

Approximate Analytical Solutions of the Improved Tietz and Improved Rosen-Morse Potential Models

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In this article, the approximate analytical solutions of the improved Tietz and improved Rosen-Morse potential models are obtained using the parametric Nikiforov-Uvarov method. The energy eigenvalues and wave functions are obtained in the relativistic realm by solving the Klein-Gordon equation. Numerical results of the energy eigenvalues are obtained and studied.

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I. INTRODUCTION

In the last decade, a lot of articles have focused on the analytical and approximate solutions of the Schrödinger, Klein-Gordon, and Dirac equations. This is because the solutions of these wave equations contain all the necessary information for the quantum system under consideration. As is well known, the Schrödinger wave equation is used to describe non-relativistic spinless particles, the Klein-Gordon equation for relativistic spin-zero particles, the Duffin-Kemmer-Petiau equation for relativistic spin-zero and spin-one particles, and the Dirac equation for relativistic spin-half particles. Many potential models have been studied using these wave equations, such as the Kratzer potential, Morse potential, Rosen-Morse potential, Manning-Rosen potential, Deng-Fan potential, and Pöschl-Teller potential among others. See for example [1–8] for details.

The Tietz potential as a potential energy function for diatomic molecules was proposed in 1963 by Tietz as [4, 7]:

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

where D_e is the dissociation energy. The parameters a , b , h , and α can be determined so as to fit the calculated values of the spectroscopic parameters to observed ones. In 2012, Jia *et al.* [9] proposed a more convenient form of the original Tietz potential energy function. The improved Tietz potential is given as [7, 9]

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

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where r_e is the equilibrium bond length. The original Tietz potential function is conventionally defined in terms of five parameters. However, it actually only has four independent parameters, as shown in Equation (2) [4, 9]. It should also be noted that a molecular Tietz potential of the form [10, 11]

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

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; its applications are given in Refs. [10, 11].

In 1932, Rosen and Morse proposed a potential function for polyatomic molecules [5]

$$V_{RM}(r) = B \tanh(r/d) - C \operatorname{sech}^2(r/d), \quad (4)$$

where B , C , and d are three adjustable parameters. The Rosen-Morse potential has been used to investigate polyatomic vibrational states [5, 12]. Many authors have studied the Rosen-Morse potential model both in non-relativistic and relativistic quantum mechanics. See Ref. [5] for details and applications of the Rosen-Morse potential. The improved Rosen-Morse potential model proposed is written as [5, 9]

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

where $\alpha = 2/d$, D_e is the dissociation energy, and r_e is the equilibrium bond length. In Equation (5), the term $1/2D_e(e^{\alpha r_e} + 1)$ 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 this paper, we attempt to obtain the energy eigenvalues and wave functions for the improved Tietz and improved Rosen-Morse potential energy models. By using the elegant parametric Nikiforov-Uvarov (NU) method, we obtain the bound state solutions of the improved Tietz potential energy model. We then make the necessary transformations to obtain the energy eigenvalues and eigen-functions for the improved Rosen-Morse potential energy model.

The paper is organized as follows: in Section II, a review of the method to be used is given (i.e., the parametric NU method). Section III contains the solutions of the improved Tietz potential model and the solutions of the improved Rosen-Morse potential, obtained by a transformation, are given in Section IV. We give the conclusion in Section V.

II. THE PARAMETRIC NIKIFOROV-UVAROV (NU) METHOD

By using the parametric NU method, the solutions of a second order differential equation of the form [13–17]

$$\frac{d^2\Psi}{ds^2} + \left[\frac{c_1 - c_2s}{s(1 - c_3s)} \right] \frac{d\Psi}{ds} + \left[\frac{-\xi_1s^2 + \xi_2s - \xi_3}{s^2(1 - c_3s)^2} \right] \Psi = 0 \quad (6)$$

are

$$c_2n - (2n + 1)c_5 + (2n + 1)(\sqrt{c_9} + c_3\sqrt{c_8}) + n(n - 1)c_3 + c_7 + 2c_3c_8 + 2\sqrt{c_8c_9} = 0 \quad (7)$$

and

$$\Psi_n = s^{c_{12}} (1 - c_3s)^{-c_{12} - \frac{c_{13}}{c_3}} P_n^{(c_{10}-1, \frac{c_{11}}{c_3} - c_{10}-1)}(1 - 2c_3s), \quad (8)$$

where

$$\begin{aligned} c_4 &= \frac{1}{2}(1 - c_1), \quad c_5 = \frac{1}{2}(c_2 - 2c_3), \quad c_6 = c_5^2 + \xi_1, \quad c_7 = 2c_4c_5 - \xi_2, \\ c_8 &= c_4^2 + \xi_3, \quad c_9 = c_3(c_7 + c_3c_8) + c_6, \quad c_{10} = c_1 + 2c_4 + 2\sqrt{c_8}, \\ c_{11} &= c_2 - 2c_5 + 2(\sqrt{c_9} + c_3\sqrt{c_8}), \quad c_{12} = c_4 + \sqrt{c_8}, \quad c_{13} = c_5 - (\sqrt{c_9} + c_3\sqrt{c_8}). \end{aligned} \quad (9)$$

