right\}. \quad (18)
$$

Introducing a new variable $Z = (1 - c_h e^{-b_h(r-r_e)})^{-1}$, and making the transformation $F_{v\kappa}(Z) = Z^{-q}(1 - Z)^{-p} f_{v\kappa}(Z)$, we rewrite eq. (14) as

$$
Z(1 - Z) \frac{\mathrm{d}^2 f_{v\kappa}(Z)}{\mathrm{d}Z^2} + [1 - 2q - (2 - 2q - 2p)Z] \frac{\mathrm{d}f_{v\kappa}(Z)}{\mathrm{d}Z} - \left[(q + p)^2 + (q + p) + \left(\frac{\xi_1}{b_h^2 c_h^2} + \frac{\xi_2}{b_h^2 c_h} \right) \right] f_{v\kappa}(Z)
$$
$$
+ \left[\frac{q^2 + \frac{\xi_1}{b_h^2 c_h^2} - \frac{\xi_3}{b_h^2 c_h} - \frac{\tilde{E}_{v\kappa}}{b_h^2}}{Z(1 - Z)} + \frac{p^2 - q^2 - \frac{\xi_1}{b_h^2 c_h^2} + \frac{\xi_3}{b_h^2 c_h}}{(1 - Z)} \right] f_{v\kappa}(Z) = 0. \quad (19)
$$

Equation (19) can be reduced to a Gauss hypergeometric equation if and only if the following two equations exist:

$$
q^2 + \frac{\xi_1}{b_h^2 c_h^2} - \frac{\xi_3}{b_h^2 c_h} - \frac{\tilde{E}_{v\kappa}}{b_h^2} = 0, \quad (20)
$$

$$
p^2 - q^2 - \frac{\xi_1}{b_h^2 c_h^2} + \frac{\xi_3}{b_h^2 c_h} = 0. \quad (21)
$$

Solving eqs. (20) and (21) gives

$$
\tilde{E}_{v\kappa} = b_h^2 p^2. \quad (22)
$$

We impose the termination condition of eqs. (20) and (21) in eq. (19) to have

$$
Z(1 - Z) \frac{\mathrm{d}^2 f_{v\kappa}(Z)}{\mathrm{d}Z^2} + [1 - 2q - (2 - 2q - 2p)Z] \frac{\mathrm{d}f_{v\kappa}(Z)}{\mathrm{d}Z}
$$
$$
- \left[\left(q + p + \frac{1}{2} + \sqrt{\frac{1}{4} - \gamma} \right) + \left(q + p + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma} \right) \right] f_{v\kappa}(Z) = 0, \quad (23)
$$

where

$$
\gamma = \frac{\xi_1}{b_h^2 c_h^2} + \frac{\xi_2}{b_h^2 c_h}. \quad (24)
$$

The solution of eq. (23) can be expressed in Gauss hypergeometric form as

$$f_{v\kappa}(Z) = {}_2F_1\left(q + p + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma}, q + p + \frac{1}{2} + \sqrt{\frac{1}{4} - \gamma}; 1 - 2p; Z\right)$$

$$= \frac{\Gamma(1 - 2p)}{\Gamma\left(q + p + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma}\right)\Gamma\left(q + p + \frac{1}{2} + \sqrt{\frac{1}{2} - \gamma}\right)}$$

$$\times \sum_{n=0}^{\infty} \frac{\Gamma\left(q + p + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma} + n\right)\Gamma\left(q + p + \frac{1}{2} + \sqrt{\frac{1}{4} - \gamma} + n\right)}{\Gamma(1 - 2p + n)} \frac{Z^n}{n!}, \tag{25}$$

where n is an integer and Γ is a Gamma function.

The wave function $f_{v\kappa}(Z)$ is likely to vanish under certain conditions if eq. (25) reduces to a polynomial of degree n when either $q + p + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma} = -n$ or $q + p + \frac{1}{2} + \sqrt{\frac{1}{4} - \gamma} = -n$.

