Original Research Article

Arbitrary l-state Solution of the Schrödinger Equation for q-deformed attractive radial plus Coulomb-like Molecular Potential within the framework of NU-Method.

Abstract

The Schrödinger equation in one dimension for the q-deformed attractive radial plus coulomb-like molecular potential (ARCMP) is solved approximately to obtain bound states eigen solutions using the parametric Nikiforov-Uvarov (NU) method. The corresponding unnormalized eigen functions are evaluated in terms of Jacobi polynomials. Interestingly, the resulting eigen energy equations can be used to study the spectroscopy of some selected diatomic atoms and molecules.

Keywords: q-deformed potential, attractive radial, Coulomb-like, Schrödinger

1 INTRODUCTION

An exact analytical solution of Schrödinger equation for central potentials has attracted enormous interest in recent years. So far, some of these potentials are the parabolic type potential [1], the Eckart Potential [2, 3], the Fermi-step Potential [2,3], the Rosen-Morse Potential [4], the Ginocchio barrier [5], the Scarf barriers [6], the Morse Potential [7] and a potential which interpolates between Morse and Eckart barriers [8]. Many researchers have investigated the exponential type potentials [9–12] and quasi-exactly solvable quadratic potentials [13–15]. Furthermore, Schrödinger, Dirac, Klein-Gordon, and Duffin-Kemmer-Petiau equations for a Coulomb type potential are solved by using different method [16–18]. Recently our group has also made significant progress in the use of combined or superposed molecular potentials to investigate the eigensolutions of relativistic and non-relativistic equations [19]. We have studied the eigen solutions (eigenvalues and eigen functions) of Klein-Gordon, Dirac and Schrödinger equations using superposed or mixed potentials. Some notable examples include Woods-Saxon plus Attractive Inversely Quadratic potential (WSAIQP) [19], Manning-Rosen plus a class of Yukawa Potential (MRCYP) [20], generalized wood-Saxon plus Mie-type Potential (GWSMP) [21], Kratzer plus Reduced Pseudoharmonic Oscillator Potential (KRPHOP) [22], Inversely Quadratic Yukawa plus Attractive Radial potentials (IQYARP) [23], Modified Echart plus Inverse Square Molecular Potentials (MEISP) [24]

In nuclear and atomic physics, the shape form of a potentials play an important role, particularly when investigating the structure of deformed nuclei or the interaction between them. Therefore, our aim, in this present work, is to investigate approximate bound state solutions of the Schrödinger equation with q-deformed attractive radial plus coulomb-like molecular potential (qARCMP) using the parametric Nikiforov-Uvarov (NU) method. The solutions of this equation will definitely give us a wider and deeper knowledge of the properties of molecules moving under the sway of the superposed potential which is the goal of this paper. The parametric NU method is very convenient and does not require the truncation of a series like the series solution method which is more difficult to use. The organization of this work is as follows. In Section 2, we briefly introduce the basic concepts of the NU method. Section 3 is devoted to the solution of the Schrödinger problem to obtain the approximate bound-state energy of q-deformed attractive radial plus coulomb-like molecular potential (qARCMP) and their corresponding eigenfunctions by applying the NU method. The results of special cases of potential consideration are discussed in Section 4. The scientific significance of this research paper includes giving an insight into possible eigensolutions of atoms and molecules moving under the influence of qARCMP potential. Secondly, the resulting eigenenergy equations can be used to study the spectroscopy of some selected diatomic atoms and molecules.

2 REVIEW OF PARAMETRIC NIKIFAROV-UVAROV METHOD

The NU method is based on the solutions of a generalized second order linear differential equation with special orthogonal functions. The Nikiforov-Uvarov method has been successfully applied to relativistic and nonrelativistic quantum mechanical problems and other field of studies as well [25].The hypergeometric NU method has shown its power in calculating the exact energy levels of all bound states for some solvable quantum systems.

$$\Psi_n''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\Psi_n'(s) + \frac{\bar{\sigma}(s)}{\sigma^2(s)}\Psi_n(s) = 0 \quad (1)$$

