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Bound State Solutions of the Schrödinger Equation with Frost-Musulin Potential Using the Nikiforov-Uvarov-Functional Analysis (NUFA) Method

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Abstract. The Schrödinger equation under the Frost-Musulin potential (FMP) energy function is solved using the Nikiforov-Uvarov-Functional Analysis (NUFA) method. We obtained the analytic solutions of the energy equation and the wave function in closed form with Greene-Aldrich approximation. The energy equation was used to obtain bound states energy eigenvalues of FMP for H_2, I_2 and N_2 diatomic molecules for various quantum states. To test the accuracy of our results, we computed the bound states energy eigenvalues of FMP which are in excellent agreement with the reports of other researchers.

KEY WORDS: Schrödinger equation; Nikiforov-Uvarov-Functional Analysis (NUFA) method; Frost-Musulin potential; Diatomic molecule.

1 Introduction

The Schrödinger equation (SE) is an essential equation in quantum mechanics. This is because it is the equation that defines a particle's action in a microscopic setting. The solutions of SE with a given central potential have an extensive variety of applications [1, 2]. Furthermore, several researchers have proposed that the SE's eigen-solutions provide important knowledge about the quantum system [3–5]. The analytical methods for solving bound state problems that arise in physics and their applications have received much attention over the past years. The development of these methods allows one to derive the analytic eigen-solutions of the relativistic and non-relativistic wave equations which play

a crucial role in interpreting the behavior of quantum mechanical systems. The frequently used analytical methods are the Nikiforov-Uvarov method (NU) [6–12], Asymptotic iterative method (AIM) [13], Laplace transformation approach [14], super-symmetric quantum mechanics approach (SUSYQM) [15, 16],the series expansion method [17, 18] and so on.

The SE can be studied for different quantum–mechanical processes with the above analytical methods [19–21]. The application of different potential model to study diatomic molecules as attracted various researchers in time part and in recent times [22–24]. For instance, Inyang et al. [25] combined Eckart and Hellmann potential function to study some selected diatomic molecules. Also, Obogo et al. [26], investigated some selected diatomic molecules through the solution of SE with a combined potential using the NU method. In addition, Edet and Ikot, [27] studied some diatomic molecules with the shifted Deng-Fan potential. Furthermore, Edet et al. [28] studied some diatomic molecules with Deng-Fan plus Eckart potentials. Motivated by the success of other researchers, we seek to solve approximately the SE with Frost-Musulin potential (FMP) to study selected diatomic molecules using a newly proposed analytical method called the Nikiforov-Uvarov-Functional Analysis (NUFA) method.

The Frost-Musulin potential (FMP) is a molecular potential function that was proposed in 1954 by Frost and Musulin [29]. Researchers have solved FMP both in relativistic and non-relativistic regime with different analytical methods [30–32].

The potential is of the form [33]

$$V(r) = D_e - \frac{D_e(r + \alpha r r_e - \alpha r_e^2)e^{-\alpha(r-r_e)}}{r}, \tag{1}$$

where D_e, r_e, r and α denote the dissociation energy, the equilibrium bound length, the internuclear separation and the range of the potential.

2 Review of Nikiforov-Uvarov-Functional Analysis (NUFA) Method

Using the concepts of the NU, parametric NU and the functional analysis methods [6,34,35], Ikot et al. [36] proposed a simple and elegant method for solving a second order differential equation of the hypergeometric type called Nikiforov-Uvarov-Functional Analysis method (NUFA) method. This method is easy and simple. The NU method is used to solve a second-order differential equation of the form [6]

$$\psi''(z) + \frac{\tilde{\tau}(z)}{\sigma(z)}\psi'(z) + \frac{\tilde{\sigma}(z)}{\sigma^2(z)}\psi(z) = 0\,, \tag{2}$$

where $\tilde{\sigma}(z)$ and $\sigma(z)$ are polynomials of maximum second degree and $\tilde{\tau}(z)$ is a polynomial of maximum first degree. Tezcan and Sever [34] latter introduced

the parametric form of NU method in the form

$$\psi'' + \frac{\alpha_1 - \alpha_2 z}{z(1-\alpha_3 z)}\psi' + \frac{1}{z^2(1-\alpha_3 z)^2}[-\xi_1 z^2 + \xi_2 z - \xi_3]\psi(s) = 0\,, \tag{3}$$

