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BOUND STATE SOLUTIONS OF SCHRÖDINGER EQUATION FOR A MORE GENERAL EXPONENTIAL SCREENED COULOMB POTENTIAL VIA NIKIFOROV-UVAROV METHOD

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Abstract: The arbitrary angular momentum solutions of the Schrödinger equation for a diatomic molecule with the general exponential screened coulomb potential of the form $V(r) = (-a/r)\{1 + (1 + b\ )e^{-2b}\}$ has been presented. The energy eigenvalues and the corresponding eigenfunctions are calculated analytically by the use of Nikiforov-Uvarov (NU) method which is related to the solutions in terms of Jacobi polynomials. The bounded state eigenvalues are calculated numerically for the 1s state of N_2 CO and NO

Keywords: Nikiforov-Uvarov method, Eigenvalues, Eigenfunctions, General Exponential Screened Coulomb Potential.

Introduction

The exact analytic solutions of the wave equations (non-relativistic and relativistic) are only possible for certain potentials of physical interest under consideration since they contain all the necessary information on the quantum system [1]. It is known that for certain potentials, the Schrödinger equation can be solved for the angular momentum quantum numbers $\ell = 0$ [2]. However, in some cases, like for the $\ell \neq 0$ states, some approximations are often used to obtain analytic solutions of the Schrödinger equation [3 – 5].

A more general exponential screened coulomb (MGESC) potential used in this paper is of the form [6]:

$$V(r) = \left(-\frac{a}{r}\right)\{1 + (1 + b\ )\exp(-2b\ )\} \quad (1)$$

where a is the strength coupling constant and b is the screened parameter. The potential in equation (1) is known to describe adequately the effective interaction in many-body environments of a variety of fields [6]. In this paper, we have decided to explore the possibility of also using it in obtaining bound state solutions of the Schrödinger equation for diatomics using Nikiforov-Uvarov (NU) method.

Overview of Nikiforov-Uvarov (NU) Method

The NU method is based on the solutions of general second order linear differential equations with some orthogonal functions [7]. For the given potential, the Schrödinger equation in the spherical coordinates is reduced to a generalized equation of hyper-geometric type with an appropriate $s = s(r)$ coordinate transformation. Thus, it has the form [8]:

$$\psi''(s)+\frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s)+\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s)=0 \qquad (2)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most second-degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. To find a particular solution of equation (2), we use the following transformation [9]:

$$\psi(s)=\phi(s)y(s) \qquad (3)$$

This reduces Schrödinger equation (2) to an equation of hyper-geometric type:

$$\sigma(s)y''+\tau(s)y'+\lambda y=0 \qquad (4)$$

where $\phi(s)$ satisfies $\phi'(s)/\phi(s)=\pi(s)/\sigma(s)$, y(s) is the hyper-geometric type function whose polynomial solutions are given by the Rodrigues relation:

$$y_n(s)=\frac{B_n}{\rho(s)}\frac{d^n}{ds^n}\left[\sigma^n(s)\rho(s)\right] \qquad (5)$$

where B_n is a normalization constant and the weight function ρ must satisfy the condition [9]:

$$\left[\sigma(s)\rho(s)\right]'=\tau(s)\rho(s) \qquad (6)$$

The function π and the parameter λ required for this method are defined as:

$$\pi=\frac{\sigma'-\tilde{\tau}}{2}\pm\sqrt{\left(\frac{\sigma'-\tilde{\tau}}{2}\right)^2-\tilde{\sigma}+k\sigma} \qquad (7)$$

and

$$\lambda=k+\pi' \qquad (8)$$

Here, $\pi(s)$ is a polynomial with the parameter s and the determination of k is necessary for $\pi(s)$ to be obtained. To find k, the expression under the square root must be square of a polynomial. A new eigenvalue equation for the Schrödinger equation thus becomes:

$$\lambda=\lambda_n=-n\tau'-\frac{n(n-1)}{2}\sigma'', \ (n=0,1,2,\cdots), \qquad (9)$$

where

$$\tau(s)=\tilde{\tau}(s)+2\pi(s) \qquad (10)$$

and $\tau'(s)$ must be negative.

Bound State Solutions via Nikiforov-Uvarov (NU) Method

The potential in equation (1) is substituted into the radial Schrödinger equation given as:

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}+V(r)\right]R_{n\ell}(r)=E_{n\ell}(r)R_{n\ell}(r), \qquad (11)$$

where n denotes the radial quantum number which together with ℓ are both named as the vibration-rotation quantum numbers in molecular chemistry, r is the internuclear separation, $E_{n\ell}$ is the exact bound state energy eigenvalues and V(r) is the internuclear potential energy function and we obtain:

$$\frac{d^2R_{n\ell}(r)}{dr^2}+\frac{2}{r}\frac{dR_{n\ell}(r)}{dr}+\frac{2\mu}{\hbar^2}\left[E_{n\ell}+\frac{a}{r}+\frac{a}{r}e^{-2b}+abe^{-2b}-\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]R_{n\ell}(r)=0. \qquad (12)$$

