A Non-Relativistic Rotational-Vibration Energy Study of Hydrogen Fluoride Molecule

[*1]Ebomwonyi, O., [2]Onate, C.A., [1]Bakare, F.O. and [1]Okunzuwa, I.S.

[1]Department of Physics, University of Benin, Benin City, Nigeria
[2]Department of Physical Sciences, Landmark University, Omu-Aran, Nigeria

Received: July 18, 2017; *Revised: October 17, 2017;* *Accepted: November 15, 2017*

Abstract

The analytical approximate solution of a three-dimensional non-relativistic Schrödinger equation was obtained with a generalized Morse potential model for any arbitrary state in the framework of the parametric Nikiforov-Uvarov method. To test the accuracy of the energy equation, numerical results for various n, ℓ and the screening parameter α were computed. These results were in good agreement when compared with other existing results. To show more practical applications of the results, the rotational-vibration transition frequencies for hydrogen fluoride molecule was calculated numerically and compared with existing results.

Keywords: Schrödinger equation, Generalized Morse potential, Diatomic molecule, Rotational-transition frequencies.

1.0 Introduction

The analytical solution of the radial Schrödinger equation is of high importance in non-relativistic quantum mechanics, since the wave function contains all the necessary information to describe a quantum system fully. There are only a few physical potentials for which radial Schrödinger equation can explicitly be solved for all n and ℓ. Thus, the exact wave function of the radial Schrödinger equation is for some given potentials [1-5]. In a situation where $\ell \neq 0$, the solution of the radial Schrödinger equation with some potentials is possible only with the introduction of the approximation scheme which deals with the centrifugal barrier [6,7]. Such approximation scheme include the Pekeris approximation [8,9], the Padé approximation [10] and the Greene-Aldrich [11].

In the past few years, the solutions of the Schrödinger equation were obtained with exponential-type potentials in the presence of the approximation scheme. These include Hulthén potential [12,13], Manning-Rosen potential [14,15], Eckart potential [16] and the generalized Morse potential [17]. So far, many methods have been developed by several researchers to obtain the bound state solutions of the Schrödinger equation. These methods include asymptotic iteration method (AIM) [18-23], the super-symmetric (SUSY) shape invariance method [24-27], the Nikiforov-Uvarov (NU) method [28]. Such useful works were reported by Ita [29], who obtained energy eigen values and the corresponding wave function by solving the Schrödinger equation with the Hellmann potential using $1/N$ expansion method and the NU method. Kocak *et al.* [30] solved the Schrödinger equation with the Hellmann potential using the asymptotic iteration method and obtained energy eigen values and wave functions. Mesa *et al.* [31] obtained bound state spectrum of the Schrödinger equation with the generalized Morse potential and Pöschl-Teller potential. Arda and Sever [32] solved the one dimensional Schrödinger equation for the generalized Morse potential with the NU method and obtained bound state solutions for the effective mass for some diatomic molecules.

***Corresponding Author: Tel: +234(0)8058865721, E-mail: osarodion.ebomwonyi@uniben.edu.ng**

It is worthy to note that in all the studies mentioned above, the authors did not apply the obtained bound state solutions to solve practical problems such as obtaining the rotational-transition frequencies of diatomic molecules. This seems to be scarce in literature. However, Zhang *et al*. [33] solved any *l*-state solutions of the Schrödinger equation with the generalized Morse potential and also calculated the rotational-transition frequencies of hydrogen fluoride (HF) diatomic molecule using the basic concept of the super-symmetric (SUSY) shape invariance formalism. Therefore, the intent of this paper is to obtain the ℓ - state solutions of the Schrödinger equation with the generalized Morse potential with the aim of computing the rotational-transition frequencies of HF diatomic molecule using an elegant parametric Nikiforov-Uvarov (NU) method. The generalized Morse potential to be studied is given by Dong and Gu [17].

$$V(r)=D_e\left(1-\frac{b}{1-e^{-\alpha r}}\right)^2, \tag{1}$$

where r is the internuclear distance with the dimension, $0\le r<\infty$, D_e is the dissociation energy, $b=e^{\alpha r_e}-1$ is the potential strength, r_e is the equilibrium bond length. A suitable approximation scheme must be employed to obtain any ℓ - state solutions of the radial Schrödinger equation with the potential in Equation (1) in order to take care of the centrifugal term. In this study, the improved approximation scheme [33] was employed.

$$\frac{\ell(\ell+1)}{r^2}\approx \ell(\ell+1)\alpha^2\left(C_0+\frac{e^{-\alpha r}}{\left(1-e^{-\alpha r}\right)^2}\right), \tag{2}$$

where C_0 is a dimensionless constant.