Using the quantization condition, $q + p + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma} = -n$, $n = 0, 1, 2, 3, \ldots$, eq. (25) can be expressed as

$$f_{v\kappa}(Z) = {}_2F_1\left(-n, n + 2q + 2p + 1; 1 - 2p; \frac{1 - (1 - 2Z)}{2}\right). \tag{26}$$

Therefore we can write eq. (26) as

$$f_{v\kappa}(Z) = \frac{\Gamma(2q)\Gamma(n)}{\Gamma(n + 2q)} P_n^{(2q,2p)}(1 - 2Z), \tag{27}$$

where $P_n^{(2q,2p)}(1 - 2Z)$ is the n-th Jacobi polynomial.

By re-transforming eq. (27) from the new variable Z to its original variable r, we obtain the wave function $F_{v\kappa}(r)$ in terms of the Jacobi Polymomial as

$$F_{v\kappa}(r) = \frac{\Gamma(2q)\Gamma(n)}{\Gamma(n + 2q)}\left(1 - c_h e^{-b_h(r - r_e)}\right)^{(q+p)}\left(-c_h e^{-b_h(r - r_e)}\right)^{-p} P_n^{(2q,2p)}\left(-\frac{1 + c_h e^{-b_h(r - r_e)}}{1 - c_h e^{-b_h(r - r_e)}}\right). \tag{28}$$

From eq. (21), we have

$$(p + q)(p - q) = \frac{\xi_1}{b_h^2 c_h^2} - \frac{\xi_3}{b_h^2 c_h}. \tag{29}$$

Combining the quantization condition, $(q + p + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma} = -n)$ and eq. (29), we have

$$-(q + p) = n + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma}, \tag{30}$$

$$-(q - p) = \frac{\frac{\xi_3}{b_h^2 c_h} - \frac{\xi_1}{b_h^2 c_h^2}}{n + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma}}. \tag{31}$$

The following expressions can be obtained by solving eqs. (30) and (31):

$$q = -\frac{1}{2}\left[n + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma} + \frac{\frac{\xi_3}{b_h^2 c_h} - \frac{\xi_1}{b_h^2 c_h^2}}{n + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma}}\right], \tag{32}$$

$$p = -\frac{1}{2}\left[n + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma} - \frac{\frac{\xi_3}{b_h^2 c_h} - \frac{\xi_1}{b_h^2 c_h^2}}{n + \frac{1}{2} - \sqrt{\frac{1}{4} - \gamma}}\right]. \tag{33}$$

Table 1. Spectroscopic parameters of the molecules used in this work.

Molecule	c_h	b_h (Å^{-1})	r_e (Å)	V_0 (cm^{-1})	$\mu/10^{-23}$ (g)	d_e (cm^{-1})
$H_2(X^1\sum_g^+)$	0.170066	1.61890	0.741	38318	0.084	0.0465
$N_2(X^1\sum_g^+)$	-0.032325	2.78585	1.097	79885	1.171	5.737×10^{-6}
$O_2(X^3\sum_g^-)$	0.027262	2.59103	1.207	42041	1.337	4.760×10^{-6}

Substituting eqs. (18) and (33) into eq. (22) and rearranging the terms, we obtain an expression of the form

$$E_{v\kappa}^2 - \mu^2 c^4 = \left(\mu c^2 + E_{v\kappa} - C_s\right)\frac{C_s}{2} - \left(\mu c^2 - E_{v\kappa}\right)C_s + \frac{\kappa(\kappa+1)\hbar^2 c^2 D_0}{r_e^2}$$

$$-b_h^2\hbar^2 c^2\left[\frac{2n+1-\sqrt{1-\frac{4V_0(\mu c^2+E_{v\kappa}-C_s)(B-c_hA)}{b_h^2 c_h^2\hbar^2 c^2}+\frac{4\kappa(\kappa+1)D_2}{b_h^2 c_h^2 r_e^2}}}{4} + \frac{\left(\frac{(\mu c^2+E_{v\kappa}-C_s)V_0 B}{b_h^2 c_h^2\hbar^2 c^2}+\frac{\kappa(\kappa+1)(c_h D_1-D_2)}{b_h^2 c_h^2 r_e^2}\right)}{2n+1-\sqrt{1-\frac{4V_0(\mu c^2+E_{v\kappa}-C_s)(B-c_hA)}{b_h^2 c_h^2\hbar^2 c^2}+\frac{4\kappa(\kappa+1)D_2}{b_h^2 c_h^2 r_e^2}}}\right]^2 .$$

(34)

Equation (34) is the relativistic energy spectra with shifted Tietz-Wei potential model.