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

$$\psi(z) = z^{\lambda}(1-z)^{v} f(z)\,. \tag{4}$$

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

$$\begin{aligned} z(1-\alpha z)f''(z) + [\alpha_1 + 2\lambda - (2\lambda\alpha_3 + 2v\alpha_3 + \alpha_2)z]f'(z) \\ - \alpha_3\left(\lambda + v + \frac{\alpha_2}{\alpha_3} - 1 + \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{\xi_1}{\alpha_3}}\right) \\ \times \left(\lambda + v + \frac{\alpha_2}{\alpha_3^2} - 1 + \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{\xi_1}{\alpha_3^2}}\right) \\ + \left[\frac{\lambda(\lambda-1) + \alpha_1\lambda - \xi_3}{z}\right. \\ \left. + \frac{\alpha_2 v - \alpha_1\alpha_3 v + v(v-1)\alpha_3 - \frac{\xi_1}{\alpha_3} + \xi_2 - \xi_3\alpha_3}{(1-\alpha_3 z)}\right] f(z) = 0\,. \end{aligned} \tag{5}$$

Equation (5) can be reduced to a Gauss hypergeometric equation if and only if the following functions are gone:

$$\lambda(\lambda-1) + \alpha_1\lambda - \xi_3 = 0\,, \tag{6}$$

$$\alpha_2 v - \alpha_1\alpha_3 v + v(v-1)\alpha_3 - \frac{\xi_1}{\alpha_3} + \xi_2 - \xi_3\alpha_3 = 0\,. \tag{7}$$

Thus Eq.(5) becomes

$$\begin{aligned} z(1-\alpha_1 z)f''(z) + [\alpha_1 + 2\lambda - (2\lambda\alpha_3 + 2v\alpha_3 + \alpha_2)z]f'(z) \\ - \alpha_3\left(\lambda + v + \frac{\alpha_2}{\alpha_3} - 1 + \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{\xi_1}{\alpha_3}}\right) \\ \times \left(\lambda + v + \frac{\alpha_2}{\alpha_3^2} - 1 + \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{\xi_1}{\alpha_3^2}}\right) f(z) = 0\,. \end{aligned} \tag{8}$$

Solving Eqs. (6) and (7) gives Eqs. (9) and (10),

$$\lambda = \frac{(1-\alpha_1)}{2} \pm \frac{1}{2}\sqrt{(1-\alpha_1)^2 + 4\xi_3}\,, \tag{9}$$

$$v=\frac{(\alpha_3+\alpha_1\alpha_3-\alpha_2)\pm\sqrt{(\alpha_3+\alpha_1\alpha_3-\alpha_2)^2+4\Big(\frac{\xi_1}{\alpha_3}+\alpha_3\xi_3-\xi_2\Big)}}{2}. \quad (10)$$

Equation (8) is the hyper geometric equation type of the form,

$$x\,(1-x)\,f''(x)+[c+(a+b+1)\,x]\,f^1(x)-abf(x)=0 \quad (11)$$

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

$$\lambda^2+2\lambda\Big(v+\frac{\alpha_2}{\alpha_3}-1+\frac{n}{\sqrt{\alpha_3}}\Big)+\Big(v+\frac{\alpha_2}{\alpha_3}-1+\frac{n}{\sqrt{\alpha_3}}\Big)^2 - \Big(\frac{\alpha_2}{\alpha_3}-1\Big)^2-\frac{\xi_1}{\alpha_3^2}=0\,, \quad (12)$$

$$\psi(z)=N_z\frac{(1-\alpha_1)+\sqrt{(1-\alpha_1)^2+4\xi_3}}{2}(1-\alpha_3 z) \times\frac{(\alpha_3+\alpha_1\alpha_3-\alpha_2)\pm\sqrt{(\alpha_3+\alpha_1\alpha_3-\alpha_2)^2+\Big(\frac{\xi_1}{\alpha_3^2}+\alpha_3\xi_3-\xi_2\Big)}}{2} \times {}_2F_1(a,b,c;z)\,, \quad (13)$$

where a, b and c are given as follows:

$$a=\sqrt{\alpha_3}\left(\lambda+v+\frac{\alpha_2}{\alpha_3}-1+\sqrt{\Big(\frac{\alpha_2}{\alpha_3}-1\Big)^2+\frac{\xi_1}{\alpha_3}}\right), \quad (14)$$

$$b=\sqrt{\alpha_3}\left(\lambda+v+\frac{\alpha_2}{\alpha_3}-1-\sqrt{\Big(\frac{\alpha_2}{\alpha_3}-1\Big)^2+\frac{\xi_1}{\alpha_3}}\right), \quad (15)$$

$$c=\alpha_1+2\lambda\,. \quad (16)$$

3 Approximate Solutions of the Schrödinger Equation with Frost-Musulin Potential

The SE takes the form [37,38]

$$\frac{d^2U(r)}{dr^2}+\Big[\frac{2\mu}{\hbar^2}\,(E_{nl}-V(r))-\frac{l\,(l+1)}{r^2}\Big]U(r)=0\,, \quad (17)$$

where E_{nl} is the energy eigenvalues of the quantum system, l is the angular momentum quantum number, μ is the reduced mass of the system, $\hbar$ is the reduced Planck's constant and $r$is radial distance from the origin.