Where, σ(s) and $\bar{\sigma}(s)$ are polynomials at most second degree and $\tilde{\tau}(s)$ is first degree polynomials. The parametric generalization of the N-U method is given by the generalized hypergeometric-type equation

$$\Psi''(s) + \frac{c_1 - c_2 s}{s(1-c_3 s)}\Psi'(s) + \frac{1}{s^2(1-c_3 s)^2}[-\epsilon_1 s^2 + \epsilon_2 s - \epsilon_3]\Psi(s) = 0 \quad (2)$$

Thus eqn. (1) can be solved by comparing it with equation (2) and the following polynomials are obtained

$$\tilde{\tau}(s) = (c_1 - c_2 s), \sigma(s) = s(1 - c_3 s), \bar{\sigma}(s) = -\epsilon_1 s^2 + \epsilon_2 s - \epsilon_3 \quad (3)$$

The parameters obtainable from equation (3) serve as important tools to finding the energy eigenvalue and eigenfunctions. They satisfy the following sets of equation respectively

$$c_2 n - (2n+1)c_5 + (2n+1)(\sqrt{c_9} + c_3\sqrt{c_8}) + n(n-1)c_3 + c_7 + 2c_3 c_8 + 2\sqrt{c_8 c_9} = 0 \quad (4)$$

$$(c_2 - c_3)n + c_3 n^2 - (2n+1)c_5 + (2n+1)(\sqrt{c_9} + c_3\sqrt{c_8}) + c_7 + 2c_3 c_8 + 2\sqrt{c_8 c_9} = 0 \quad (5)$$

While the wave function is given as

$$\Psi_n(s) = N_{n,l} S^{c_{12}}(1 - c_3 s)^{-c_{12} - \frac{c_{13}}{c_3}} P_n^{\left(c_{10} - 1, \frac{c_{11}}{c_3} - c_{10} - 1\right)}(1 - 2c_3 s) \quad (6)$$

Where,

$c_4 = \frac{1}{2}(1 - c_1)$, $c_5 = \frac{1}{2}(c_2 - 2c_3)$, $c_6 = c_5{}^2 + \epsilon_1$, $c_7 = 2c_4 c_5 - \epsilon_2$, $c_8 = c_4{}^2 + \epsilon_3$,

$c_9 = c_3 c_7 + c_3{}^2 c_8 + c_6$, $c_{10} = c_1 + 2c_4 + 2\sqrt{c_8}$, $c_{11} = c_2 - 2c_5 + 2(\sqrt{c_9} + c3\sqrt{c_8})$

$c_{12} = c_4 + \sqrt{c_8}$, $c_{13} = c_5 - (\sqrt{c_9} + c3\sqrt{c_8})$ (7)

And P_n is the orthogonal polynomials.

$$\text{Given that } P_n^{(\alpha,\beta)} = \sum_{r=0}^{n} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(\alpha+r+1)\Gamma(n+\beta-r+1)(n-r)!r!}\left(\frac{x-1}{2}\right)^r\left(\frac{x+1}{2}\right)^{n-r} \quad (8)$$

This can also be expressed in terms of the Rodriguez's formula

$$P_n(x)^{(\alpha,\beta)} = \frac{1}{2^n n!}(x-1)^{-\alpha}(x+1)^{-\beta}\left(\frac{d}{dx}\right)^n\left((x-1)^{n+\alpha}(x+1)^{n+\beta}\right)$$

3 EIGENSOLUTIONS OF THE SHRODINGER EQUATION WITH qARCMP

The l-State Schrödinger Equation with vector V(r), potential is given as [26-29]

$$\frac{d^2 R(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[(E - V(r)) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]R(r) = 0 \tag{9}$$

Where, E is the energy eigenvalue, ℓ is the angular momentum quantum number

The q-deformed attractive radial potential is given as [26]

$$V(r) = -\left(\frac{V_1 e^{-4\alpha r} + V_2 e^{-2\alpha r} + V_3}{(1-qe^{-2\alpha r})^2}\right) \tag{10}$$

Where, $V_1 = \frac{\alpha^2}{4}, V_2 = \frac{(A-8)\alpha^2}{4}, V_3 = \frac{(4-A)\alpha^2}{4}$

Where, screening parameter α determines the range of the potential, and V_1, V_2, V_3 are the coupling parameters describing the depth of the potential well. In general q-deformed hyperbolic functions are defined as

$$Sinh_q(r) = \frac{1}{Cosech_q(r)} = \frac{e^r - qe^{-r}}{2}, Cosh_q(r) = \frac{e^r + qe^{-r}}{2}, Coth_q(r) = \frac{Cosh_q(r)}{Sinh_q(r)} \tag{11}$$