In Equation (8), $P_n^{\alpha,\beta}(x)$ is the Jacobi polynomial. In the special case $c_3 = 0$, we have

$$\lim_{c_3 \rightarrow 0} P_n^{(c_{10}-1, \frac{c_{11}}{c_3} - c_{10}-1)}(1 - 2c_3s) = L_n^{c_{10}-1}(c_{11}s), \quad (10)$$

$$\lim_{c_3 \rightarrow 0} (1 - 2c_3s)^{-c_{12} - \frac{c_{13}}{c_3}} = e^{c_{13}s}, \quad (11)$$

and the wave function in Equation (8) turns to

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

where $L_n^\alpha(x)$ is the Laguerre polynomial.

III. SOLUTIONS OF THE KLEIN-GORDON EQUATION WITH THE IMPROVED TIETZ POTENTIAL

The radial part of the time-independent Klein-Gordon equation with equal scalar $S(r)$ and vector $V(r)$ potentials, describing a spin-zero particle can be written as [19–22]

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell + 1)}{r^2} + \frac{(E^2 - M^2c^4)}{\hbar^2c^2} - \frac{2}{\hbar^2c^2} (E + Mc^2) V(r) \right] R_{n\ell}(r) = 0, \quad (13)$$

where E refers to the energy spectrum and M is the rest mass of the confined particle. If we substitute Equation (2) into Equation (13), we obtain

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{(E^2 - M^2 c^4)}{\hbar^2 c^2} - \frac{2}{\hbar^2 c^2} (E + M c^2) D_e \left(1 - \frac{e^{\alpha r_e} + q}{e^{\alpha r} + q} \right)^2 \right] R_{n\ell}(r) = 0. \quad (14)$$

Equation (14) cannot be solved exactly except for the s-wave ($\ell = 0$) state. So we employ the approximation given in Ref. [4] where the centrifugal potential was expanded in a series around zero as

$$V_{CP}(r) = \frac{\ell(\ell+1)\hbar^2 c^2}{r^2} = \frac{\ell(\ell+1)\hbar^2 c^2}{r_e^2} \frac{1}{(1+x)^2} = \gamma(1 - 2x + 3x^2 + \dots), \quad (15)$$

which is then replaced by

$$V_{CP}(r) = \rho \left(f_0 + f_1 \frac{1}{e^{\alpha r} + q} + f_2 \frac{1}{(e^{\alpha r} + q)^2} \right), \quad (16)$$

where

$$\rho = \frac{\ell(\ell+1)\hbar^2 c^2}{r_e^2}, \quad (17)$$

$$f_0 = 1 + \frac{3 - 3\alpha r_e + 6q e^{-\alpha r_e} + 3q^2 e^{-2\alpha r_e} - 2q\alpha r_e e^{-\alpha r_e} + q^2 \alpha r_e e^{-2\alpha r_e}}{\alpha^2 r_e^2}, \quad (18)$$

$$f_1 = \frac{-18q + 6q\alpha r_e - 6e^{\alpha r_e} + 4\alpha r_e e^{\alpha r_e} - 18q^2 e^{-\alpha r_e} - 6q^3 e^{-2\alpha r_e} - 2q^3 \alpha e^{-2\alpha r_e}}{\alpha^2 r_e^2}, \quad (19)$$

$$f_2 = \frac{18q^2 + 12q e^{\alpha r_e} + 3e^{2\alpha r_e} - 2q\alpha r_e e^{\alpha r_e} - \alpha r_e e^{2\alpha r_e} + 12q^3 e^{-\alpha r_e} + 3q^4 e^{-2\alpha r_e} + 2q^3 \alpha r_e e^{-\alpha r_e} + q^4 \alpha r_e e^{-2\alpha r_e}}{\alpha^2 r_e^2}, \quad (20)$$

and we made use of the coordinate transformation $x = (r - r_e)/r_e$. Substituting Equation (16) into Equation (14), we obtain

$$\left[\frac{d^2}{dr^2} - \frac{\eta_1}{e^{\alpha r_e} + q} - \frac{\eta_2}{(e^{\alpha r_e} + q)^2} e^{\alpha r_e} + \eta_{n\ell} \right] R_{n\ell} = 0, \quad (21)$$

