SOLUTIONS OF THE SCHRÖDINGER EQUATION WITH INVERSELY QUADRATIC HELLMANN PLUS MIE-TYPE POTENTIAL USING NIKIFOROV – UVAROV METHOD

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ABSTRACT

The solutions of the Schrödinger equation with inversely quadratic Hellmann plus Mie-type potential for any angular momentum quantum number have been presented using the Nikiforov-Uvarov method. The bound state energy eigenvalues and the corresponding un-normalized eigenfunctions are obtained in terms of the Laguerre polynomials. Several cases of the potential are also considered and their eigen values obtained.

KEYWORDS

Schrödinger equation, inversely quadratic Hellmann potential, Mie-type potential, Nikiforov – Uvarov method, Laguerre polynomials, PACS Nos 03.65.W; 03.65.Ge.

1. Introduction

The bound state solutions of the Schrödinger equation (SE) are only possible for some potentials of physical interest [1-5]. Quite recently, several authors have tried to solve the problem of obtaining exact or approximate solutions of the Schrödinger equation for a number of special potentials [6-11]. Some of these potentials are known to play very important roles in many fields of Physics such as Molecular Physics, Solid State and Chemical Physics [8].

The purpose of the present work is to present the solution of the Schrodinger equation with the inversely quadratic Hellmann plus Mie-type potential (IQHMP) of the form

\[ V(r) = -\frac{a}{r} + \frac{b}{r^2} e^{\delta r} + \left(-\frac{A}{r} + \frac{B}{r^2} + C\right) \]

where \( A, B, C \) are constants that relates to the coulombic interactions between two electrons.

This potential can be written as

\[ V(r) = \frac{B+b}{r^2} - \frac{A+b\delta}{r} + (C + b\delta^2) \]

(1)
Where \( r \) represents the internuclear distance, \( \alpha \) and \( \beta \) are the strengths of the Coulomb and Yukawa potentials, respectively, and \( \delta \) is the screening parameter. Equation (1) is then amenable to Nikiforov-Uvarov method. Okon et al [12] have obtained analytical solutions of the Schrodinger equation with Mie-type potential using factorization method. Sever et al [13] have obtained bound state solutions of the Schrodinger equation for Mie potential. They applied their results to several diatomic molecules. Potoff and Bernard-Brunel [14] obtained Mie potentials for phase equilibria calculations and obtained excellent results when applied to alkanes and perfluoroalkanes. Also Edalat et al [15] used the second virial coefficient data and obtained optimized coefficients as well as exponents of the Mie potential energy function for a number of symmetric groups of molecules. Furthermore, Barakat et al [16] studied the effect of Mie-type potential range on the cohesive energy of metallic nanoparticles using the size-dependent potential parameters method. Aydogdu and Sever [17] investigated the exact solutions of the Dirac equation for Mie-type potentials under the conditions of pseudospin and spin symmetry limits. The bound state energy equations and the corresponding two-component spinor wave functions of the Dirac particles for the Mie-type potentials with pseudospin and spin symmetry were obtained. Agboola [18] solved the N-dimensional Schrodinger equation with Mie-type potentials and obtained exact solutions. Yong et al [19] obtained the Mie potential and equation of state for bulk metallic glass from thermal expansion and ultrasonic data. Ita [20] has solved the Schrödinger equation for the Hellman potential and obtained the energy eigenvalues and their corresponding wave functions using expansion method and Nikiforov-Uvarov method. Also, Hamzavi and Rajabi [21] have used the parametric Nikiforov-Uvarov method to obtain tensor coupling and relativistic spin and pseudospin symmetries of the Dirac equation with the Hellmann potential. Kocak et al [22] solved the Schrödinger equation with the Hellmann potential using asymptotic iteration method and obtained energy eigenvalues and the wave functions. However, not much has been achieved in the area of solving the radial Schrodinger equation for any angular momentum quantum number, \( l \), with IQHMP using Nikiforov – Uvarov method in the literature.

