Exact and Approximate Solutions of Some Potential Energy Functions for Diatomic Molecules

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Abstract

In this article, a one-body problem is solved analytically using the parametric Nikiforov-Uvarov method. By using the certain approximation schemes, we solved (in the non-relativistic case) the Schrödinger equation for improved Tietz potential model. We also obtained the solutions of the Schrödinger equation for improved Rosen-Morse and improved Manning-Rosen potential models from the results of the improved Tietz potential by using a certain transformation. Numerical results are obtained by considering some diatomic molecules such as NO^+ , O_2^+ , Cl_2 , and N_2^+ . Also the bound state solutions of the positive energy subspace and negative energy subspace of Dirac equation are obtained exactly in the relativistic case for s-wave only.

1.0 Introduction

The exact and approximate analytical solutions of Schrödinger, Klein-Gordon, Duffin-Kemmer-Petiau, and Dirac equations for different potential models have been studied extensively in recent years due to the importance of these wave equations in non-relativistic and relativistic quantum mechanics, and quantum chemistry. Some of the potential models that have been considered are Harmonic oscillator potential, Coulomb potential, Woods-Saxon potential, Morse potential, Eckart potential, ring-shaped nonspherical harmonic oscillator, Pöschl-Teller potential,Yukawa potential, Mie-type potential, Deng-Fan potential, Tietz potential among others [1-7]. Different methods have also been employed to obtain the solutions of these wave equations. Some of the methods are supersymmetry quantum mechanics [8, 9], Nikiforov-Uvarov method [1, 5, 10], asymptotic iteration method [11-14], factorization method [15], Laplace integral transform [16], proper quantization rule and exact quantization rule [17, 18] among others.

The Tietz potential has a potential energy function for diatomic molecules which was proposed in 1963, by Tietz as [19]:

$$V_T(r) = D_e + D_e \frac{(a+b)e^{-2\alpha r} - be^{-\alpha r}}{(1+he^{-\alpha r})^2},$$
(1)

where D_e is the dissociation energy. The parameters a, b, h, and α can be determined so as to fit calculated values of spectroscopic parameters to observed ones. In 2012, Jia et al. [20] proposed a more convenient form of the original Tietz potential energy function called the improved Tietz potential given as [20, 21]

$$V_{IT}(r) = D_e \left(1 - \frac{e^{\alpha r_e} + q}{e^{\alpha r} + q} \right)^2,$$
 (2)

where r_e is the equilibrium bond length. The original Tietz potential function is conventionally defined in terms of five parameters. However, it only has four independent parameters as shown in equation (2) [19, 20]. It should be noted that a molecular Tietz potential of the form [14, 22].

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$$V(r) = D_e \left(\frac{\sinh\left(\frac{r-r_e}{a}\right)}{\sinh\left(\frac{r}{a}\right)} \right)$$
(3)

has also been proposed and has been solved for the Klein-Gordon equation and the Schrödinger equation. This molecular potential is quite different from the improved Tietz potential model and the applications are given in Refs. [14, 22]. In 1932, Rosen and Morse proposed a potential function for polyatomic molecules [23]

$$V_{RM}(r) = B \tanh(r/d) - C \sec h^2(r/d), \qquad (4)$$

where B, C, and d are three adjustable parameters. The Rosen-Morse potential has been used to investigate polyatomic vibrational states [23]. Many authors have studied the Rosen- Morse potential model both in the non-relativistic and relativistic quantum mechanics. See Ref. [23] for details and applications of the Rosen-Morse potential. The improved Rosen-Morse potential model proposed is written as [20, 23]

$$V_{IRM}(r) = D_e \left(1 - \frac{e^{\alpha r_e} + 1}{e^{\alpha r} + 1} \right)^2,$$
(5)

where $\alpha = 2/d$, D_e is the dissociation energy, and r_e is the equilibrium bond length. In equation (5), the term $1/2D_e\left(e^{\alpha r_e}+1\right)$ is added to the Rosen-Morse potential in equation (4). The improved expression of some potential functions are more convenient for their applications. It should also be noted that when q = 1 in the improved Tietz potential of equation (2), we obtain the improved Rosen-Morse potential given in equation (5). In 1933, Manning and Rosen proposed a potential function for diatomic molecules,

$$V_{MR}(r) = \frac{\hbar^2}{8\mu\pi^2 b^2} \left[\frac{\beta(\beta-1)}{1-e^{r_e b}} - \frac{Ae^{r_e b}}{1-e^{r_e b}} \right]$$
(6)

in which β and A are two dimensionless parameters, parameter b is related to the range of the potential and has dimension of length. In 2012, Wang et al. proposed an improved Manning-Rosen potential energy model. The improved Manning-Rosen potential is written as,

$$V_{IMR}(r) = D_e \left(1 - \frac{e^{\alpha r_e} - 1}{e^{\alpha r} - 1} \right)^2,$$
(7)

where D_e is the dissociation energy, r_e is the equilibrium bond length. By employing the conventional Greene-Aldrich approximation scheme to deal with the centrifugal term, the bound state solution and scattering state solution of the Schrödinger equation with original Manning-Rosen potential has been obtained [24]. In Ref [25], the solutions of the improved Tietz and improved Rosen-Morse potential models were obtained by solving Klein-Gordon equation which is used to describe relativistic spinless particles. Also, in Ref. [21], the energy eigenvalues of the improved Tietz potential model was obtained using wave function ansazt. In this paper, we shall obtain the solutions of the improved Tietz, improved Rosen-Morse, and improved Manning-Rosen potential energy models by solving Schrödinger equation (used to describe nonrelativistic particles) and Dirac equation (used to describe relativistic spin-half particles). We will compare our results with that of Ref. [21] to check the validity of our results (the energy eigenvalues) for the non-relativistic case of the improved Tietz potential model. In Ref. [21], only the energy eigenvalues were obtained. We will obtain both the energy eigenvalues and wave functions for the three potential models. To the best of our knowledge, this is the first attempt to obtain the energies and wave functions of Dirac equation for the three potential models.

One of the applications of the solutions of non-relativistic and relativistic wave equations is in information theory. Information theory arises as a branch of applied Mathematics, Physics and electrical engineering involving the quantification of information. See Refs [26-28] for details of the importance and applications of the information-theoretic measures.

The paper is organised as follows. In Sec 2, the parametric Nikiforov-Uvarov (NU) method is briefly described. The bound state solutions of Schrödinger equation for the potential models will be obtained in Sec 3. Sec 4 contains the bound state solutions of Dirac equation for the potential models while the conclusion is given in Sec 5.