Equation (17) cannot be solved exactly with the proposed potential. So we introduce an approximation scheme proposed by Greene-Aldrich [39] to deal with the centrifugal barrier. This approximation is a good approximation to the centrifugal term which is valid for $\alpha \ll 1$, and it becomes

$$\frac{1}{r^2} \approx \frac{\alpha^2}{(1-e^{-\alpha r})^2}. \tag{18}$$

Substituting Eqs. (1) and (18) into Eq. (17), and by defining a variable of the form $x = e^{-\alpha r}$, with some algebraic simplifications, we achieve Eq. (19) as;

$$\frac{d^2U(x)}{dx^2} + \frac{1-x}{x(1-x)}\frac{dU(x)}{dx} + \frac{1}{x^2(1-x)^2}\Big[-(\varepsilon-\beta_0-\beta_1+\beta_2)x^2 + (2\varepsilon+\beta_3-\beta_4+\beta_5+\beta_6)x - (\varepsilon+\beta_2-\beta_7+\gamma)\Big]U(x) = 0\,, \tag{19}$$

where

$$\begin{aligned} -\varepsilon &= \frac{2\mu E_{nl}}{\hbar^2}, \quad \beta_0 = \frac{2\mu}{\hbar^2}D_e\alpha r_e e^{\alpha r_e}(r_e+1), \quad \beta_1 = \frac{2\mu}{\hbar^2}D_e e^{\alpha r_e}, \\ \beta_2 &= \frac{2\mu}{\hbar^2}D_e, \quad \beta_3 = -\frac{2\mu}{\hbar^2}D_e\alpha r_e e^{\alpha r_e}(r_e+2), \quad \beta_4 = -\frac{4\mu D_e E_{nl}}{\hbar^2}, \\ \beta_5 &= -\frac{4\mu e^{\alpha r_e}}{\hbar^2}, \quad \beta_6 = -\frac{4\mu D_e}{\hbar^2}, \quad \beta_7 = \frac{2\mu D_e}{\hbar^2}(1+\alpha r_e)e^{\alpha r_e}, \quad \gamma = l(l+1) \end{aligned} \tag{20}$$

Comparing Eq. (19) and Eq. (3), we obtain the relevant polynomials as

$$\begin{aligned} &\alpha_1 = \alpha_2 = \alpha_3 = 1, \\ &\xi_1 = \varepsilon - \beta_0 - \beta_1 + \beta_2, \\ &\xi_2 = 2\varepsilon + \beta_3 - \beta_4 + \beta_5 + \beta_6, \\ &\xi_3 = \varepsilon - \beta_2 - \beta_7 + \gamma \end{aligned} \tag{21}$$

Inserting the polynomials given by Eq. (21) into Eqs. (9) and (10), we have

$$\lambda = \sqrt{(\varepsilon - \beta_2 - \beta_7 + \gamma)}\,, \tag{22}$$

$$v = \frac{1 \pm \sqrt{1 + 4(\gamma - \beta_0 - \beta_1 - \beta_3 + \beta_4 - \beta_5 - \beta_6 - \beta_7)}}{2} \tag{23}$$

Substituting Eqs. (21), (22), (23) and (20) into Eq. (12), we obtain the energy equation of the FMP as;

$$E_{nl} = D_e(1-\alpha^2 r_e^2 e^{\alpha r_e}) - D_e(1+\alpha r_e)e^{\alpha r_e} - \frac{\hbar^2\alpha^2}{2\mu}\left[\frac{(l+n+1)^2 + \frac{2\mu D_e r_e^2 e^{\alpha r_e}}{\hbar^2} + (l+l^2)}{2(l+n+1)}\right]^2. \tag{24}$$

The corresponding unnormalized wave function is given as

$$\psi(x) = N\frac{\sqrt{4(\varepsilon-\beta_2-\beta_7+\gamma)}}{2}(1-z)$$
$$\times\frac{1+\sqrt{1+4(\gamma-\beta_0-\beta_1-\beta_3+\beta_4-\beta_5-\beta_6-\beta_7)}}{2}F_1(a,b,c;z), \quad (25)$$

where

$$a = \frac{1}{2}\sqrt{4(\varepsilon-\beta_2-\beta_7+\gamma)} + \frac{1\pm\sqrt{1+4(\gamma-\beta_0-\beta_1-\beta_3+\beta_4-\beta_5-\beta_6-\beta_7)}}{2} + \sqrt{\varepsilon-\beta_0-\beta_1+\beta_2} \quad (26)$$

$$b = \frac{1}{2}\sqrt{4(\varepsilon-\beta_2-\beta_7+\gamma)}, + \frac{1\pm\sqrt{1+4(\gamma-\beta_0-\beta_1-\beta_3+\beta_4-\beta_5-\beta_6-\beta_7)}}{2} - \sqrt{\varepsilon-\beta_0-\beta_1+\beta_2}, \quad (27)$$