2. Overview of the Nikiforov-Uvarov Method

The Nikiforov-Uvarov (NU) method is based on the solutions of a generalized second-order linear differential equation with special orthogonal functions [20]. The Schrödinger equation of the type as:

\[
\psi''(r) + [E - V(r)]\psi(z) = 0
\]

could be solved by this method. Where in equation (2) \( \psi(r) \) is a wave function whose argument is \( r \), \( E \) is the Energy eigen value and \( V(r) \) is the potential energy function. The prim \((')\) means derivative with respect to the coordinate \( r \) and double prime stands for double derivative with respect to the coordinate \( r \). This can be done by transforming equation (2) into an equation of hypergeometric type with appropriate coordinate transformation \( z = z(r) \) to get

\[
\psi''(z) + \frac{\sigma(z)}{\sigma(z)} \psi'(z) + \frac{\bar{\sigma}(z)}{\bar{\sigma}(z)} \psi(z) = 0
\]

In equation (3) \( \sigma(z) \) and \( \bar{\sigma}(z) \) are polynomials at most second-degree, \( \bar{\sigma}(z) \) is a first-degree polynomial and \( \psi(z) \) is a function of hypergeometric-type.
To find the exact solution to equation (3), we write $\psi(z)$ as

$$\psi(z) = \phi(z)\chi(z)$$  \hfill (4)

$\phi(z)$ and $\chi(z)$ are two functions which have to be chosen appropriately. Substitution of equation (4) into equation (3) yields equation (5) of hypergeometric type as

$$\sigma(z)\chi''(z) + \tau(z)\chi'(z) + \lambda\chi(z) = 0$$  \hfill (5)

Where $\lambda$ is a constant.

In equation (4), the wave function $\phi(z)$ is defined as the logarithmic derivative [21]

$$\frac{\phi'(z)}{\phi(z)} = \frac{\pi(z)}{\sigma(z)}$$  \hfill (6)

With $\pi(z)$ being at most first order polynomials. Also, the hypergeometric-type functions in equation (5) for a fixed integer $n$ is given by the Rodrigue relation as

$$\chi_n(z) = \frac{B_n}{\rho_n d^n z^n} [\sigma^n(z) \rho(z)]$$  \hfill (7)

where $B_n$ is the normalization constant and the weight function $\rho(z)$ must satisfy the condition

$$\frac{d}{dz} [\sigma^n(z) \rho(z)] = \tau(z) \rho(z)$$  \hfill (8)

With

$$\tau(z) = \tau(z) + 2\pi(z)$$  \hfill (9)

In order to accomplish the condition imposed on the weight function $\rho(z)$ it is necessary that the polynomial $\tau(z)$ be equal to zero at some point of an interval $(a, b)$ and its derivative at this interval at $\sigma(z) > 0$ will be negative [22]. That is

$$\frac{d\tau(z)}{dz} < 0$$  \hfill (10)

The function $\pi(z)$ and the parameter $\lambda$ required for the NU method are then defined as [22]

$$\pi(z) = \sigma' - \frac{1}{2} \pm \sqrt{\left(\frac{\sigma' - \tau}{2}\right)^2 - \bar{\sigma} + k\sigma}$$  \hfill (11)

$$\lambda = k + \pi'(z)$$  \hfill (12)

The $z$-values in equation (11) are possible to evaluate if the expression under the square-root be square of polynomials. This is possible if and only if its discriminant is zero. Therefore, the new eigenvalue equation becomes [23]
\[ \lambda = \lambda_n = -n \frac{d^2}{dz^2} - \frac{n(n-1)}{z} \frac{d^2\sigma}{dz^2}, n = 0, 1, 2, ... \] (13)

A comparison between equations (12) and (13) yields the energy eigenvalues.

### 3. The Schrödinger Equation

In spherical coordinate, Schrödinger equation with the potential \( V(r) \) is given as [24]

\[
-\frac{\hbar^2}{2\mu} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin\theta \frac{\partial}{\partial \theta} \left( \sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta \frac{\partial^2}{\partial \phi^2}} \right] \psi(r, \theta, \phi) + V(r)\psi(r, \theta, \phi) = E\psi(r, \theta, \phi) \] (14)

Using the common ansatz for the wave function:

\[
\psi(r, \theta, \phi) = \frac{R(r)}{r} Y_{lm}(\theta, \phi) \] (15)

in equation (8) we get the following set of equations:

\[
\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left( E - V(r) - \frac{\lambda \hbar^2}{2\mu r^2} \right) R_{nl}(r) = 0 \] (16)

\[
\frac{d^2 \theta_{ml}(\theta)}{d\theta^2} + \cot\theta \frac{d\theta_{ml}(\theta)}{d\theta} \left( \lambda - \frac{m^2}{\sin^2\theta} \right) \theta_{ml}(\theta) = 0 \] (17)

\[
\frac{d^2 \phi_{m}(\phi)}{d\phi^2} + m^2 \Phi_m(\phi) = 0 \] (18)

Where \( \lambda = l(l+1) \) and \( m^2 \) are the separation constants. \( Y_{lm}(\theta, \phi) = \theta_{ml}(\theta)\Phi_m(\phi) \) is the solution of equations (17) and (18) and their solutions are well known as spherical harmonic functions [24].