Equation (12) can be rearranged to give:

$$\frac{d^2R_{n\ell}(r)}{dr^2}+\frac{2}{r}\frac{dR_{n\ell}(r)}{dr}+\frac{1}{r^2}\frac{2\mu}{\hbar^2}\left[\left(E_{n\ell}+abe^{-2b}\right)r^2+\left(a+ae^{-2b}\right)r-\frac{\ell(\ell+1)\hbar^2}{2\mu}\right]R_{n\ell}(r)=0. \qquad (13)$$

Introducing the following dimensional parameters:

$$\varepsilon^2=\frac{2\mu}{\hbar^2}\left[E_{n\ell}+abe^{-2b}\right], \qquad (14)$$

$$-\beta=\frac{2\mu}{\hbar^2}\left[a+ae^{-2b}\right] \qquad (15)$$

$$\gamma=\ell(\ell+1) \qquad (16)$$

equation (13) is written as:

$$\frac{d^2R_{n\ell}(r)}{dr^2}+\frac{2}{r}\frac{dR_{n\ell}(r)}{dr}+\frac{1}{r^2}\left(\varepsilon^2r^2-\beta r-\gamma\right)R_{n\ell}(r)=0. \qquad (17)$$

A comparison of equations (2) and (17) reveals the following polynomials:

$$\tilde{\tau}(r)=2, \quad \sigma(r)=r, \quad \tilde{\sigma}(r)=\varepsilon^2r^2-\beta r-\gamma \qquad (18)$$

Substituting these polynomials into equation (7), we get $\pi(r)$ as:

$$\pi(r)=-\frac{1}{2}\pm\frac{1}{2}\sqrt{-4\varepsilon^2r^2+4(k+\beta)r+4\gamma+1} \qquad (19)$$

and $\sigma'(r)$ is taken equal to 1. The discriminant of the expression under the square root in equation (19) has to be zero for it to have equal roots. Therefore, we get:

$$\left[4(k+\beta)\right]^2-4\left(-4\varepsilon^2\right)(4\gamma+1)=0, \qquad (20)$$

On solving equation (20) for k we get:

$$k_{\pm}=-\beta\pm i\varepsilon\sqrt{4\gamma+1}, \qquad (21)$$

where

$$k_{-}=-\beta-i\varepsilon\sqrt{4\gamma+1} \qquad (22)$$

and

$$k_{+}=-\beta+i\varepsilon\sqrt{4\gamma+1}. \qquad (23)$$

Substituting $k_{\pm}$ into equation (19), gives the following four possible solutions obtained for $\pi(r)$ as:

$$\pi(r)=-\frac{1}{2}\pm\begin{cases} i\varepsilon r-\frac{1}{2}\sqrt{4\gamma+1}, & \text{for } k_{-}=-\beta-i\varepsilon\sqrt{4\gamma+1} \\ i\varepsilon r+\frac{1}{2}\sqrt{4\gamma+1}, & \text{for } k_{+}=-\beta+i\varepsilon\sqrt{4\gamma+1}. \end{cases} \qquad (24)$$

From the four possible forms of $\pi(r)$ in equation (24), we select the one for which the function $\tau(s)$ in equation (10) has a negative derivative. $\tau(s)$ satisfies these requirements with:

$$\tau(r)=1-2i\varepsilon r+\sqrt{4\gamma+1} \qquad (25)$$

and

$$\tau'(r)=-2i\varepsilon<0 \qquad (26)$$

From equation (8), we obtain:

$$\lambda=-\beta-i\varepsilon\sqrt{4\gamma+1}-i\varepsilon \qquad (27)$$

and also

$$\lambda=\lambda_n=2i\eta\varepsilon, \ n=0,1,2,3,\cdots. \qquad (28)$$

We then obtain the parameters ε^2 as:

$$\varepsilon^2=\left[\frac{-\beta}{1+2n+\sqrt{4\gamma+1}}\right]^2. \qquad (29)$$

Substituting the values of ε^2, β and γ from equations (14) – (16) into equation (29), yields:

$$E_{n\ell}=-abe^{-2b}+\frac{2\mu}{\hbar^2}\left[\frac{a+ae^{-2b}}{(1+2n)+\sqrt{4\left[\ell(\ell+1)\right]+1}}\right]^2 \qquad (30)$$

,

To find y(r), we first obtain $\rho(r)$ from equation (6) as:

$$\rho(r) = r^{1+\sqrt{4\gamma+1}} e^{-2i\varepsilon r} \quad (31)$$

Substituting this into the Rodrigues relation given in equation (5), we get:

$$y_{n\ell}(r) = B_{n\ell} r^{-\left(1+\sqrt{4\gamma+1}\right)} e^{2i\varepsilon r} \frac{d^n}{dr^n}\left[r^{\left(n+1+\sqrt{4\gamma+1}\right)} e^{-2i\varepsilon r} \right] \quad (32)$$