2.0 The Parametric Nikiforov-Uvarov (NU) Method

By using the parametric NU method, the solutions of a second order differential equation of the form [29].

$$\frac{d^{2}\Psi}{ds^{2}} + \frac{(\alpha_{1} - \alpha_{2}s)}{s(1 - \alpha_{3}s)}\frac{d\Psi}{ds} + \left[\frac{-\xi_{1}s^{2} + \xi_{2}s - \xi_{3}}{s(1 - \alpha_{3}s)}\right]\Psi = 0, (8)$$

are

and

$$\alpha_{2}n - (2n+1)\alpha_{5} + (2n+1)\left(\sqrt{\alpha_{9}} + \alpha_{3}\sqrt{\alpha_{8}}\right) + n(n-1)\alpha_{3} + \alpha_{7} + 2\alpha_{3}\alpha_{8} + 2\sqrt{\alpha_{8}\alpha_{9}} = 0$$
(9)

$$\Psi_{n} = s^{\alpha_{12}} (1 - \alpha_{3} s)^{-\alpha_{12} - \frac{\alpha_{13}}{\alpha_{3}}} P_{n}^{\left(\alpha_{10} - 1, \frac{\alpha_{11}}{\alpha_{3}} - \alpha_{10} - 1\right)} (1 - 2\alpha_{3} s),$$
(10)

where $P_n^{(\alpha,\beta)}(x)$ is the Jacobi polynomials and

$$\alpha_{4} = \frac{1}{2}(1 - \alpha_{1}), \alpha_{5} = \frac{1}{2}(\alpha_{2} - 2\alpha_{3}), \alpha_{6} = \alpha_{5}^{2} + \xi_{1}, \alpha_{7} = 2\alpha_{4}\alpha_{5} - \xi_{2}$$

$$\alpha_{8} = \alpha_{4}^{2} + \xi_{3}, \alpha_{9} = \alpha_{3}(\alpha_{7} + \alpha_{3}\alpha_{8}) + \alpha_{6}, \alpha_{10} = \alpha_{1} + 2\alpha_{4} + 2\sqrt{\alpha_{8}}$$

$$\alpha_{11} = \alpha_{2} - 2\alpha_{5} + 2(\sqrt{\alpha_{9}} + \alpha_{3}\sqrt{\alpha_{8}}), \alpha_{12} = \alpha_{4} + \sqrt{\alpha_{8}}, \alpha_{13} = \alpha_{5} - (\sqrt{\alpha_{9}} + \alpha_{3}\sqrt{\alpha_{8}}). \quad (11)$$

In the special case $\alpha_3 = 0$, we have

$$\lim_{\alpha_{3}\to 0} P_{n}^{\left(\alpha_{10}^{-1},\frac{\alpha_{11}}{\alpha_{3}}-\alpha_{10}^{-1}\right)} (1-2\alpha_{3}s) = L_{n}^{\alpha_{10}^{-1}}(\alpha_{11}s), \quad (12)$$

$$\lim_{\alpha_3 \to 0} (1 - 2\alpha_3 s)^{\alpha_{12} \alpha_3} = e^{\alpha_{13} s}, \quad (13)$$

and the wave function in equation (10) turns to

$$\Psi = s^{c_{12}} e^{c_{13}s} L_n^{c_{10}-1}(c_{11}s), \qquad (14)$$

where $L_n^{\alpha}(x)$ is the Laguerre polynomials. Detailed derivation of the formulae given in this Section can be found in [29]

3.0 Solution of the Schrödinger Equation for the Potential Models

In this section we shall obtain the bound state solutions of the Schrödinger equation for the improved Tietz, improved Rosen-Morse, and improved Manning-Rosen potential energy models.

3.1 Solution of Schrödinger equation for the Improved Tietz potential model

The Schrödinger equation in spherical polar coordinate can be written as [14]

$$-\frac{\hbar^{2}}{2\mu}\left\{\frac{\partial^{2}}{\partial r^{2}}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^{2}}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^{2}\theta}\frac{\partial^{2}}{\partial\phi^{2}}\right]+V(r)\right\}\Psi_{n\ell\mu}(r,\theta,\phi)=E\Psi_{n\ell\mu}(r,\theta,\phi).$$
(15)

Defining $\Psi_{n\ell\mu}(r,\theta,\phi) = U_{n\ell}Y_{\ell\mu}(\theta,\phi)$, we obtain the radial part of the Schrödinger equation as

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)U_{n\ell}(r) - \frac{2\mu}{\hbar^2}\left(V(r) + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right)U_{n\ell} + \frac{2\mu E_{n\ell}}{\hbar^2}U_{n\ell} = 0.$$
 (16)

If we define $U_{n\ell}(r) = \frac{R_{n\ell}(r)}{r}$, the radial equation appears as

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left(E_{n\ell} - V(r) - \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} \right) R_{n\ell}(r) = 0.$$
(17)

Substitution of the molecular Tietz potential in equation (5) into equation (17), we have

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$$\frac{-\hbar^2}{2\mu}\frac{d^2R(r)}{dr^2} + \left[D_e\left(1 + \frac{e^{\alpha r_e} + q}{e^{\alpha r} + q}\right)^2 + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]R(r) = ER(r).$$
(18)

Equation (18) cannot be solved exactly (except for $\ell = 0$ case called s-wave) because of the centrifugal term, we thus resort to the approximation used in Ref [21, 25] given as (see Ref. [21] for details of the approximation scheme)

$$V_{CT}(r) = \frac{\ell(\ell+1)}{2\mu r^2} \hbar^2 = \frac{\ell(\ell+1)}{2\mu r_e^2} \hbar^2 \frac{1}{(1+x)^2} = \gamma(1-2x+3x^2+...)$$
(19)

The centrifugal potential is then replaced by

$$V_{CT}(r) = \gamma \left(d_0 + d_1 \frac{1}{e^{\alpha r} + q} + d_2 \frac{1}{\left(e^{\alpha r} + q\right)^2} \right), \tag{20}$$

where

$$\begin{split} \gamma &= \frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}, \quad (21) \\ d_o &= 1 + \frac{3 - 3\alpha r_e + 6q e^{-\alpha r_e} + 3q^2 e^{-2\alpha r_e} - 2q \alpha r_e e^{-\alpha r_e} + q^2 \alpha r_e e^{-2\alpha r_e}}{\alpha^2 r_e^2}, \quad (22) \\ d_1 &= \frac{2\left(-9q + 3q \alpha r_e - 3e^{-\alpha r_e} + 2\alpha r_e e^{\alpha r_e} - 9q^2 e^{-\alpha r_e} - 3q^3 e^{-2\alpha r_e} - q^3 \alpha r_e e^{-2\alpha r_e}\right)}{\alpha^2 r_e^2}, \quad (23) \\ d_2 &= \frac{\left(18q^2 + 12q e^{\alpha r_e} + 3e^{2\alpha r_e} - 2q \alpha r_e e^{\alpha r_e} - \alpha r_e e^{2\alpha r_e} + 12q^3 e^{-\alpha r_e} + 3q^4 e^{-2\alpha r_e} + 2q^3 \alpha r_e e^{-2\alpha r_e} + q^4 \alpha r_e e^{-2\alpha r_e}\right)}{\alpha^2 r_e^2}, \quad (24) \end{split}$$