3 Discussion

We first of all consider the non-relativistic limit by carrying out the mapping $\mu c^2 + E_{v\kappa} \to 2\mu c^2$ and $E_{v\kappa} - \mu c^2 \to E_{vJ}$ in eq. (34). This results in exact symmetry condition ($C_s = 0$) of the form

$$E_{vJ} = \frac{J(J+1)\hbar^2 D_0}{2\mu r_e^2} - \frac{b_h^2\hbar^2}{2\mu}$$

$$\times\left[\frac{2v+1-\sqrt{1-\frac{8\mu V_0(B-c_hA)}{b_h^2 c_h^2\hbar^2}+\frac{4J(J+1)D_2}{b_h^2 c_h^2 r_e^2}}}{4} + \frac{\left(\frac{2\mu V_0 B}{b_h^2 c_h^2\hbar^2}+\frac{J(J+1)(c_h D_1-D_2)}{b_h^2 c_h^2 r_e^2}\right)}{2v+1-\sqrt{1-\frac{8\mu V_0(B-c_hA)}{b_h^2 c_h^2\hbar^2}+\frac{4J(J+1)D_2}{b_h^2 c_h^2 r_e^2}}}\right]^2 .$$

(35)

Equation (35) is the non-relativistic rotation-vibrational energy spectra within the framework of shifted Tietz potential energy model. Here, we have considered the case of an unaligned spin ($\kappa = J$) and also denoted $E_{v\kappa}$ by E_{vJ} (with $n = v$) in eq. (34). Our numerical computations is focused on non-relativistic ro-vibrational energy spectra with the shifted Tietz-Wei potential, due to lack of literatures for comparison [27].

We have used the experimental data obtained from the ref. [28] as given in table 1 to calculate thero-vibrational energies of $H_2(X^1\sum_g^+)$, $N_2(X^1\sum_g^+)$, and $O_2(X^3\sum_g^-)$ numerically as shown in table 2, with the help of eq. (35). The following conversion has been employed in our numerical calculation: $1\,\text{cm}^{-1} = 1.239841875 \times 10^{-4}\,\text{eV}$. Our computations have been compared with the work of Roy [27]. It is worthy to note here that d_e is the dissociation energy.

The variation of energies with different parameters are also shown in figs. 1–7 for $N_2(X^1\sum_g^+)$. Figure 1 indicates that the potential well depth increases directly as the energy decreases. In fig. 2, there is a sharp decrease in energy as the molecular bond length increase from zero to 0.1 Å; thereafter, the energy remains constant with increase in molecular bond length for various vibrational quantum numbers. In fig. 3, maximum value of the energy is observed when the value of A is approaching zero. As A moves away from zero, the energy begins to decrease abruptly. Figure 4 shows a steady state decrease in energy as the value of B increases. It is worthy to note here that A and B are functions of the optimization parameter. Figure 5 shows an almost constant energy value for all values of the screening parameter. The value of the energy here decreases as the vibrational quantum number increases. In fig. 6, there is a sharp increase in energy as the value of b_h increases for different values of vibrational quantum numbers. The variation of energy with the optimization parameter is shown in fig. 7. As the optimization parameter increases, the energy decreases. The trend in energy decrease strongly depends on the vibrational quantum number. As the vibrational quantum number increases, the energy decreases more rapidly. The rotational quantum number is maintained at $J = 1$ throughout our plots.

Table 2. Ro-vibrational energies for various values of v and J.