### 4. Solutions to the Radial Schrodinger Equation

Equation (16) is the radial part of the Schrodinger equation which we are interested in solving. Equation (16) together with the potential in equation (1) and with the transformation \( z = r^2 \) yields the following equation:

\[
\frac{d^2 \tilde{R}(z)}{dz^2} + \frac{1}{2z} \frac{d\tilde{R}(z)}{dz} + \frac{1}{4z^2} \left( -\alpha z^2 + \beta z - \gamma \right) \tilde{R}(z) = 0 \] (19)

Where the radial wave function is \( \tilde{R}(z) \) and

\[
\alpha = -\frac{2\mu(E - C - Db^2)}{\hbar^2}, \beta = \frac{2\mu(A + Db)}{\hbar^2}, \gamma = \frac{2\mu(B + D)}{\hbar^2} + l(l + 1) \] (20)

Equation (13) is then compared with equation (3) and the following expressions are obtained
\[ \bar{\xi} = 2, \alpha(z) = z, \bar{\alpha} = -\alpha z^2 + \beta z - \gamma \]  

We then obtain the function \( \pi \) by substituting equation (21) into equation (11):

\[ \pi = \frac{1}{2} \pm \frac{1}{2} \sqrt{4\alpha^2 + (k - \beta)z + 1 + 4\gamma} \]  

According to the NU method, the quadratic form under the square-root sign of equation (22) must be solved by setting the discriminant of this quadratic equation equal to zero, i.e., \( D = b^2 - 4ac = 0 \). This discriminant gives a new equation which can be solved for the constant \( k \) to get the two roots as

\[ k_\pm = \beta \pm \sqrt{\alpha(1 + 4\gamma)} \]  

Thus we have

\[ k_- = \beta - \sqrt{\alpha(1 + 4\gamma)} \]  
\[ k_+ = \beta + \sqrt{\alpha(1 + 4\gamma)} \]  

When the two values of \( k \) given in equations (24) and (25) are substituted into equation (22), the four possible forms of \( \pi(z) \) are obtained as

\[ \pi(z) = -\frac{1}{2} \pm \frac{1}{2} \left\{ \begin{array}{ll} 2\sqrt{\alpha z + \sqrt{1 + 4\gamma}} & \text{for} \\ k_+ = \beta + \sqrt{\alpha(1 + 4\gamma)} & \\ 2\sqrt{\alpha z - \sqrt{1 + 4\gamma}} & \text{for} \\ k_- = \beta - \sqrt{\alpha(1 + 4\gamma)} & \end{array} \right. \]  

One of the four values of the polynomial \( \pi(z) \) is just proper to obtain the bound state solution since \( \tau \) given in equation (3) must have negative derivative. Therefore, the most suitable expression of \( \pi(z) \) is chosen as

\[ \pi(z) = -\frac{1}{2} - \frac{1}{2} \left( \bar{\alpha} z - \sqrt{1 + 4\gamma} \right) \]  

for \( k_- = \beta - \sqrt{\alpha(1 + 4\gamma)} \). We obtain \( \tau(z) = 1 + \sqrt{1 + 4\gamma} - 2 \bar{\alpha} z \) from equation (9) and the derivative of this expression would be negative, i.e., \( \tau'(z) = -\frac{4}{\sqrt{1 + 4\gamma}} \bar{\alpha} < 0 \). From equations (18) and (19) we obtain

\[ \lambda = \beta - \sqrt{\alpha(1 + 4\gamma)} - 2 \bar{\alpha} z \]  
\[ \lambda_n = 2n \bar{\alpha} \]  

When we compare these expressions, \( \lambda = \lambda_n \), we obtain the energy of the IQEMP as
\[ E = C + \delta b^2 - \frac{\mu(d^2+2b^2)/2\hbar^2}{(n+\frac{1}{2})^2 + \frac{2\mu B + l^2}{\hbar^2} + (l+\frac{1}{2})^2} \]  

(30)