where we have also made use of the coordinate transformation $x = (r - r_e)/r_e$. In order to solve equation (18) (after substituting the approximation to the centrifugal term given in equation (20)) using the parametric NU method, we make use of the transformation $s = \frac{e^{\alpha r}}{e^{\alpha r} + q}$ to obtain $\left[\frac{d^2}{ds^2} + \frac{1}{s}\frac{(1-2s)}{(1-s)}\frac{d}{dr} + \frac{1}{s^2(1-s)^2}\left\{Bs^2 - (A+2B)s + \overline{\varepsilon} + A + B\right\}\right]R(s) = 0, \quad (25)$

where

$$\overline{\varepsilon} = \frac{\left(D_e + \gamma d_0 - E\right)}{\alpha^2} \left(\frac{-2\mu}{\hbar^2}\right),\tag{26}$$

$$\gamma d_e = 2D \left(e^{\alpha r} + e^{\alpha}\right)(-2\mu)$$

$$\mathsf{A} = \frac{\mathcal{H}_1 - 2D_e \left(e^{\alpha r} + q\right)}{q\alpha^2} \left(\frac{-2\mu}{\hbar^2}\right),\tag{27}$$

$$\mathsf{B} = \frac{\gamma d_2 + D_e \left[e^{\alpha r_e} + q \right]^r}{q^2 \alpha^2} \left(\frac{-2\mu}{\hbar^2} \right). \tag{28}$$

Comparing equation (25) with equation (8), we have

 $\alpha_1 = 1, \ \alpha_2 = 2, \ \alpha_3 = 1, \ \xi_1 = -B, \ \xi_2 = -(A + 2B), \ \xi_3 = -(\overline{\varepsilon} + A + B).$ (29) Making use of equation (11), we obtain

$$\begin{aligned} &\alpha_4 = 0, \, \alpha_5 = 0, \, \alpha_6 = -\mathsf{B}, \, \alpha_7 = \mathsf{A} + 2\mathsf{B}, \, \alpha_8 = -(\overline{\varepsilon} + \mathsf{A} + \mathsf{B}) \\ &\alpha_9 = -\overline{\varepsilon}, \, \alpha_{10} = 1 + 2\sqrt{-(\overline{\varepsilon} + \mathsf{A} + \mathsf{B})}, \, \alpha_{11} = 2 + 2\left(\sqrt{-\overline{\varepsilon}} + \sqrt{-(\overline{\varepsilon} + \mathsf{A} + \mathsf{B})}\right) \\ &\alpha_{12} = \sqrt{-(\overline{\varepsilon} + \mathsf{A} + \mathsf{B})}, \, \alpha_{13} = -\left(\sqrt{-\overline{\varepsilon}} + \sqrt{-(\overline{\varepsilon} + \mathsf{A} + \mathsf{B})}\right) \end{aligned}$$
(30)

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Substituting equations (29) and (30) into equation (9), we obtain the energy equation as [30]

 $2n + (2n+1)\left(\sqrt{-\overline{\varepsilon}} + \sqrt{-(\overline{\varepsilon} + A + B)}\right) + n(n-1) + A + 2B - 2(\overline{\varepsilon} + A + B) + 2\sqrt{\overline{\varepsilon}(\overline{\varepsilon} + A + B)} = 0, \quad (31)$

from which the energy eigenvalues can be obtained. The wave function is obtained by substituting equations (29) and (30) into equation (10) as

 $R(s) = N_n s^{\sqrt{-(\overline{\varepsilon} + \mathsf{A} + \mathsf{B})}} (1 - s)^{\sqrt{-\overline{\varepsilon}}} P_n^{\left(2\sqrt{-(\overline{\varepsilon} + \mathsf{A} + \mathsf{B})}, 2\sqrt{-\overline{\varepsilon}}\right)} (1 - 2s), \quad (32)$

where N_n is the normalization constant. We give the numerical results obtained for the energy eigenvalues with the improved Tietz potential model in Table 2. In all our numerical results, both in Tables and Figures (except stated otherwise), we have used $\alpha = 0.01$, $2\mu = 1$, $\hbar = 0.5$. The values of D_e , r_e , and q for some diatomic molecules are given in Table 1. The values are obtained from Refs [28, 31]. It can be observed from Table 2 and the Figures 1 - 4 that the energy eigenvalues for the Tietz potential increase linearly with n for the various values of ℓ considered.

Diatomic molecule	$D_e(eV)$	$r_e(\text{\AA})$	q
Cl_2	2.513903386	1.987	7.73121
O_2^+	6.780447246	1.116	0.47836
N_2^+	8.848131541	1.116	0.28175
NO^+	10.99665353	1.063	0.53878

Table 1: Spectroscopic constants of the diatomic molecules used in this study



Figure 1: The graph of Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic improved Tietz potential for O_2^+ molecule, with various values of ℓ

Table 2: The Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic molecular Tietz potential for some diatomic molecules with $\ell = 0$

n	O_2^+	Cl_2	NO^+	N_2^+
0	0.0077043	0.000919119	0.0116278	0.0108118
1	0.0231029	0.00273260	0.0348673	0.0324262
2	0.0384841	0.00451116	0.0580824	0.0540246
3	0.0538479	0.00625455	0.0812729	0.0756071
4	0.0691944	0.00796249	0.1044390	0.0971735
5	0.0845236	0.00963474	0.1275800	0.1187240
6	0.0998354	0.01127100	0.1506980	0.1402580
7	0.1151300	0.01287110	0.1737900	0.1617770
8	0.1304070	0.01596150	0.1968580	0.1832790
9	0.1456660	0.01443470	0.2199010	0.2047650
10	0.1609080	0.01745120	0.2429200	0.2262360

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Figure 2: The graph of Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic improved Tietz potential for Cl_2 molecule, with various values of ℓ



Figure 3: The graph of Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic improved Tietz potential for NO^+ molecule, with various values of ℓ



Figure 4: The graph of Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic improved Tietz potential for N_2^+ molecule, with various values of ℓ

In order to check the validity of the results we obtained, we will compare the energy eigenvalues obtained with that obtained in Ref. [21]. This is shown in Table 3. It can be observed from the Table that our results are in perfect agreement. This shows also the strength of the method we have used here.

n	E_n (our result)	E_n (Ref. [21])	
0	0.0216167	0.0216167	
1	0.0648136	0.0648136	
2	0.1079460	0.1079460	
3	0.1510150	0.1510150	
4	0.1940200	0.1940200	
5	0.2369600	0.2369600	
6	0.2798370	0.2798370	
7	0.3226490	0.3226490	
8	0.3653960	0.3653960	
9	0.4080790	0.4080790	
10	0.4506980	0.4506980	

Table 3: Comparison of the energy eigenvalues obtained here with that obtained in Ref. [21] using the data for NO^+ with $\alpha = 0.01$, $\mu = 0.5$, and $\hbar = 1$ for s – wave ($\ell = 0$).