v	J	$(E_{vJ} - d_e)$ (eV)		$(E_{vJ} - d_e)$ (eV)		$(E_{vJ} - d_e)$ (eV)	
		$H_2(X^1 \sum_g^+)$		$N_2(X^1 \sum_g^+)$		$O_2(X^3 \sum_g^-)$	
		Present	Roy [28]	Present	Roy [28]	Present	Roy [28]
0	0	−4.749286824	−4.481579782	−9.901147431	−9.758805832	−5.210727503	−5.116322311
	1	−4.782024241	−4.466980157	−9.862718246	−9.758315584	−5.243078227	−5.115978444
	2	−4.805829976	−4.437915462	−9.834493625	−9.757335106	−5.266692953	−5.115290722
	3	−4.829004636		−9.806761600		−5.289777766	
	4	−4.851875739		−9.779139125		−5.312655128	
1	0	−4.749370234		−9.901161339		−5.210714723	
	1	−4.848448897		−9.786857362		−5.308809185	
	2	−4.920466391		−9.702457834		−5.379880085	
	3	−4.990890641		−9.619672476		−5.449473967	
	4	−5.060705238		−9.537353305		−5.518559120	
2	0	−4.749194757		−9.901521691		−5.211026375	
	1	−4.915441390		−9.711872566		−5.375445371	
	2	−5.035669081		−9.571297577		−5.493971974	
	3	−5.153342476		−9.433458426		−5.610074702	
	4	−5.270100231		−9.296442707		−5.725367311	
3	0	−4.749335694		−9.902122518		−5.211546044	
	1	−4.983004079		−9.637764780		−5.442987920	
	2	−5.151439508		−9.441013291		−5.608968968	
	3	−5.316360945		−9.248120058		−5.771580072	
	4	−5.480061313		−9.056407370		−5.933080026	
4	0	−4.749570801		−9.902963820		−5.212273732	
	1	−5.051139358		−9.564535077		−5.511437833	
	2	−5.267778936		−9.311605684		−5.724871761	
	3	−5.479947163		−9.063657583		−5.933990771	
	4	−5.690589327		−8.817247640		−6.141697574	

Recently, Falaye *et al.* [25] studied the Schrödinger equation with the shifted Tietz-Wei potential model for a set of different diatomic molecules, using the exact quantization rule (EQR). In their studies, the eigenfunction, in addition to the arbitrary values of n and l quantum numbers were obtained via formula method. Also, a similar potential called Tietz-Hua potential was modified by Onate *et al.* [29], with the aim to evaluate Shannon entropy and information energy under the modified Tietz-Hua potential. The shifted Tietz-Wei potential can effectively describe the vibrational energy levels of diatomic molecules, hence our motivation for the study.
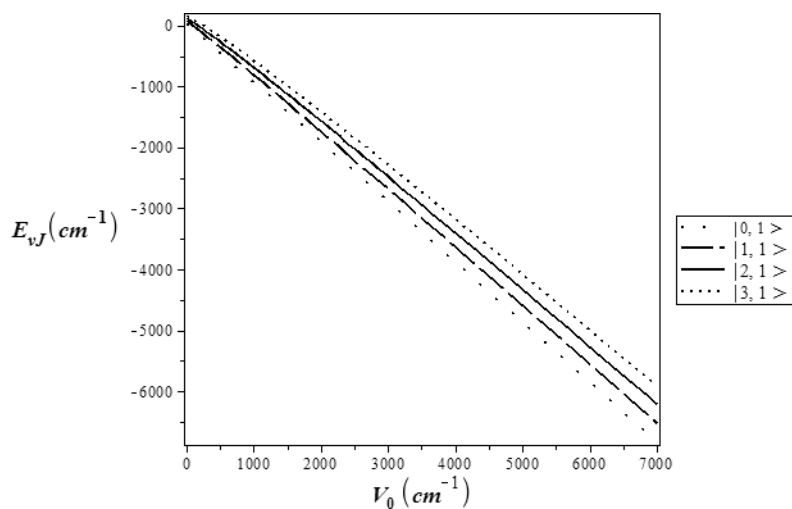
Fig. 1. Energy variation with potential well depth for various vibrational quantum numbers for $N_2(X^1\sum_g^+)$.
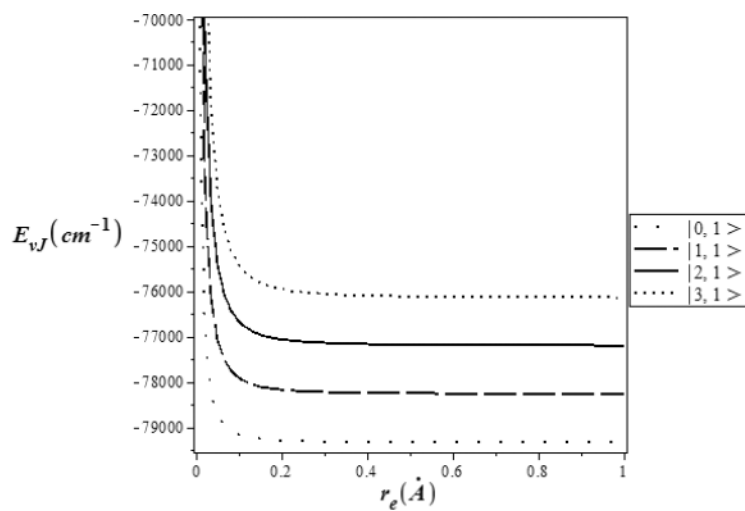