The Coulomb-like Potential, $V(r) = -\frac{A}{r}$ (12)

Making the transformation $s = e^{-2\alpha r}$the sum of the potentials (qARCMP) in equations (10) and (12) becomes

$$V(s) = \left(\frac{V_1 s^2 + V_2 s + V_3}{(1-qs)^2} - \frac{2A\alpha}{(1-qs)}\right) \tag{13}$$

By applying the Pekeris-like approximation [27, 28] to the inverse square term, $\frac{1}{r^2} = \frac{4\alpha^2}{(1-s)^2}$ to eq. (13) enable us to completely solve eq. (9).

Again, applying the transformation $s = e^{-2\alpha r}$ to get the form that Nikiforov-Uvarov (NU) method is applicable, equation (9) gives a generalized hypergeometric-type equation as

$$\frac{d^2 R(s)}{ds^2} + \frac{(1-s)}{(1-s)s}\frac{dR(s)}{ds} + \frac{1}{(1-s)^2 s^2}[(2\beta^2 q^2 - B)s^2 + (-Hq - P - 4\beta^2 q)s + (2\beta^2 + H - J + \lambda)]R(s) = 0 \tag{14}$$

Where,

$$-\beta^2 = \left(\frac{\mu E}{4\alpha^2\hbar^2}\right),\ B = \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1, \lambda = l(l+1), P = \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_2, H = \left(\frac{\mu}{\alpha\hbar^2}\right)A, J = \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3 \tag{15}$$

$$c_1 = c_2 = c_3 = q, c_4 = 0, c_5 = -\frac{q}{2}, c_6 = \frac{q^2}{4} + 2\beta^2 q^2 - B, c_7 = -4\beta^2 q - P - Hq,$$

$$c_8 = 2\beta^2 - J + H + \lambda, c_9 = \frac{q^2}{4} + pq + Jq^2 + \lambda q^2 + B, c_{10} = q + 2\sqrt{2\beta^2 - J + H + \lambda},$$

$$c_{11} = 2 + 2\left(\sqrt{\frac{q^2}{4} + pq + Jq^2 + \lambda q^2 + B} + \sqrt{2\beta^2 - J + H + \lambda}\right), c_{12} = \sqrt{2\beta^2 - J + H + \lambda}\,,$$

$$c_{13} = -\frac{1}{2} - \left(\sqrt{\frac{q^2}{4} + pq + Jq^2 + \lambda q^2 + B} + \sqrt{2\beta^2 - J + H + \lambda}\right), \varepsilon_1 = 2\beta^2 q^2 + B,$$

$$\varepsilon_2 = 4\beta^2 q + P + Hq, \varepsilon_3 = 2\beta^2 + H - J + \lambda \qquad (16)$$

Now using equations (6), (15) and (16) we obtain the energy eigen spectrum of the q-deformed ARCMP as

$$\beta^2 = \left[\frac{(2Jq - P - \lambda q) - q\left(n^2 + n + \frac{1}{2}\right) - (2n+1)\sqrt{\frac{q^2}{4} + pq + Jq^2 + \lambda q^2 + B}}{q\left(n + \frac{1}{2}\right) + 2\sqrt{\frac{q^2}{4} + pq + Jq^2 + \lambda q^2 + B}}\right]^2 - (J - H - \lambda) \qquad (17)$$

The above equation can be solved explicitly and the energy eigen spectrum of q-deformed ARCMP becomes

$$E = \frac{4\alpha^2\hbar^2}{\mu}\left\{\left[\frac{\left(2q\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3 - \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_2 - l(l+1)q\right) - q\left(n^2 + n + \frac{1}{2}\right) - (2n+1)\sqrt{\frac{q^2}{4} + q\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_2 + q^2\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3 + l(l+1)q^2 + \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1}}{q\left(n + \frac{1}{2}\right) + 2\sqrt{\frac{q^2}{4} + q\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_2 + q^2\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3 + l(l+1)q^2 + \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1}}\right]\right\} - \left(\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3 - \left(\frac{\mu}{\alpha\hbar^2}\right)A - l(l+1)\right) \qquad (18)$$