3.2 Solution of Schrödinger Equation for the Improved Rosen-Morse Potential Model

The improved Rosen-Morse potential model is given in equation (5). If we compare equations (2) and (5), we observe that equation (5) can be obtained from equation (2) if we let q = 1. Therefore, the energy eigenvalues and wave functions for the improved Rosen-Morse potential model can be obtained from the energy eigenvalues and wave functions for the improved Tietz potential energy model by setting q = 1 in the results obtained from the improved Tietz potential model. Hence the energy equation for the improved Rosen-Morse potential model is obtained as

$$2n + (2n+1)\left(\sqrt{-\omega} + \sqrt{-(\omega+\mathsf{Z}+\varphi)}\right) + n(n-1) + \mathsf{Z} + 2\varphi - 2(\omega+\mathsf{Z}+\varphi) + 2\sqrt{\omega(\omega+\mathsf{Z}+\varphi)} = 0, \quad (33)$$

ere

where

$$\omega = \frac{\left(D_{e} + \gamma d_{0} - E\right)}{\alpha^{2}} \left(\frac{-2\mu}{\hbar^{2}}\right),
Z = \frac{\gamma d_{1} - 2D_{e} \left(e^{\alpha r} + 1\right)}{\alpha^{2}} \left(\frac{-2\mu}{\hbar^{2}}\right),
\varphi = \frac{\gamma d_{2} + D_{e} \left(e^{\alpha r_{e}} + 1\right)^{2}}{\alpha^{2}} \left(\frac{-2\mu}{\hbar^{2}}\right), (34)
d_{0} = 1 + \frac{\left(3 - 3\alpha r_{e} + 6e^{-\alpha r_{e}} + 3e^{-2\alpha r_{e}} - 2\alpha r_{e}e^{-\alpha r_{e}} + \alpha r_{e}e^{-2\alpha r_{e}}\right)}{\alpha^{2} r_{e}^{2}}, (35)
d_{1} = \frac{2\left(-9 + 3\alpha r_{e} - 3e^{-\alpha r_{e}} + 2\alpha r_{e}e^{\alpha r_{e}} - 9e^{-\alpha r_{e}} - 3e^{-2\alpha r_{e}} - \alpha r_{e}e^{-2\alpha r_{e}}\right)}{\alpha^{2} r_{e}^{2}}, (36)$$

and

$$d_{2} = \frac{\left(18 + 12e^{\alpha r_{e}} + 3e^{2\alpha r_{e}} - 2\alpha r_{e}e^{\alpha r_{e}} - \alpha r_{e}e^{2\alpha r_{e}} + 12e^{-\alpha r_{e}} + 3e^{-2\alpha r_{e}} + 2\alpha r_{e}e^{-2\alpha r_{e}} + \alpha r_{e}e^{-2\alpha r_{e}}\right)}{\alpha^{2} r_{e}^{2}}.$$
 (37)

We give the numerical results of the energy eigenvalues for the improved Rosen-Morse potential model in Table 4. It can be observed that the energy eigenvalues increase with increasing ℓ and n. It can also be observed from Figures 5 – 8 that the energy eigenvalues for the improved Rosen-Morse potential increase with increasing n and ℓ .

Table 4: The Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic molecular Rosen-Morse potential for some diatomic molecules with $\ell = 0$

n	O_2^+	Cl_2	NO^+	N_2^+
0	0.0057056	0.0009191	0.0040001	0.0074748
1	0.0171106	0.0027326	0.0119941	0.0224182
2	0.0285031	0.0045111	0.0199756	0.0373491
3	0.0398831	0.0062545	0.0279446	0.0522675
4	0.0512506	0.0079624	0.0359010	0.0671734
5	0.0626056	0.0079624	0.0438450	0.0820668
6	0.0739481	0.0112710	0.0517765	0.0969477
7	0.0852781	0.0128711	0.0596954	0.1118160
8	0.0965955	0.0144347	0.0676019	0.1266720
9	0.1079010	0.0159615	0.0754958	0.1415150
10	0.1191930	0.0174512	0.0833773	0.1563460



Figure 5: The graph of Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic improved Rosen-Morse potential for O_2^+ molecule, with various values of ℓ



Figure 6: The graph of Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic improved Rosen-Morse potential for Cl_2 molecule, with various values of ℓ



Figure 7: The graph of Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic improved Rosen-Morse potential for NO^+ molecule, with various values of ℓ



Figure 8: The graph of Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic improved Rosen-Morse potential for N_2^+ molecule, with various values of ℓ

3.3 Solution of the Schrödinger Equation for the Improved Manning-Rosen Potential Model

The radial part of the D-dimension Schrödinger equation with a central force potential V(r) is given as

$$\left[\frac{-\hbar^2}{2\mu}\frac{1}{r^{D-1}}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right) + V(r) + \frac{\hbar^2 J(J+D-2)}{2\mu r^2}\right]R_{vj} = E_{vj}^D(r), \quad (38)$$

where D is a positive integer and $D \ge 2$, μ is the reduced mass of a diatomic molecule, \hbar denotes the reduced Planck's constant, E_{vj}^{D} the rotational vibrational energy of the diatomic molecule system, v and j are the vibrational and rotational $\frac{D-1}{2}$

quantum numbers respectively. Defining $R_{vj} = r^{\frac{1}{2}} u_{vj}$, we obtain the radial part of the Schrödinger equation as

$$\frac{-\hbar^2}{2\mu}\frac{d^2 U_{vj}(r)}{dr^2} + \left[U(r) + \frac{K(K+1)\hbar^2}{2\mu r^2}\right]U_{vj}(r) = E_{vj}^D(r), \quad (39)$$

where $K = J + \frac{1}{2}(D-3)$. Substitution of the molecular improved Manning-Rosen potential in equation (7) into equation (39), we have

$$\frac{-\hbar^2}{2\mu}\frac{d^2 U_{vj}(r)}{dr^2} + \left[D_e \left(1 - \frac{e^{\alpha r_e} - 1}{e^{\alpha r} - 1}\right)^2 + \frac{K(K+1)\hbar^2}{2\mu r^2}\right]U_{vj}(r).$$
(40)

By using the improved Greene-Aldrich approximation scheme

$$\frac{1}{r^2} \approx \alpha^2 \left(\frac{1}{12} + \frac{e^{\alpha r}}{\left(e^{\alpha r} - 1\right)^2} \right)$$
(41)

to deal with the centrifugal term, we obtain

$$\frac{-\hbar^2}{2\mu}\frac{d^2U(r)}{dr^2} + \left[\frac{D_e(e^{\alpha r_e}-1)^2 + K(K+1)\alpha^2 e^{\alpha r}}{(e^{\alpha r}-1)^2} - \frac{D_e(e^{2\alpha r_e}-1)}{e^{\alpha r_e}-1} + \left(D_e - E + \frac{K(K+1)\frac{\hbar^2}{2\mu}}{12}\right)\right] = 0.$$
(42)