where

$$\eta_1 = \frac{1}{\hbar^2 c^2} \left[\rho f_1 - 2(\mu c^2 + E_{n\ell}) D_e(e^{\alpha r_e} + q) + \frac{\rho f_2 + (\mu c^2 + E_{n\ell}) D_e(e^{\alpha r_e} + q)^2}{q} \right], \quad (22)$$

$$\eta_2 = -\frac{\rho f_2 + (\mu c^2 + E_{n\ell})D_e(e^{\alpha r_e} + q)^2}{\hbar^2 c^2 q}, \quad (23)$$

$$\eta_{n\ell} = \frac{E_{n\ell}^2 - \mu^2 c^4 - (\mu c^2 + E_{n\ell})D_e - \rho f_0}{\hbar^2 c^2}, \quad (24)$$

In order to solve Equation (21) using the parametric NU method, we make use of the transformation $z = \frac{e^{\alpha r}}{e^{\alpha r} + q}$. Hence, Equation (21) transforms to

$$\frac{d^2 R_{n\ell}}{dz^2} + \frac{(1-2z)}{z(1-z)} \frac{dR_{n\ell}}{dz} + \frac{1}{z^2(1-z)^2} [Az^2 + Bz + C] R_{n\ell}(z) = 0, \quad (25)$$

where

$$A = \frac{\eta_2}{\alpha^2 q}, \quad B = \frac{\eta_1 - \eta_2}{\alpha^2 q}, \quad C = \frac{q\eta_{n\ell} - \eta_1}{\alpha^2 q}. \quad (26)$$

Comparing Equation (25) with Equation (6), we have

$$c_1 = 1, \quad c_2 = 2, \quad c_3 = 1, \quad \xi_1 = -A, \quad \xi_2 = B, \quad \xi_3 = -C. \quad (27)$$

Making use of Equation (9), we obtain

$$\begin{aligned} c_4 &= 0, \quad c_5 = 0, \quad c_6 = -A, \quad c_7 = -B, \quad c_8 = -C, \\ c_9 &= -A - B - C, \quad c_{10} = 1 + 2\sqrt{-C}, \quad c_{11} = 2 + 2(\sqrt{-A - B - C} + \sqrt{-C}), \\ c_{12} &= \sqrt{-C}, \quad c_{13} = -\left[(\sqrt{-A - B - C} + \sqrt{-C})\right]. \end{aligned} \quad (28)$$

Substituting Equation (28) into Equation (7), we obtain the energy equation as

$$2n + (2n+1) \left[\sqrt{(-A - B - C)} + \sqrt{-C} \right] + n(n-1) - B - 2C + 2\sqrt{-C}(-A - B - C) = 0, \quad (29)$$

from which the energy eigenvalues can be obtained. The wave function is also obtained by substituting Equations (27) and (28) into Equation (8) as

$$R_{n\ell} = z^{\sqrt{-C}} (1-z)^{\sqrt{(-A-B-C)}} P_n^{2\sqrt{-C}, 2\sqrt{(-A-B-C)}}(1-2z). \quad (30)$$

We give the numerical results obtained for the energy eigenvalues with the improved Tietz potential model in Tables I and II below. It can be observed from Table I that the energy eigenvalues for the improved Tietz potential energy model when $\ell = 0$ decreases as q increases, but it increases with increasing n . We also observe from Table II that the energy eigenvalues for the improved Tietz potential energy model when $\ell = 1$ increases with increasing q and n .

TABLE I: Energy eigenvalues for the improved Tietz potential energy model for some values of the parameter q with $D_e = 10.0$, $r_e = 1.5$, $\alpha = 0.01$, $\hbar = 2\mu = c = 1$, $\ell = 0$.

n	$q = 1$	$q = 2$	$q = 3$	$q = 4$
0	0.515793	0.510577	0.507948	0.506364
1	0.546653	0.531373	0.523607	0.518905
2	0.576613	0.551706	0.538952	0.531198
3	0.605760	0.571610	0.554002	0.543254
4	0.634171	0.591112	0.568771	0.555082
5	0.661907	0.610239	0.583274	0.566692
6	0.689023	0.629013	0.597523	0.578093
7	0.715567	0.647455	0.611531	0.589292
8	0.741579	0.665583	0.625307	0.600297
9	0.767097	0.683413	0.638863	0.611115
10	0.792153	0.700962	0.652207	0.621751

TABLE II: Energy eigenvalues for the improved Tietz potential energy model for some values of the parameter q with $D_e = 10.0$, $r_e = 1.5$, $\alpha = 0.01$, $\hbar = 2\mu = c = 1$, $\ell = 1$.