Fig. 2. Energy variation with molecular bond length for various vibrational quantum numbers for $N_2(X^1\sum_g^+)$.
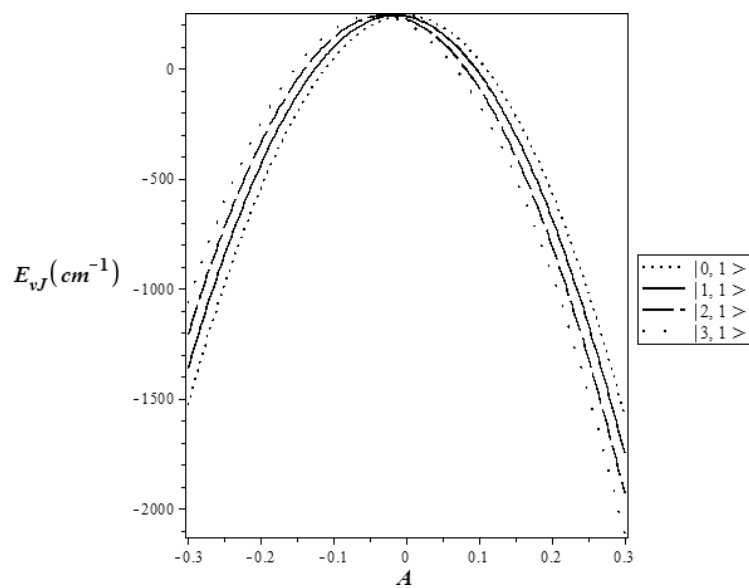

Fig. 3. Energy variation with A for various vibrational quantum numbers for $N_2(X^1\sum_g^+)$.
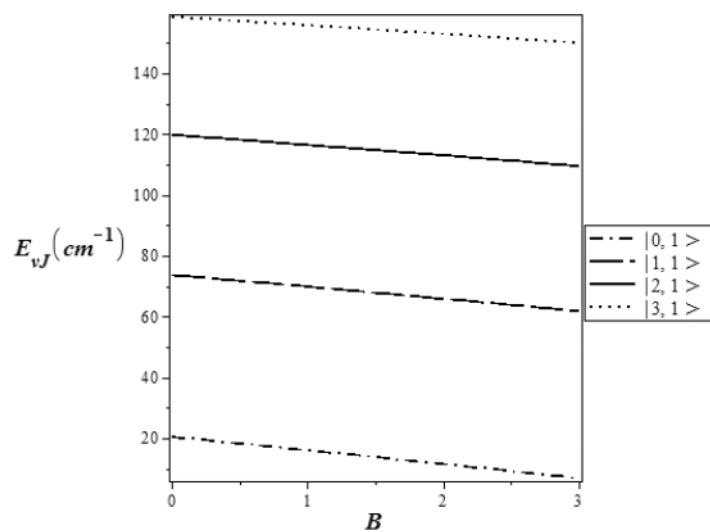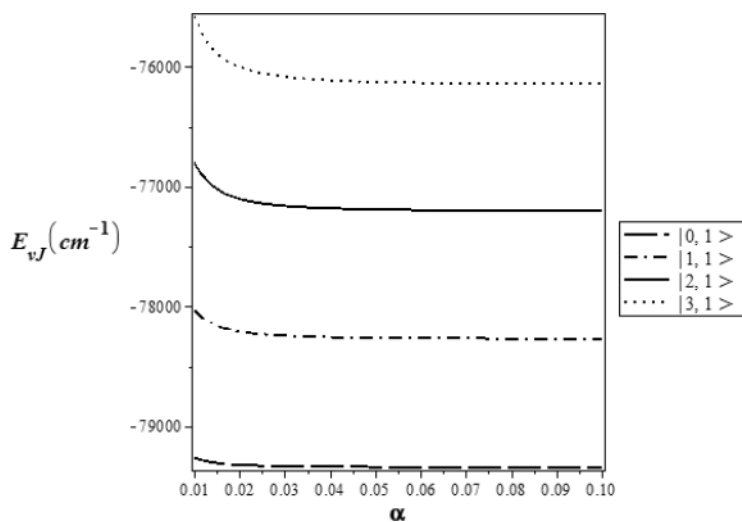
Fig. 4. Energy variation with B for various vibrational quantum numbers for $N_2(X^1\sum_g^+)$.