It should be noted that for 3D case, K = J. In order to solve equation (42) using the parametric NU method, we make use $e^{\alpha r}$

of the transformation $z = \frac{e^{\alpha r}}{e^{\alpha r} - 1}$. Hence, equation (42) transforms to $\frac{d^2 U}{d^2 U} \pm \frac{1}{2} \frac{(1 - 2z)}{dU} \frac{dU}{dU} + \frac{1}{2} \frac{(\sigma - \Lambda z)}{(\sigma - \Lambda z)} \sigma \frac{dU}{dU}$

$$\frac{d^2 U}{dz^2} + \frac{1}{z} \frac{(1-2z)}{(1-z)} \frac{dU}{dr} + \frac{1}{z^2 (1-z)^2} \left[\sigma - \Lambda z (1-z) - \chi (1-z) \right] U = 0,$$
(43)

where

$$\sigma = \left(D_e - E + \frac{K(K+1)\frac{\hbar^2}{2\mu}}{12} \right) \left(\frac{-2\mu}{\hbar^2 \alpha^2} \right), \quad (44)$$
$$\Lambda = \left(\frac{2\mu}{\hbar^2} D_e (e^{\alpha r_e} - 1)^2 + K(K+1) \right) \left(\frac{-2\mu}{\hbar^2 \alpha^2} \right), \quad (45)$$
$$\chi = \frac{2\mu}{\hbar^2} D_e \left(e^{2\alpha r_e} - 1 \right) \left(\frac{-2\mu}{\hbar^2 \alpha^2} \right). \quad (46)$$

Comparing equation (43) with the equation (8) we have

$$\alpha_1 = 1, \, \alpha_2 = 2, \, \alpha_3 = 1, \, \xi_1 = \Lambda, \, \xi_2 = (\chi + \Lambda), \, \xi_3 = -(\sigma - \chi).$$
 (47)

Making use of equation (11), we obtain

$$\alpha_{4} = 0, \alpha_{5} = 0, \alpha_{6} = \Lambda, \alpha_{7} = -(\Lambda + \chi), \alpha_{8} = \chi - \sigma \alpha_{9} = -\sigma, \alpha_{10} = 1 + 2\sqrt{\chi} - \sigma$$
$$\alpha_{11} = 2 + 2\left(\sqrt{-\sigma} + \sqrt{\chi} - \sigma\right)\alpha_{12} = \sqrt{\chi} - \sigma, \alpha_{13} = -\left(\sqrt{-\sigma} + \sqrt{\chi} - \sigma\right) \quad (48)$$
tion (47) and (48) into equation (0), we obtain the energy equation of

Substituting equation (47) and (48) into equation (9), we obtain the energy equation as

$$2n + (2n+1)\left(\sqrt{-\sigma} + \sqrt{\chi - \sigma}\right) + n(n-1) + \chi - \Lambda - 2\sigma + 2\sqrt{(\chi - \sigma)(-\sigma)} = 0$$
(49)

from which the energy eigenvalues can be obtained. The wave function is obtained by substituting equations (47) and (48) into equations (10) as

$$U(z) = N_n z^{\sqrt{\chi - \sigma}} \quad (1 - z)^{\sqrt{-\sigma}} \quad P_n^{(2\sqrt{\chi - \sigma}, 2\sqrt{-\sigma})} (1 - 2z), \tag{50}$$

where N_n is the normalization constant. It can be observed from Table (5) that the energy eigenvalues for the Manning-Rosen potential increases with the increasing values of n considered for the case K = 0. Note that the results are obtained in 3D only. The results obtained in this subsection could also have been obtained from the results obtained for the improved Tietz potential by setting q = -1 in the 3D case only.

n	O_2^+	Cl_2	NO^+	N_2^+
0	5.13880	2.41268	2.27882	10.7616
1	5.14057	2.41426	2.28124	10.7640
2	5.14227	2.41583	2.28364	10.7664
3	5.14395	2.41738	2.28603	10.7688
4	5.14562	2.41892	2.28841	10.7712
5	5.14728	2.42046	2.29077	10.7735
6	5.14892	2.42197	2.29313	10.7759
7	5.15056	2.42348	2.29547	10.7782
8	5.15218	2.42497	2.29780	10.7805
9	5.15378	2.42645	2.30011	10.7829
10	5.15538	2.42792	2.30241	10.7852

Table 5: The Energy eigenvalues $E_{n\ell}$ (in eV) of the non-relativistic molecular Manning-Rosen potential for some diatomic molecules with K = 0 i.e. in 3D (D = 3)

4.0 Solutions of Dirac equation for the potential models

The Dirac equation with both the scalar potential S(r) and vector potential V(r) can be written as $(\hbar = c = 1)$ [5, 32]

$$\left\{\boldsymbol{\alpha} \cdot \mathbf{p} + V(r) + \boldsymbol{\beta}[M + S(r)]\right\} \Psi(r) = E \Psi(r), \quad (51)$$

where M is the mass of the particle and E denotes the particle energy. The α and β are the usual 4×4 matrices given by

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$
(52)

where σ is the Pauli's 2×2 matrices. In Ref [5], a second-order differential equation was derived for the upper component spinor F(r) of Dirac equation for equally mixed scalar and vector potentials with the same sign. The following equation was derived for s – wave case (where $\ell = 0$)

$$\left[-\frac{d^2}{dx^2} + 2(E+M)V(x)\right]F(x) = \tilde{E}F(x), \qquad (53)$$

The lower component spinor G(x), is given by [5]

$$G(x) = \frac{1}{M+E} \frac{dF(x)}{dx},$$
 (54)

where $\tilde{E} = E^2 - M^2$, $E + M \neq 0$, for the positive energy solution.

Similarly, for an equally mixed scalar and vector potentials with the opposite sign, we have the lower and upper component spinor, respectively as,

$$\left\lfloor \frac{-d^2}{dx^2} + 2(E - M)V(x) \right\rfloor G(x) = \widetilde{E}G(x), \tag{55}$$

and

$$F(x) = \frac{1}{M - E} \frac{dG(x)}{dx},$$
 (56)

where $\tilde{E} = E^2 - M^2$, $E - M \neq 0$, for the negative energy solution. In this Section, we shall obtain the bound state solutions of the improved Tietz, improved Rosen-Morse, and improved Manning-Rosen potentials using the method described in Sec 2.

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4.1 Solutions of s-wave Dirac Equation for Improved Tietz Potential Model

The solutions of Dirac equation for the three potential models we are considering will be obtained analytically without any approximations. This means that we will solve only for the s-wave Dirac equation.