$B_{n\ell}$ is the normalization constant. The polynomial solutions of $y_{n\ell}(r)$ in equation (32) are expressed in terms of the associated Laguerre polynomials, which is one of the orthogonal polynomials. We write:

$$y_{n\ell}(r) = L_n^{1+\sqrt{4\gamma+1}}(v) \quad (33)$$

where $v = 2i\varepsilon r$, therefore,

$$r = (2i\varepsilon)^{-1} v \quad (34)$$

By substituting $\pi(r)$ and $\sigma(r)$ into the expression $\phi'(r)/\phi(r) = \pi(r)/\sigma(r)$ and solving the resulting differential equation, the other part of the wave function in equation (3) is obtained as:

$$\phi(r) = r^{\frac{1}{2}\sqrt{4\gamma+1}-\frac{1}{2}} e^{-i\varepsilon r} \quad (35)$$

or in terms of v,

$$\phi(v) = (2i\varepsilon)^{-\frac{3}{2}+\frac{1}{2}\sqrt{4\gamma+1}} v^{-\frac{1}{2}+\frac{1}{2}\sqrt{4\gamma+1}} e^{-\frac{v}{2}} \quad (36)$$

Combining the Laguerre polynomials and $\phi(v)$ in equation (3), enables the radial wave function to be constructed as:

$$R_{n\ell}(r) = A_{n\ell} \psi_{n\ell}(r) \quad (37)$$

$$\therefore R_{n\ell}(r) = A_{n\ell} (2i\varepsilon)^{-\frac{3}{2}+\frac{1}{2}\sqrt{4\gamma+1}} v^{-\frac{1}{2}+\frac{1}{2}\sqrt{4\gamma+1}} e^{-\frac{v}{2}} L_n^{1+\sqrt{4\gamma+1}}(v) \quad (38)$$

If we introduce the variable $\alpha = \frac{1}{2}\sqrt{4\gamma+1}$, equation (38) becomes:

$$R_{n\ell}(r) = A_{n\ell} (2i\varepsilon)^{-\frac{3}{2}+\alpha} v^{-\frac{1}{2}+\alpha} e^{-\frac{v}{2}} L_n^{1+2\alpha}(v) \quad (39)$$

To find $A_{n\ell}$, a new normalization constant, we write:

$$\int_0^\infty R_{n\ell}^2(r)\,dr = 1. \quad (40)$$

Therefore,

$$A_{n\ell}^2 (2i\varepsilon)^{2\alpha-3} \int_0^\infty v^{2\alpha-1} e^{-v} \left[L_n^{2\alpha+1}(v)\right]^2 dv = 1. \quad (41)$$

The above integral can be evaluated by using the recursion relation for Laguerre polynomials and $A_{n\ell}$ is found to be:

$$A_{n\ell} = \left[\frac{(n-2\alpha+1)!(2i\varepsilon)^{3-2\alpha}}{(2n-2\alpha+2)(n!)^3} \right]^{\frac{1}{2}} \quad (42)$$

Therefore, $R_{n\ell}(r)$ becomes:

$$R_{n\ell}(r) = \left[\frac{(n-2\alpha+1)!(2i\varepsilon)^{3-2\alpha}}{(2n-2\alpha+2)(n!)^3} \right]^{\frac{1}{2}} (2i\varepsilon)^{-\frac{3}{2}+\alpha} v^{\alpha-\frac{1}{2}} e^{-\frac{v}{2}} L_n^{2\alpha+1}(v). \quad (43)$$

Conclusion

The analytical solutions of the Schrödinger equation for the general exponential screened coulomb potential has been presented. The Nikiforov-Uvarov method employed in the solutions enables us to explore an effective way of obtaining the eigenvalues and corresponding eigenfunctions of the Schrödinger equation for any ℓ - state.

Finally, we calculate the energies of the exponential screened coulomb potential for diatomic molecules by means of equation (30) for the ℓ - state. The explicit values of the energy at different values of the screened parameter are shown in Table 1.

Table 1. Bound State Eigenvalues for $0 \le b \le 0.05$ for the 1s State of Diatomic Molecules in Atomic Units $(\hbar = \mu = a = 1)$

b	E_{1s}(ev)		
	N_2	CO	NO
0.01	0.2348302	0.2346764	0.2345716
0.02	0.2202668	0.2199730	0.2197791
0.03	0.2062752	0.2058684	0.2056002
0.04	0.1928410	0.1932419	0.1920133
0.05	0.1799455	0.17937370	0.1789975

Note: The r values for N_2 (1.0940), CO (1.21282) and NO (1.1508) were adapted from M. Karplus and R. N. Porter, Atoms and Molecules: An Introduction for Student's of Physical Chemistry, Benjamin, Menlo Park, CA, 1970.

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