The Schrödinger Equation with Deng-Fan-Eckart Potential (DFEP): Nikiforov-Uvarov-Functional Analysis (NUFA) Method

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ABSTRACT

In this study, the radial part of the Schrödinger equation with the Deng-Fan-Eckart potential (DFEP) is solved analytically by employing the improved Greene and Aldrich approximation to bypass the centrifugal barrier and using the Nikiforov-Uvarov-Functional Analysis method (NUFA). The energy expression and wave function are obtained respectively. The numerical energy spectra for some diatomic molecules have been studied and compared with the findings of earlier studies and it has been found to be in good agreement. The NUFA method used in this study is easy and very less cumbersome compared to other methods that currently exist and it is recommended that researchers in this area adopt this method. The findings of this study will find direct applications in molecular physics.

Keywords: bound state, NUFA method, non-relativistic, potential model.

I. INTRODUCTION

Solving the Schrödinger equation remains a relevant and interesting task in non-relativistic quantum mechanics. This is because the solution of this equation provides the energy spectrum and wave function which are relevant tools for the description of a quantum system. In view of this, researchers over the years have paid great attention to solve this equation with myriads of potential [1-10]. These solutions with several models have been applied to study several physical systems, example: quantum dots [11], quarks [12], diatomic molecules [13], etc. Amongst the numerous potentials proposed and adopted for studying diatomic molecules is the Deng-Fan-Eckart potential (DFEP) proposed by Ikot et al. [14]. This model is given as:

\[
V(r) = D_e \left(1 - \frac{b}{e^{-\alpha r} - 1}\right)^2 - \frac{V_1 e^{-\alpha r}}{1 - e^{-\alpha r}} + \frac{V_2 e^{-\alpha r}}{1 - e^{-\alpha r}}
\]

where \(r_e\) is the molecular bond length, \(D_e\) is the dissociation energy, \(r\) is the inter-nuclear distance, \(\alpha\) the range of the potential well, \(V_1\) and \(V_2\) are the potential strengths. A number of authors have adopted this model to carry out some interesting studies. For instance, Ikot et al. [14] in a maiden study solved the Dirac equation under spin and pseudo-spin symmetries with Deng-Fan-Eckart potential with Coulomb-like and Yukawa-like tensor interaction terms using the Nikiforov-Uvarov method [14]. Edet et al. [15] applied the model to study the diatomic molecules and its thermal properties. Amadi et al. [15] applied this model study the information entropies for \(H_2\) and \(ScF\) diatomic molecules. A number of authors have solved the SE with various potentials and with applications to various physical systems [16]-[20]. Ikot et al. [21] studied effects of magnetic and AB fields on the energy spectra and thermo-magnetic properties of the screened Kratzer potential (SKP). Edet and Ikot [22] studied the effects of magnetic and AB fields on the energy spectra and thermal properties of some diatomic molecules using the Hulthen-Kratzer potential (HKP) model. Nwabuzor et al. [23] studied the impacts of topological defect on the energy spectra and thermal properties of LiH, TiC and I\(_2\) diatomic molecules. Edet and Ikot [4] studied the effects of magnetic and AB fields on the energy spectra and thermo-magnetic properties of CO diatomic molecule using screened modified Kratzer. Ushie et al. [25] studied the effects of the deformation parameter on the non-relativistic energy spectra of Hulthen-quadratic exponential-type potential model for \(H_2\), HCl, CO and LiH diatomic molecules.

In view of the above, this study will focus on the solutions of the SE with DFEP using the NUFA. The results will be compared with that of Edet et al [15] to show the efficiency of this method.

The paper is organized as follows. In section 2, a brief review of the NUFA method is presented. In section 3, the solution of the 3D Schrödinger equation with the DFEP is presented. In section 4, result is discussed. Finally, a brief
concluding remark is given in section 5

II. NU-FUNCTIONAL ANALYSIS (NUFA) METHOD

Igot et al. [26] proposed the Nikiforov-Uvarov-Functional Analysis method (NUFA) as a simple and elegant method for solving a second order differential equation of the hypergeometric form. The Nikiforov Uvarov (NU) method [27], the parametric NU method [28], and the functional analysis method [29]-[31] were used. This method, like the parametric NU method, is simple and straightforward. The NU is well-known for solving a second-order differential equation with the form [28]:

$$\psi''(s) + \frac{\sigma(s)}{s} \psi'(s) + \frac{\sigma'(s)}{\sigma(s)} \psi(s) = 0$$  \hspace{1cm} (2)$$

where $\sigma(s)$ and $\sigma'(s)$ are polynomials, at most of second degree, and $\sigma(s)$ is a first-degree polynomial. Tezcan and Sever [28] latter introduced the parametric form of NU method in the form:

$$\psi'' + \frac{\alpha_i - \alpha s}{s(1 - \alpha s)} \psi' + \frac{1}{s^2 (1 - \alpha s)^2} \left[ -\xi_i s^2 + \xi_i s - \xi_i \right] \psi(s) = 0$$  \hspace{1cm} (3)$$

where $\alpha_i$ and $\xi_i (i = 1,2,3)$ are all parameters. It can be observed in equation (3) that the differential equation has two singularities at $s \to 0$ and $s \to 1$, thus we take the wave function in the form:

$$\psi(s) = s^{\lambda - 1} \phi(s)$$  \hspace{1cm} (4)$$

Substituting equation (4) into equation (3) leads to the following equation:

$$x(1-\alpha s) f'(s) + [\alpha_i + 2 \lambda - (2 \lambda \alpha_i + 2 \alpha_i s + \alpha_i s) s] f''(s) - \alpha_i \left[ \lambda + \frac{-\alpha_i}{\alpha_i} + \frac{\alpha_i - 1}{\alpha_i} \sqrt{\frac{\alpha_i - 1}{\alpha_i}} \right] + \alpha_i \left[ \lambda + \frac{-\alpha_i}{\alpha_i} + \frac{\alpha_i - 1}{\alpha_i} \sqrt{\frac{\alpha_i - 1}{\alpha_i}} \right] - \frac{\alpha_i}{\alpha_i} = 0$$  \hspace{1cm} (5)$$

Equation (5) can be reduced to a Gauss hypergeometric equation if and only if the following functions vanished,

$$\lambda (\lambda - 1) + \alpha \lambda - \xi = 0$$  \hspace{1cm} (6)$$

$$\alpha_i \nu - \alpha_i \alpha_i + \nu (\nu - 1) \alpha_i - \frac{\xi_i}{\alpha_i} + \xi_i - \xi_i \alpha = 0$$  \hspace{1cm} (7)$$

Thus, equation (5) becomes:

$$x(1-\alpha s) f'(s) + [\alpha_i + 2 \lambda - (2 \lambda \alpha_i + 2 \alpha_i s + \alpha_i s) s] f''(s) - \alpha_i \left[ \lambda + \frac{-\alpha_i}{\alpha_i} + \frac{\alpha_i - 1}{\alpha_i} \sqrt{\frac{\alpha_i - 1}{\alpha_i}} \right] + \alpha_i \left[ \lambda + \frac{-\alpha_i}{\alpha_i} + \frac{\alpha_i - 1}{\alpha_i} \sqrt{\frac{\alpha_i - 1}{\alpha_i}} \right] - \frac{\alpha_i}{\alpha_i} = 0$$  \hspace{1cm} (8)$$

Solving equations (6) and (7) completely give:

$$\lambda = \frac{(1-\alpha)}{2} \left[ (1-\alpha^2)^2 + 4 \xi^2 \right]$$  \hspace{1cm} (9)$$

$$v = \frac{2}{(1-\alpha)}$$  \hspace{1cm} (10)$$

Equation (8) is the hypergeometric equation type of the form:

$$x(1-x) f'(x) + \left[ c + (a + b + 1)x \right] f''(x) - abf(x) = 0$$  \hspace{1cm} (11)$$

Using equations (4), (8) and (11), we obtain the energy equation and the corresponding wave equation respectively for the NUFA method as follows:

$$\lambda^2 + 2\lambda \left[ \frac{\nu + \frac{\alpha_i}{\alpha_i} - 1 + \frac{n}{\sqrt{\alpha_i}}}{\sqrt{\alpha_i}} \right] + \left[ \frac{\nu + \frac{\alpha_i}{\alpha_i} - 1 + \frac{n}{\sqrt{\alpha_i}}}{\sqrt{\alpha_i}} \right] - \frac{\alpha_i}{\alpha_i} = 0$$  \hspace{1cm} (12)$$

$$\psi(s) = N_\alpha \left[ 1 - \alpha_i x \right] f_\alpha(a,b,c,s)$$  \hspace{1cm} (13)$$

where $a$, $b$, $c$ are given as follows:

$$a = \sqrt{\alpha_i} \left[ \lambda + \alpha_i - 1 + \frac{\alpha_i - 1}{\sqrt{\alpha_i}} \right]$$  \hspace{1cm} (14)$$

$$b = \sqrt{\alpha_i} \left[ \lambda + \alpha_i - 1 + \frac{\alpha_i - 1}{\sqrt{\alpha_i}} \right]$$  \hspace{1cm} (15)$$

$$\alpha_i + 2 \lambda$$  \hspace{1cm} (16)$$

III. SCHRODINGER EQUATION WITH DENG-FAN-ECKART POTENTIAL

The radial part of the Schrödinger equation is given by [15], [32], [33]:

$$\frac{d^2 \psi(r)}{dr^2} + \frac{2 \mu}{\hbar^2} \left[ E_{n\ell} - V(r) - \frac{\hbar^2 \ell (\ell + 1)}{2 \mu r^2} \right] \psi(r) = 0$$  \hspace{1cm} (17)$$