In the standard case of the attractive radial potential where q = 1, our energy eigen spectrum formula (eq. [18]) matches up with the results of parametric Nikifrov-Uvarov approach in ref. [29]

We now calculate the radial wave function of the q-deformed ARCMP as follows

$$\rho(s) = s^u(1 - qs)^v \qquad (19)$$

Where, $u = 2\beta^2 - J + H + \lambda$, and $v = 2q\sqrt{\frac{q^2}{4} + pq + Jq^2 + \lambda q^2 + B}$

$X_n(s) = p_n^{(u,v)}(1 - 2qs)$, where $p_n^{(u,v)}$ are Jacobi polynomials

$$\varphi(s) = s^{u/2}(1 - qs)^{1+v/2} \qquad (20)$$

Radial wavefunction

$$R_n(s) = N_n\varphi(s)X_n(s) \qquad (21)$$

$$R_n(s) = N_n s^{u/2}(1 - qs)^{1+v/2}P_n^{(u,v)}(1 - 2qs)$$

And using equation (16) we get

$$\varphi(s) = s^{U/2}(1-s)^{V-1/2}, \tag{22}$$

We then obtain the radial wave function from the equation

$$R_n(s) = N_n \varphi(s) \chi_n(s),$$

As

$$R_n(s) = N_n s^{U/2}(1-s)^{(V-1)/2} P_n^{(U,V)}(1-2s), \tag{23}$$

Where n is a positive integer and N_n is the normalization constant

4 DICUSSION

We consider the following cases from equation (19)

CASE I: If we choose $V_1 = V_2 = V_3 = 0$ then the energy eigen values of the Coulomb-like molecular potential is given as

$$E = \frac{4\alpha^2\hbar^2}{\mu}\left\{\left[\frac{(l(l+1)q) - q\left(n^2+n+\frac{1}{2}\right) - (2n+1)\sqrt{\frac{q^2}{4}+l(l+1)q^2}}{q\left(n+\frac{1}{2}\right)+2\sqrt{\frac{q^2}{4}+l(l+1)q^2}}\right]\right\} - \left(\left(\frac{\mu}{\alpha\hbar^2}\right)A - l(l+1)\right) \tag{24}$$

CASE II: If we choose $A = 0$ then the energy eigen values of the q-deformed Attractive Radial Potential

$$E = \frac{4\alpha^2\hbar^2}{\mu}\left\{\left[\frac{\left(2q\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3 - \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_2 - l(l+1)q\right) - q\left(n^2+n+\frac{1}{2}\right) - (2n+1)\sqrt{\frac{q^2}{4}+q\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_2+q^2\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3+l(l+1)q^2+\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1}}{q\left(n+\frac{1}{2}\right)+2\sqrt{\frac{q^2}{4}+q\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_2+q^2\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3+l(l+1)q^2+\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1}}\right]\right\} - \left(\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3 - l(l+1)\right) \tag{25}$$

CASE III: If we choose $l = 0$ then the eigen energy spectrum of the s-wave 1-dimensional Schrödinger equation with q-deformed ARCMP

$$E = \frac{4\alpha^2\hbar^2}{\mu}\left\{\left[\frac{\left(2q\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3 - \left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_2\right) - q\left(n^2+n+\frac{1}{2}\right) - (2n+1)\sqrt{\frac{q^2}{4}+q\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_2+q^2\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3+\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1}}{q\left(n+\frac{1}{2}\right)+2\sqrt{\frac{q^2}{4}+q\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_2+q^2\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3+\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_1}}\right]\right\} - \left(\left(\frac{\mu}{2\alpha^2\hbar^2}\right)V_3 - \left(\frac{\mu}{\alpha\hbar^2}\right)A\right) \tag{26}$$

5 CONCLUSION

In this work, using the parametric generalization of the NU method, we have obtained approximately energy eigenvalues and the corresponding wave functions of the Schrödinger equation for q-deformed attractive radial plus Coulomb-like molecular potential. The corresponding unnormalized eigen functions are evaluated in terms of Jacobi polynomials. Interestingly, the Klein-Gordon and Dirac equation with the arbitrary angular momentum values for this potential can be solved by this method. The resulting eigen energy equations can be used to study the spectroscopy of some selected diatomic atoms and molecules.

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