n	$q = 1$	$q = 2$	$q = 3$	$q = 4$
0	152.432	228.454	304.476	380.499
1	152.439	228.459	304.480	380.502
2	152.447	228.464	304.484	380.505
3	152.454	228.468	304.487	380.508
4	152.461	228.473	304.491	380.511
5	152.468	228.478	304.495	380.514
6	152.476	228.483	304.498	380.517
7	152.483	228.488	304.502	380.520
8	152.490	228.493	304.505	380.522
9	152.497	228.497	304.509	380.525
10	152.505	228.502	304.513	380.528

IV. SOLUTIONS OF THE KLEIN-GORDON EQUATION WITH THE IMPROVED ROSEN-MORSE POTENTIAL

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.

Hence the energy equation for the improved Rosen-Morse potential model is obtained as

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

where

$$A = \frac{\eta_2}{\alpha^2}, \quad B = \frac{\eta_1 - \eta_2}{\alpha^2}, \quad C = \frac{\eta_{n\ell} - \eta_1}{\alpha^2}, \quad (32)$$

$$f_0 = 1 + \frac{3 - 3\alpha r_e + 6e^{-\alpha r_e} + 3e^{-2\alpha r_e} - 2\alpha r_e e^{-\alpha r_e} + \alpha r_e e^{-2\alpha r_e}}{\alpha^2 r_e^2}, \quad (33)$$

$$f_1 = \frac{-18 + 6\alpha r_e - 6e^{\alpha r_e} + 4\alpha r_e e^{\alpha r_e} - 18e^{-\alpha r_e} - 6e^{-2\alpha r_e} - 2\alpha e^{-2\alpha r_e}}{\alpha^2 r_e^2}, \quad (34)$$

$$f_2 = \frac{18 + 12e^{\alpha r_e} + 3e^{2\alpha r_e} - 2\alpha r_e e^{\alpha r_e} - \alpha r_e e^{2\alpha r_e} + 12e^{-\alpha r_e} + 3e^{-2\alpha r_e} + 2\alpha r_e e^{-\alpha r_e} + \alpha r_e e^{-2\alpha r_e}}{\alpha^2 r_e^2}, \quad (35)$$

$$\eta_1 = \frac{1}{\hbar^2 c^2} \left[\rho f_1 - 2(\mu c^2 + E_{n\ell}) D_e (e^{\alpha r_e} + 1) + \rho f_2 + (\mu c^2 + E_{n\ell}) D_e (e^{\alpha r_e} + 1)^2 \right], \quad (36)$$

$$\eta_2 = -\frac{\rho f_2 + (\mu c^2 + E_{n\ell}) D_e (e^{\alpha r_e} + 1)^2}{\hbar^2 c^2}, \quad (37)$$

$$\eta_{n\ell} = \frac{E_{n\ell}^2 - \mu^2 c^4 - (\mu c^2 + E_{n\ell}) D_e - \rho f_0}{\hbar^2 c^2}. \quad (38)$$

We give the numerical results of the energy eigenvalues for the improved Rosen-Morse potential model in Table III. It can be observed that the energy eigenvalues increase with increasing ℓ and n .

TABLE III: Energy eigenvalues for the improved Rosen-Morse potential energy model for some values of ℓ with $D_e = 10.0$, $r_e = 1.5$, $\alpha = 0.01$, $\hbar = 2\mu = c = 1$.

n	$\ell = 0$	$\ell = 1$	$\ell = 2$	$\ell = 3$
0	0.515793	152.432	264.017	373.374
1	0.546653	152.439	264.024	373.381
2	0.576613	152.447	264.031	373.388
3	0.605760	152.454	264.038	373.396
4	0.634171	152.461	264.045	373.403
5	0.661907	152.468	264.053	373.410
6	0.689023	152.476	264.060	373.417
7	0.715567	152.483	264.067	373.424
8	0.741579	152.490	264.074	373.431
9	0.767097	152.497	264.081	373.439
10	0.792153	152.505	264.089	373.446

V. CONCLUSION

We have obtained the approximate analytical solutions of the improved Tietz and improved Rosen-Morse potential energy models via the parametric Nikiforov-Uvarov method. By solving the Klein-Gordon equation, we obtained the energy eigenvalues and wave functions. Numerical results are obtained. The energy eigenvalues for the improved Tietz potential decreases as q increases when $\ell = 0$, but the energy eigenvalues increases as q increases when $\ell = 1$. For the improved Rosen-Morse potential model, the energy eigenvalues increase with increasing ℓ and n .

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