$$c = 1+2\sqrt{(\varepsilon-\beta_2-\beta_7+\gamma)} \quad (28)$$

4 Results and Discussion

We used Eq. (26) and apply the spectroscopic data (Table 1) and the conversion $\hbar c = 1973.29$ eVÅ obtained from Ref. [40], to compute the vibrational energies of FMP for H_2, I_2 and N_2 diatomic molecules as shown in Table 2. It is observed that for each vibrational quantum number, the vibrational energies increase with increase in the rotational quantum number, for each of the selected diatomic molecules. We computed the bound states energy eigenvalues of FMP to check the accuracy of the NUFA method with $\hbar = \mu = 1$, using $\alpha = 0.1$, $r_e = 0.4$ and $D_e = 15$ Ref. [33] as presented in Table 3. The result shows, as the angular quantum number increases, there is a decrease in energy eigenvalues. The result is in good agreement with the earlier result of Ref. [33] with Function analysis method.

Table 1. Spectroscopic parameters of selected diatomic molecules used in this study [40]

Molecules	D_e (eV)	α (Å^{-1})	r_e (Å)	μ (MeV)
N_2	11.93819	2.6986	1.0940	0.65235787010
H_2	4.744600	1.9426	0.7416	0.05021684305
I_2	1.555600	1.8643	2.6660	5.91053779800

Table 2. Bound state energy spectra E_{nl} (eV) of Frost-Musulin potential for H_2, I_2 and N_2 diatomic molecules

n	l	E_{nl} (eV) of H_2	E_{nl} (eV) of I_2	E_{nl} (eV) of N_2
0	0	-0.651520223	-2.986849670	-2.740002210
1	0	-0.694545926	-2.793156331	-2.237811440
	1	-0.837306330	-1.808307281	-2.166221765
2	0	-0.768651215	-1.794847748	-2.149557432
	1	-0.937373235	-1.453835269	-2.135514463
	2	-1.209312076	-1.300850879	-2.145938459
3	0	-0.872713066	-1.446058147	-2.124272714
	1	-1.069404202	-1.290443844	-2.127449959
	2	-1.365597788	-1.209922884	-2.145041222
	3	-1.767342813	-1.164647314	-2.173027661
4	0	-1.006593123	-1.285296867	-2.118718092
	1	-1.232063881	-1.202407843	-2.129592631
	2	-1.554585330	-1.155846187	-2.151297128
	3	-1.979646890	-1.128590987	-2.182002364
	4	-2.511388384	-1.112668258	-2.221075461
5	0	-1.170257245	-1.198689586	-2.122224156
	1	-1.424894724	-1.150074928	-2.137681506
	2	-1.774901763	-1.121521338	-2.162362683
	3	-2.225143077	-1.104661980	-2.195324529
	4	-2.779627564	-1.095194564	-2.236258592
	5	-2.779627564	-1.090737210	-2.285096241

5 Conclusion

In this research, the bound state solutions to the Schrödinger equation with FMP have been studied within the Greene-Aldrich approximation scheme. The energy equation and the wave function are obtained using the NUFA method. We then apply the energy equation to compute the numerical value for three selected diatomic molecules by imputing the experimental values of each molecular parameter. The results show that the bound state energy spectra of these diatomic molecules increases as various quantum numbers n and l increase.

To test the accuracy of our results, we computed the bound states energy (eV) eigenvalues of FMP which agree with the report of other researcher. Our results obtained are accurate and our method is highly efficient and less bulky compared to other methods.

Table 3. Bound state energy eigenvalues in$(eV)$of the Frost-Musulin potential with $\hbar = \mu = 1$, $\alpha = 0.1$, $r_e = 0.4$ Å and $D_e = 15$ eV [33]

n	l	Present work	Ref. [33]
0	0	-1.306566	-1.306565933
1	0	-1.286917	-1.286916932
	1	-1.297165	-1.297164835
2	0	-1.288834	-1.288833784
	1	-1.302941	-1.302940898
	2	-1.326413	-1.326412747
4	0	-1.296067	-1.296067182
	1	-1.312814	-1.312814390
	2	-1.338316	-1.338315516
	3	-1.372736	-1.372736151
4	0	-1.306615	-1.306615212
	1	-1.325817	-1.325816658
	2	-1.353452	-1.353451695
	3	-1.389759	-1.389759069
	4	-1.435009	-1.435009157
5	0	-1.319984	-1.319983895
	1	-1.341616	-1.341615798
	2	-1.371479	-1.371478782
	3	-1.409825	-1.409824986
	4	-1.456927	-1.456927198
	5	-1.513019	-1.513019253

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