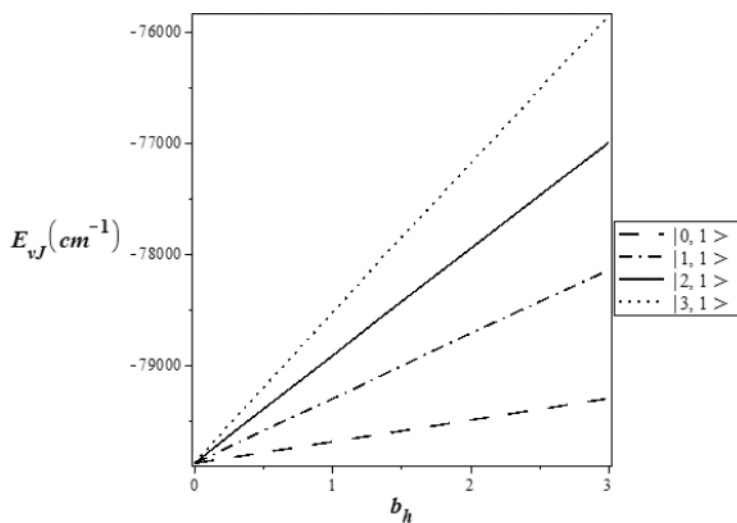**Fig. 5.** Energy variation with screening parameter for various vibrational quantum numbers for $N_2(X^1\sum_g^+)$.

Fig. 6. Energy variation with b_h for various vibrational quantum numbers for $N_2(X^1\sum_g^+)$.
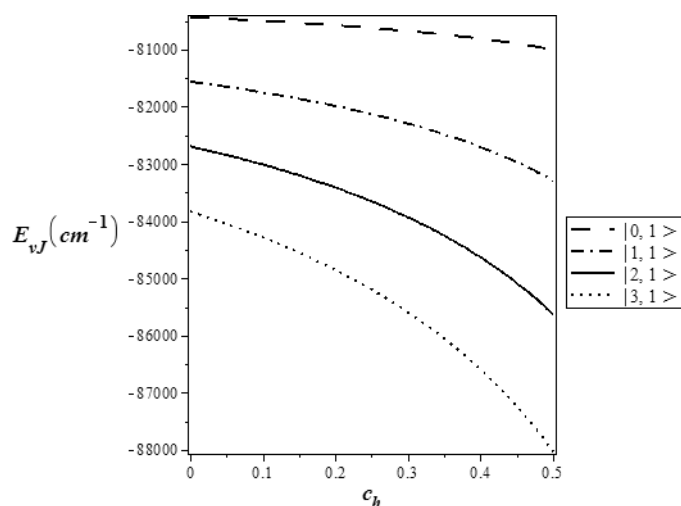
Fig. 7. Energy variation with optimization parameter for various vibrational quantum numbers for $N_2(X^1\sum_g^+)$.

4 Conclusion

In this article, we have solved the Dirac equation using modified factorization method and suitable approximation to replace the centrifugal term. We have also presented the relativistic and non-relativistic ro-vibrational energy spectra with the shifted Tietz-Wei potential model for some diatomic molecules. Computation of energies have been done numerically and the results discussed extensively using graphical relations. We have shown that there is an inverse relationship between the ro-vibrational energy and the optimization parameter. This relation strongly depends on the vibrational quantum number. Our results agree with those of Roy in ref. [27]. We found that the shifted Tietz-Wei potential can effectively describe the vibrational energy levels of diatomic molecules. Finally, this study has many applications in different areas of physics such as nuclear physics, particles physics and minimal length [30–33] among others.

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