4.1.1 Solutions of the Positive Energy Subspace for Tietz Potential Model

Substitution of the potential function $V_{IT}(r)$ given in equation (2) into equation (53), and taking into consideration the Alhaidari's suggestion [33], equation (53) gives

$$\left\{\frac{d^2}{dr^2} + \left[\widetilde{E} - 2AD_e \left(1 - \frac{e^{\alpha r_e} + q}{e^{\alpha r} + q}\right)^2\right]\right\} F(r) = 0, \quad (57)$$

where

 $(M+E) = A. \tag{58}$

In order to solve equation (57) using the parametric NU method, we make use of the transformation $z = \frac{e^{\alpha r}}{e^{\alpha r} + q}$. Hence,

equation (57) transforms to

$$\left\{\frac{d^2}{dz^2} + \left(\frac{1-2z}{1-z}\right)\frac{1}{z}\frac{d}{dz} + \frac{1}{z^2(1-z)^2}\left[\rho + \phi - \Omega - z(\phi - 2\Omega) - z^2\Omega\right]\right\}F(z) = 0, \quad (59)$$

where

$$\rho = \frac{\widetilde{E} - 2AD_e}{\alpha^2},\tag{60}$$

$$\phi = \frac{4AD_e(e^{\alpha r_e} + q)}{\alpha^2},$$
 (61)

and

$$\Omega = \frac{2AD_e (e^{\alpha r_e} + q)^2}{\alpha^2}.$$
 (62)

Comparing equation (59) with equation (8), we obtain the following

$$\alpha_1 = 1, \ \alpha_2 = 2, \ \alpha_3 = 1, \ \xi_1 = \Omega, \ \xi_2 = -(\phi - 2\Omega), \ \xi_3 = (\Omega - \phi - \rho)$$
(63)

Substituting equation (63) into equation (11), we obtain

$$\begin{aligned} \alpha_4 &= 0, \ \alpha_5 = 0, \ \alpha_6 = \Omega, \ \alpha_7 = (\phi - 2\Omega), \ \alpha_8 = (\Omega - \phi - \rho), \\ \alpha_9 &= -\phi \ \alpha_{10} = 1 + 2\sqrt{\Omega - \phi - \rho}, \ \alpha_{11} = 2 - 2(\sqrt{-\phi} + \sqrt{\Omega - \phi - \rho}), \\ \alpha_{12} &= \sqrt{\Omega - \phi - \rho}, \ \alpha_{13} = -(\sqrt{-\phi} + \sqrt{\Omega - \phi - \rho}). \end{aligned}$$

Substituting equation (64) into equation (9), we obtain the energy equation as [33]

$$n^{2} + n(2n+1)(\sqrt{-\phi}) - 2\rho - \phi + 2\sqrt{(\Omega - \phi - \rho)(-\phi)} = 0$$
(65)

from which the energy eigenvalues can be obtained. The upper spinor wave function is obtained as

$$F_n(z) = z^{\sqrt{\Omega - \phi - \rho}} (1 - z)^{\sqrt{-\phi}} P_n^{2\sqrt{\Omega - \phi - \rho}, 2 + 2\sqrt{-\phi}} (1 - 2z).$$
(66)

If we substitute equation (66) into (54) we obtain the lower spinor component as

$$G_{n} = \frac{1}{M + E_{n}} \left\{ -(1-z)^{\sqrt{-\phi}} z^{\sqrt{\Omega-\phi-\rho}} \left(3 + n + 2\sqrt{-\phi} + a\right) P_{n-1}^{(1+a,b)} (1-2z) \quad (67) \\ -(1-z)^{-1+\sqrt{-\phi}} z^{\sqrt{\Omega-\phi-\rho}} \sqrt{-\phi} P_{n}^{\left[2\sqrt{\Omega-\phi-\rho}, 2+2\sqrt{-\phi}\right]} (1-2z) \\ +(1-z)^{\sqrt{-\phi}} z^{(-1+\sqrt{\Omega-\phi-\rho})} \sqrt{\Omega-\phi-\rho} P_{n}^{(2\sqrt{\Omega-\phi-\rho}, 2+2\sqrt{-\phi})} (1-2z) \right\}$$

where $a = 2\sqrt{\Omega - \phi - \rho}$ and $b = 3 + 2\sqrt{-\phi}$.

4.1.2 Solutions of the Negative Energy Subspace for Tietz Potential Model

The solutions of the negative energy subspace of the Dirac equation for the improved Tietz potential is obtained, after using the Nikiforov-Uvarov method. the energy equation is obtained as

$$-\left[n^{2} + n(2n+1)(\sqrt{-\phi'}) - 2\rho' - \phi + 2\sqrt{(\Omega - \phi - \rho)(-\phi)}\right] = 0, \quad (68)$$

from which the energy eigenvalues can be obtained. The lower and upper component spinors are, respectively,

$$G_n(r) = C_n z^{\sqrt{\Omega - \phi - \rho}} (1 - z)^{\sqrt{-\phi}} P_n^{2\sqrt{\Omega - \phi - \rho}, 2 + 2\sqrt{-\phi}} (1 - 2z),$$
(69)

and

$$F_{n} = C_{n} \frac{1}{M - E_{n}} \left\{ -(1 - z)^{\sqrt{-\phi}} z^{\sqrt{\Omega - \phi - \rho}} \left(3 + n + 2\sqrt{-\phi} + a\right) P_{n-1}^{(1 + a, b)} (1 - 2z) \right.$$
(70)
$$-(1 - z)^{-1 + \sqrt{-\phi}} z^{\sqrt{\Omega - \phi - \rho}} \sqrt{-\phi} P_{n}^{\left[2\sqrt{\Omega - \phi - \rho}, 2 + 2\sqrt{-\phi}\right]} (1 - 2z) + (1 - z)^{\sqrt{-\phi}} z^{(-1 + \sqrt{\Omega - \phi - \rho})} \sqrt{\Omega - \phi - \rho} P_{n}^{(2\sqrt{\Omega - \phi - \rho}, 2 + 2\sqrt{-\phi})} (1 - 2z) \right\}$$

where C_n is the normalization constant, $a = 1 + 2\sqrt{\Omega - \phi - \rho}$ and $b = 3 + 2\sqrt{-\phi}$. The symbols used are the same as those used for the positive energy subspace of the Dirac equation but the energy is now negative of the energy obtained in that case.

4.2 Solutions of Dirac Equation for Improved Rosen-Morse Potential

We follow the method described in the previous subsection to obtain the solutions of the Dirac equation for the improved Rosen-Morse potential model.