Substituting Eq. (1) into Eq. (17), the radial Schrödinger equation is obtained in the following form:
\[ d^4 \psi(t) \over dt^4 + \frac{2\mu}{R}
\left[ \begin{array}{c}
E_n - \left( D + \frac{D_{h^2}}{h^2} \right) + \frac{2D_b e^{-\gamma t}}{1-e^{-\gamma t}} + \frac{V_{e} e^{-\gamma t}}{1-e^{-\gamma t}} \end{array} \right] \psi(t) = 0
\] (18)

Eq. (18) in its current form cannot be solved with any standard mathematical procedure analytically for \( \ell \neq 0 \) because of the centrifugal barrier. This calls for a need to adopt and apply an approximation to the centrifugal term. The following approximation is adopted [34, 35]:

\[ \frac{1}{r^2} = \alpha^2 \left[ d_o + \frac{e^{\alpha r}}{1-e^{-\alpha r}} \right] \] (19)

Inserting Eqs. (19) into Eq. (18) where we have the \( \frac{1}{r^2} \) term, we have:

\[ d^4 \psi(t) \over dt^4 + \frac{2\mu}{R} \left[ \begin{array}{c}
E_n - \left( D + \frac{D_{h^2}}{h^2} \right) + \frac{2D_b e^{-\gamma t}}{1-e^{-\gamma t}} + \frac{V_{e} e^{-\gamma t}}{1-e^{-\gamma t}} \end{array} \right] \psi(t) = 0
\] (20)

The following dimensionless parameters have been introduced:

\[ -\varepsilon^2 = \frac{2\mu(E_n - D)}{h^2\alpha^2}, u_n = \frac{2\mu D_b h^2}{h^2\alpha^2}, u_t = \frac{2\mu D_b h^2}{h^2\alpha^2}, P_i = \frac{2\mu V_{e}}{h^2\alpha^2}, P_o = \frac{2\mu V_{e}}{h^2\alpha^2} \]

and

\[ \gamma = \ell (\ell + 1) \] (21)

Hence, Eq. (20) can be rewritten in a less ambiguous form as:

\[ d^4 \psi(t) \over dt^4 + \frac{2\mu}{R^2} \left[ -\varepsilon^2 \left( 1-e^{-\varepsilon^2} \right) - u_n e^{2\varepsilon^2} + u_t e^{-\varepsilon^2} \right] \psi(t) = 0 \] (22)

The transformation \( t = e^{-\varepsilon^2} \) is utilized and it transforms Eq. (22) to the hypergeometric-type of the form:

\[ d^4 \psi(t) \over dt^4 + \frac{1}{4t} \frac{d^2 \psi(t)}{dt^2} + \frac{1}{t^2 (1-t)^2} \left[ -\varepsilon^2 + u_n + P_i + \gamma d_e \right] \psi(t) = 0 \] (23)

Comparing (23) and (3), we obtain the following:

\[ \alpha_1 = \alpha_2 = \alpha_3 = 1, \]
\[ \lambda = \sqrt{\varepsilon^2 + \gamma d_e} \] (24)

The energy is then obtained from (12) as follows:

\[ (\lambda + \nu) - \sqrt{\varepsilon^2 + u_1 + u_2 + P_1 + \gamma d_e} = -n \quad n = 0, 1, 2... \] (25)

from which we obtain:

\[ \varepsilon^2 = -\ nu_1 - \frac{1}{4} \left( n + \frac{1}{2} \pm \sqrt{1 + u_1 + P_2 + \nu} \right) \] (26)

On substitution of the value of the dimensionless parameters in Eq. (21) into Eq. (26), the solutions is obtained as follows:

\[ E_n = D + \frac{h^2\alpha^2}{2\mu} \left( n + \frac{1}{2} \right)^{2} + \frac{2\mu D_b b^2}{h^2\alpha^2} + \frac{4\mu D_b b^2}{h^2\alpha^2} + \frac{8\mu V_{e}}{h^2\alpha^2} \] (27)

where

\[ \nu = 1 + \frac{1}{2} \sqrt{2(\ell + 1)^2 + \frac{8\mu D_b b^2}{h^2\alpha^2} + \frac{8\mu V_{e}}{h^2\alpha^2}} \] (28)