Let us now calculate the radial wave function, \( R(z) \). Using \( \sigma \) and \( \pi \) equations (6) and (8), the following expressions are obtained

\[ \phi(z) = z^{(-1+\sqrt{1+4\gamma})/2} e^{-\sqrt{\gamma}z} \]  

(31)

\[ \rho(z) = z^{\sqrt{1+4\gamma}} e^{-\sqrt{\gamma}z} \]  

(32)

Then from equation (7) one has

\[ \chi_n(z) = B_n z^{-\sqrt{1+4\gamma}} e^{\sqrt{\gamma}z} \frac{d^n}{dz^n} \left(z^{n+\sqrt{1+4\gamma}} e^{-\sqrt{\gamma}z}\right) \]  

(33)

\( B_n \) is a normalization constant. The wave function \( R(z) \) can be obtained in terms of the generalized Laguerre polynomials as

\[ R(z) = N_n z^{(-1+\sqrt{1+4\gamma})/2} e^{-\sqrt{\gamma}z} L_n^{\sqrt{1+4\gamma}}(2\sqrt{\gamma}z) \]  

(34)

\( N_n \) is the normalization constant.

5. Results and Discussion

Having obtained the energy eigen values (equation 30) and corresponding eigen functions (equation 34) of the IQHMP, we now consider the following cases of the potential:

Case 1: If we set the parameters, \( a = b = C = D = 0, A = z \epsilon^2 \), it is easy to show that equation (30) reduces to the bound state energy spectrum of a particle in the Coulomb potential, i.e., \( E_C = -\frac{Z^2 \mu e^4}{2\hbar^2} n_p^2 \), where \( n_p = n + l + 1 \), is the principal quantum number.

Case 2: Similarly, if we set \( a = b = 0, A \neq 0, B \neq 0, C \neq 0 \) equation (30) results in the bound state energy spectrum of a vibrating-rotating diatomic molecule subject to the Mie-type potential as follows:

\[ E_M = C - \frac{\mu(A)^2/2\hbar^2}{(n+\frac{1}{2})^2 + \frac{2\mu B}{\hbar^2} + (l+\frac{1}{2})^2} \]  

(35)

Case 3: If we set \( a = b = C = 0, A \neq 0, B \neq 0 \) we obtain the energy spectrum of the Kratzer-Feus potential as

\[ E_{KF} = -\frac{\mu(A)^2/2\hbar^2}{(n+\frac{1}{2})^2 + \frac{2\mu B}{\hbar^2} + (l+\frac{1}{2})^2} \]  

(36)
Case 4: If we set \( a = B = C = 0, b \neq 0, A \neq 0 \), we have the energy spectrum of the coulomb plus inversely quadratic effective potential as

\[
E_{IQEC} = Db^2 - \frac{\mu (A + b \delta)^2 / 2b^2}{\left(n + \frac{1}{2} \sqrt{k^2 + \left(t + \frac{1}{2}\right)^2}\right)^2}
\]  

(37)

Case 5: If we set \( a = B = A = C = 0, b \neq 0 \), we have the energy spectrum of the inversely quadratic effective potential as

\[
E_{IQE} = \delta b^2 - \frac{\mu (b \delta)^2 / 2b^2}{\left(n + \frac{1}{2} \sqrt{k^2 + \left(t + \frac{1}{2}\right)^2}\right)^2}
\]  

(38)

Case 6: If we set \( A = B = C = 0, a \neq 0, b \neq 0 \), we have the energy spectrum of the inversely quadratic Hellmann potential as

\[
E_{IQH} = \delta b^2 - \frac{\mu (a - b \delta)^2 / 2b^2}{\left(n + \frac{1}{2} \sqrt{k^2 + \left(t + \frac{1}{2}\right)^2}\right)^2}
\]  

(39)

Case 7: If we set \( b = A = C = 0, a \neq 0, B \neq 0 \), we have the energy spectrum of the inversely quadratic plus coulomb potential as

\[
E_{IQ+C} = -\frac{\mu (a)^2 / 2b^2}{\left(n + \frac{1}{2} \sqrt{k^2 + \left(t + \frac{1}{2}\right)^2}\right)^2}
\]  

(40)

Equations (35) and (36) are similar to the ones obtained in reference [12].

6. Conclusion

The bound state solutions of the Schrodinger equation have been obtained for the inversely quadratic Hellmann plus Mie-type potential using Nikiforov-Uvarov method. With appropriate choice of parameters, several cases of the potential are obtained and their energy eigen spectra calculated.

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References

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