4.2.1 Solutions of the positive energy subspace for Rosen-Morse potential

The energy equation is obtained as

$$n^{2} + n + (2n+1)(\sqrt{-\Pi}) - \Pi - 2\mu + 2\sqrt{(\Gamma - \Pi - \mu)(-\Pi)} = 0, \quad (71)$$

where

$$\mu = \frac{\tilde{E} - 2AD_e}{\alpha^2}, \quad (72)$$
$$\Pi = \frac{4AD_e(e^{\alpha r_e} + 1)}{\alpha^2}, \quad (73)$$

and

$$\Gamma = \frac{2AD_e(e^{\alpha r_e} + 1)^2}{\alpha^2}.$$
 (74)

The upper spinor wave function is obtained as

$$F_n(z) = C_n z^{\sqrt{\Gamma - \Pi - \mu}} (1 - z)^{\sqrt{-\Pi}} P_n^{2\sqrt{\Gamma - \Pi - \mu}, 2 + 2\sqrt{-\Pi}} (1 - 2z),$$
(75)

while the lower spinor wave function is also obtained as

$$G_{n}(z) = C_{n} \frac{1}{M+E} \left\{ -(1-z)^{\sqrt{-\Pi}} z^{\sqrt{\Gamma-\Pi-\mu}} \left(3+n+2\sqrt{-\phi}+\Xi\right) P_{n-1}^{[1+\Xi,\varsigma]}(1-2z) \right. (76) \\ \left. -(1-z)^{(-1+\sqrt{-\Pi})} z^{(\sqrt{\Gamma-\Pi-\mu})} \sqrt{-\Pi} P_{n}^{[2\sqrt{\Gamma-\Pi-\mu},2+2\sqrt{-\Pi}]}(1-2z) \right. \\ \left. +(1-z)^{\sqrt{-\Pi}} z^{(1-\sqrt{\Gamma-\Pi-\mu})} \sqrt{\Gamma-\Pi-\mu} P_{n}^{[2\sqrt{\Gamma-\Pi-\mu},2+2\sqrt{-\Pi}]}(1-2z) \right\}$$
where $\Xi = 2\sqrt{\Gamma-\Pi-\mu}$ and $\varsigma = 3+2\sqrt{-\Pi}$.

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Solutions of the negative energy subspace for Rosen-Morse Potential 4.2.2

The solutions of the negative energy subspace of the Dirac equation for the improved Rosen-Morse potential model is obtained as

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$$-\left[n^{2}+n+(2n+1)(\sqrt{-\Pi})-\Pi-2\mu+2\sqrt{(\Gamma-\Pi-\mu)(-\Pi)}\right]=0,$$
 (77)

from where the energy eigenvalues can be obtained. The lower and upper component spinors are obtained as

$$G_n(z) = C_n z^{\sqrt{\Gamma - \Pi - \mu}} (1 - z)^{\sqrt{-\Pi}} P_n^{2\sqrt{\Gamma - \Pi - \mu}, 2 + 2\sqrt{-\Pi}} (1 - 2z),$$
(78)

and

$$F_{n}(z) = C_{n} \frac{1}{M - E} \left\{ -(1 - z)^{\sqrt{-\Pi}} z^{\sqrt{\Gamma - \Pi - \mu}} \left(3 + n + 2\sqrt{-\phi} + \Xi \right) P_{n-1}^{[1 + \Xi, \varsigma]} (1 - 2z) - (1 - z)^{(-1 + \sqrt{-\Pi})} z^{(\sqrt{\Gamma - \Pi - \mu})} \sqrt{-\Pi} P_{n}^{[2\sqrt{\Gamma - \Pi - \mu}, 2 + 2\sqrt{-\Pi}]} (1 - 2z) + (1 - z)^{\sqrt{-\Pi}} z^{(1 - \sqrt{\Gamma - \Pi - \mu})} \sqrt{\Gamma - \Pi - \mu} P_{n}^{[2\sqrt{\Gamma - \Pi - \mu}, 2 + 2\sqrt{-\Pi}]} (1 - 2z) \right\}$$
(79)

The symbols used are the same as those used for the positive energy subspace of the Dirac equation (for the improved Rosen-Morse potential model) but the energy is now negative of the energy obtained in that case.

4.3 Solutions of s-wave Dirac equation for improved Manning-Rosen Potential

In this subsection, we will obtain the solutions of the Dirac equation for the improved Manning-Rosen potential model.

4.3.1 Solutions of the positive energy subspace for Manning-Rosen potential

Following similar technique used earlier in this section, the energy equation for the positive energy subspace of the Dirac equation with the manning-Rosen potential model is obtained as

$$n^{2} + n + (2n+1)(\sqrt{-\sigma}) - \tau - 2\sigma + 2\sqrt{(\nu - \tau - \sigma)(-\sigma)} = 0,$$
 (80)

where

$$\sigma = \frac{\widetilde{E} - 2AD_e}{\alpha^2}, \qquad (81)$$
$$\tau = \frac{4AD_e(e^{\alpha r_e} - 1)}{\alpha^2}, (82)$$

and

$$v = \frac{2AD_{e}(e^{\alpha r_{e}} - 1)^{2}}{\alpha^{2}}.$$
 (83)

The upper spinor wave function is obtained as

$$F_{n}(z) = C_{n} z^{\sqrt{\nu - \tau - \sigma}} (1 - z)^{\sqrt{-\sigma}} P_{n}^{2\sqrt{\nu - \tau - \sigma}, 2 + 2\sqrt{-\sigma}} (1 - 2z),$$
(84)

and the lower spinor wave function as

$$G_{n}(z) = C_{n} \frac{1}{M+E} \left\{ -(1-z)^{\sqrt{-\sigma}} z^{\sqrt{\nu-\tau-\sigma}} (3+n+2\sqrt{-\sigma}+\varpi) P_{(n-1)}^{[1+\varpi,3+2\sqrt{-\sigma}]} (1-2z) + (1-z)^{(-1+\sqrt{-\sigma})} z^{\sqrt{\nu-\tau-\sigma}} \sqrt{-\sigma} P_{n}^{[2\sqrt{\nu-\tau-\sigma},2+2\sqrt{-\sigma}]} (1-2z) + (1-z)^{\sqrt{-\sigma}} z^{(-1+\sqrt{\nu-\tau-\sigma})} \sqrt{\nu-\tau-\sigma} P_{n}^{[2\sqrt{\nu-\tau-\sigma},2+2\sqrt{-\sigma}]} (1-2z) \right\},$$
(85)

where $\overline{\omega} = 2\sqrt{\upsilon - \tau - \sigma}$.

4.3.2 Solutions of the negative energy subspace for Manning-Rosen potential

The solutions of the negative energy subspace of the Dirac equation for the improved Manning-Rosen potential models are given in this subsection. The energy equation (from which the energy eigenvalues can be obtained) is obtained as

$$-[n^{2} + n + (2n+1)(\sqrt{-\sigma}) - \tau - 2\sigma + 2\sqrt{(\upsilon - \tau - \sigma)(-\sigma)}] = 0.$$
(86)

The upper spinor wave function is obtained as

$$G_{n}(z) = C_{n} z^{\sqrt{\nu - \tau - \sigma}} (1 - z)^{\sqrt{-\sigma}} P_{n}^{2\sqrt{\nu - \tau - \sigma}, 2 + 2\sqrt{-\sigma}} (1 - 2z)$$
(87)

and the lower spinor wave function as ;

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$$F_{n}(z) = C_{n} \frac{1}{M-E} \left\{ -(1-z)^{\sqrt{-\sigma}} z^{\sqrt{\nu-\tau-\sigma}} (3+n+2\sqrt{-\sigma}+\varpi) P_{(n-1)}^{[1+\varpi,3+2\sqrt{-\sigma}]} (1-2z) + (1-z)^{(-1+\sqrt{-\sigma})} z^{\sqrt{\nu-\tau-\sigma}} \sqrt{-\sigma} P_{n}^{[2\sqrt{\nu-\tau-\sigma},2+2\sqrt{-\sigma}]} (1-2z) + (1-z)^{\sqrt{-\sigma}} z^{(-1+\sqrt{\nu-\tau-\sigma})} \sqrt{\nu-\tau-\sigma} P_{n}^{[2\sqrt{\nu-\tau-\sigma},2+2\sqrt{-\sigma}]} (1-2z) \right\},$$
(88)

where $\varpi = 2\sqrt{\upsilon - \tau - \sigma}$.