Similarly, the wave function is obtained as:

\[ \psi(t) = N_e t^{\ell/2} e^{-\gamma t/2} \left( 1-t \right)^{\ell/2} \left( 1-e^{-\gamma t} \right) F_1 \left( -n, n + 2(\lambda + \nu); 2\lambda + 1; t \right) \] (29)

### IV. DISCUSSION OF RESULTS

In order to show the validity of the results obtained in this study, the numerical energy levels is computed by utilizing Eq. (27) for different quantum numbers \( n \) and \( \ell \) with for four Diatomic molecules (\( H_2, CO, ScN \) and \( ScF \)). To achieve this objective, spectroscopic parameters shown in Table I are adopted from the NIST database and the following conversions:

\[ 1 \text{amu} = 931.494028 \text{MeV}/c^2, \]
\[ 1 \text{cm}^{-1} = 1.239841875 \times 10^{-4} \text{eV} \text{ Å} \text{ are used} [15]. \]

The numerical energy values obtained by adopting the experimental fitting parameters are presented in Table II and Table III for several vibrational and rotational quantum numbers. To firmly establish the validity and accuracy of our results, the numerical energy is compared with the results of Edet et al. [15] and from observation, it is clearly seen that there is an excellent agreement.
The energy equation and wave function are obtained respectively. The numerical energy spectra for some diatomic molecules have been studied and compared with the findings of Edet et al. [15] and it has been found to be in perfect agreement. However, it is interesting to point out here that the NUFAs method used in this study is easy and very less cumbersome compared the other methods that currently exist. The findings of this study will find direct applications in molecular physics.

### Table II: Comparison of Bound State Energies $E_n (eV)$ for $H_2$ and CO Molecules Obtained by Using Nikiforov-Uvarov\- Functional Analysis Method (NUFA) with Factorization Method for Different Values of the $n$ and $\ell$ Quantum Numbers

| $n$ | $\ell$ | $H_2$ (NUFA) | $H_2$ (FAA) | $H_2$ (CO) | $H_2$ (FAA) |
|-----|--------|--------------|-------------|-----------|------------|
| 0   | 0      | 0.3161089    | 0.316109    | 0.3653484 | 0.3653484 |
| 1   | 0      | 0.3304972    | 0.3304972   | 0.3658917 | 0.3658917 |
| 2   | 0      | 0.9626475    | 0.9626475   | 0.6487759 | 0.6487759 |
| 3   | 1      | 1.5464922    | 1.5464922   | 0.9281702 | 0.9281702 |
| 4   | 1      | 1.5858663    | 1.5858663   | 0.9287056 | 0.9287056 |
| 5   | 1      | 1.5832386    | 1.5832386   | 0.9297766 | 0.9297766 |

### Table III: Comparison of Bound State Energies $E_n (eV)$ for $\text{N}_2$ and CO Molecules Obtained by Using Nikiforov-Uvarov\- Functional Analysis Method (NUFA) with Factorization Method for Different Values of the $n$ and $\ell$ Quantum Numbers

| $n$ | $\ell$ | $\text{N}_2$ (NUFA) | $\text{N}_2$ (FAA) | CO (NUFA) | CO (FAA) |
|-----|--------|---------------------|-------------------|-----------|----------|
| 0   | 0      | 0.5678234           | 0.5678234         | 0.780749  | 0.780749 |
| 1   | 0      | 0.5679634           | 0.5679634         | 0.7808573 | 0.7808573|
| 2   | 0      | 0.6573524           | 0.6573524         | 0.8685782 | 0.8685782|
| 3   | 0      | 0.6574917           | 0.6574917         | 0.8686851 | 0.8686851|
| 4   | 0      | 0.7547977           | 0.7547977         | 0.9555848 | 0.9555848|
| 5   | 0      | 0.7549361           | 0.7549361         | 0.9559415 | 0.9559415|
| 6   | 0      | 0.7462130           | 0.7462130         | 0.9559042 | 0.9559042|
| 7   | 0      | 0.8331616           | 0.8331616         | 1.0417712 | 1.0417712|
| 8   | 0      | 0.8332993           | 0.8332993         | 1.0418772 | 1.0418772|
| 9   | 0      | 0.8335745           | 0.8335745         | 1.0420891 | 1.0420891|
| 10  | 0      | 0.8339876           | 0.8339876         | 1.0424072 | 1.0424072|

### V. Conclusion

In this study, the three-dimensional Schrödinger equation with the Deng-Fan-Eckart potential (DFEP) is solved using the Nikiforov-Uvarov functional analysis (NUFA) method.
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