It should be noted that the solutions of Dirac equation have been obtained for s-wave bound states only, but the method we have used here can also be used to obtain the solutions for arbitrary ℓ – states as well as scattering state solutions. To the best of our knowledge, this is the first attempt to obtain the solutions of Dirac equation for the three potential models studied here.

5.0 Conclusion

We have studied the Schrödinger equation and Dirac equation with the interaction potentials improved Tietz, improved Rosen-Morse and improved Manning-Rosen. We employed the parametric Nikiforov-Uvarov and some approximation schemes to solve the one-body problems of Schrödinger equation and obtained exact solutions (without any approximations) for Dirac equation with the potential models for s-wave state only. In order to check the validity of the results we obtained in the non-relativistic case, we compared the energy eigenvalues obtained for improved Tietz potential with that obtained in Ref. [21]. Our results are in perfect agreement. In the relativistic case (using the Dirac equation), we obtained the energy equations and spinors for the positive energy subspace and negative energy subspace cases (bound states only). From our numerical results (shown in Tables and Figures), it can be observed that the energy eigenvalues for the potential models considered increase linearly with n and ℓ in the non-relativistic case. We have again demonstrated the power of the parametric Nikiforov-Uvarov method in solving one-body problem analytically by solving a bound state problem. The method is simple enough to follow and the work can be extended to scattering states solutions. We strongly believe that many-body problems should also have simplified methods to tackle them. In this respect, we shall, in future, carry out a research to formulate simple methods to deal with many-body problems (of course employing some approximations initially). The results we have obtained can be applied to scattering problems and to obtain information-theoretic measures in quantum information theory. Scattering state solutions of some wave equations are currently under investigation. Other methods can be used to solve Dirac equation for the three potential models to test the accuracy/validity of our results (and the method used).

6.0 References

- [1] Hassanabadi, H., Zarrinkamar, S., Hamzavi, M., and Rajabi, A. A. (2011). Few-Body Syst. 51, 69.
- [2] Hamzavi, M. and Ikhdair, S. M. (2012). Mol. Phys. **110**, 3031.
- [3] Ikhdair, S. M. and Sever, R. J. (2011). Phys. A: Math. Theor., 44, 355301.
- [4] Yahya, W. A., Oyewumi, K. J., Akoshile, C. O. and Ibrahim, T. T. (2010). J. Vec. Rel. 5, 27.
- [5] Yahya, W. A. and Oyewumi, K. J. (2013). J. Math. Phys. 54, 013508.
- [6] Yahya, W. A., Falaye, B. J., Oluwadare, O. J. and Oyewumi, K. J. (2013). Int. J. Mod. Phys. E 22(8), 1350062.
- [7] Zhang, M. C., Sun, G. H., and Dong, S. H. (2010). Phys. Lett. A., **374**, 704.
- [8] Oyewumi, K. J., and Akoshile, C. O. (2010). Eur. Phys. J. A. 45, 311.
- [9] Hassanabadi, H., Maghsoodi, E., and Zarrinkamar, S. (2012). Eur. Phys. J. Plus, 127, 31.
- [10] Sun, G. H. and Dong, S. H. (2010). Mod. Phys. Lett. A.25, 2849.
- [11] Çiftçi, H., Hall, R. L., and Saad, N. (2003). J. Phys. A: Math Gen. 36, 11807.
- [12] Falaye, B. J. (2012). J. Math. Phys. 53, 082107.
- [13] Boztosun, I., Karakoç, M., Yasuk, F., and Durmus, A. (2006). J. Math. Phys. 47, 062301.
- [14] Yahya, W. A., Issa, K., Falaye, B.J., and Oyewumi, K. J. (2014). Can J. Chem. 92, 215.
- [15] Dong, S. H. (2007). Factorization Method in Quantum Mechanics, Springer, Dordrecht, The Netherlands.
- [16] Ortakaya, S. (2012). Chin. Phys. B **21**(7), 070303.
- [17] Ma, Z. Q., and Xu, B. W. (2005). Eur. Phys. Lett. 69, 685.
- [18] Qiang, W. C., and Dong, S. H.(2007). Phys. Lett. A **363**, 169.
- [19] Liu, J. Y., Du, J. F., and Jia, C. S. (2013). J. Eur. Phys. **128**, 139.
- [20] Jia, C. S., Diao, Y. F., Liu, X. J., Wang, P. Q., Liu, J. Y., and Zhang, G. D. (2012). J. Chem. Phys. 137(1), 014101.
- [21] Tang, H. M., Liang, G. C., Zhang, L. H., Zhao, F., and Jia, C. S. (2014). Can. J. Chem. 92, 201. dx.doi.org/10.1139/cjc-2013-0466.
- [22] Nikoofard, H., Maghshoodi, E., Zarrinkamar, S., Farhadi, M., and Hassanabadi, H. (2013). Turkish J. Phys. 37, 74.
- [23] Chen, T., Lin, S. R., and Jia, C. S. (2013): Eur. Phys. J. Plus 128, 69.

- [24] Hu, X. T., Zhang, L. H., and Jia, C. S. (2014). D-dimension energies for the lithium dimer, J. Mol. Spec., **294**, 21-24.
- [25] Yahya, W. A. and Issa, K. (2015). Chin. J. Phys. **53**(3), 060401.
- [26] Dehesa, J. S., Lopez-Rosa, S., and Martinez-Finkelshtein, A. (2010). Int. J. Quantum Chem. 110, 1529.
- [27] Yahya, W. A., Oyewumi, K. J., and Sen, K. D. (2014). Indian J. Chem. **53A**, 1307.
- [28] Yahya, W. A., Oyewumi, K. J., and Sen, K. D. (2015). Int. J. Quant. Chem. DOI:10.1002/qua.24971.
- [29] Tezcan, C., and Sever, R. (2009). Int. J. theor. Phys, 48, 337.
- [30] Olufadi, Y. (2015). Non-relativistic solutions of some molecular potential models with applications. Undergraduate research project, Kwara State University, Malete, Nigeria.
- [31] Jia, C. S., Chen, T., Yi, L. Z., and Lin, S. R. (2013). J. Math. Chem. 51, 2165.
- [32] Alhaidari, A. D., Bahlouli, H., and Al-Hasan, A. (2006). Phys. Lett. A 349, 87.
- [33] Salami, I. (2015). Exact solutions of the s-wave Dirac equations for some potential models. Undergraduate research project, Kwara State University, Malete, Nigeria