2.0 Methodology

2.1 The Parametric Nikiforov-Uvarov (NU) Method

The parametric NU method is an effective method to solve second-order differential equations derived by Tezcan and Sever [35] from the conventional Nikiforov-Uvarov method. The general form of a Schrödinger equation obtained is given by

$$\left[\frac{d^2}{ds^2}+\frac{\theta_1-\theta_2 s}{s(1-\theta_3 s)}\frac{d}{ds}+\frac{-\xi_1 s^2+\xi_2 s-\xi_3}{s^2(1-\theta_3 s)^2}\right]\psi=0. \tag{3}$$

Based on Equation (3) above, the condition for the wave function and energy equation are respectively given as

$$\psi=s^{\theta_{12}}\left(1-\theta_3 s\right)^{-\theta_{12}-\frac{\theta_{13}}{\theta_3}}P_n^{(\theta_{10}-1,\theta_{11}\theta_3^{-1}-\theta_{10}-1)}\left(1-2\theta_3 s\right), \tag{4}$$

$$\theta_2 n-(1+2n)\theta_5+(2n+1)\left(\sqrt{\theta_9}+\theta_3\sqrt{\theta_8}\right)+n(n-1)\theta_3+\theta_7+2\theta_3\theta_8+2\sqrt{\theta_8\theta_9}=0, \tag{5}$$

where $P_n^{(\theta_{10}-1,\theta_{11}\theta_3^{-1}-\theta_{10}-1)}$ are the orthogonal Jacobi polynomials and the parametric constants are deduced as

$$\theta_4=\frac{1}{2}(1-\theta_1),\ \theta_5=\frac{1}{2}(\theta_2-2\theta_3),\ \theta_6=\theta_5^2+\xi_1,\ \theta_7=2\theta_4\theta_5-\xi_2,\ \theta_8=\theta_4^2+\xi_3,$$

$$\theta_9=\theta_3\theta_7+\theta_3^2\theta_8+\theta_6,\ \theta_{10}=\theta_1+2\theta_4+2\sqrt{\theta_8},\ \theta_{11}=\theta_2-2\theta_5+2\sqrt{\theta_9}+2\theta_3\sqrt{\theta_8}, \tag{6}$$

$$\theta_{12}=\theta_4+\sqrt{\theta_8},\ \theta_{13}=\theta_5-\left(\sqrt{\theta_9}+\theta_3\sqrt{\theta_8}\right).$$

3.0 Results

3.1 Bound State Solution

The radial Schrödinger equation is given of the form [28]

$$\frac{d^2U_{n,\ell}(r)}{dr^2}+\frac{2\mu}{\hbar^2}\left[E_{n,\ell}-V(r)-\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]U_{n,\ell}(r)=0, \tag{7}$$

where μ is the reduced mass, E is the non-relativistic energy, $V(r)$ is the interacting potential and ℓ is the angular momentum quantum number. Substituting both the generalized Morse potential in Equation (1) and approximation scheme in Equation (2) into Equation (7) gives

$$\left[\frac{d^2}{dr^2}+\frac{2\mu E_{n,\ell}-2\mu D_e}{\hbar^2}-\ell(\ell+1)C_0\alpha^2+\frac{\frac{2\mu bD_e(2+b)}{\hbar^2}}{1-e^{-\alpha r}}e^{-\alpha r}+\frac{\frac{-2\mu D_e b^2}{\hbar^2}-\ell(\ell+1)\alpha^2}{\left(1-e^{-\alpha r}\right)^2}e^{-\alpha r}\right]U_{n,\ell}(r)=0. \tag{8}$$

By defining a variable of the form $y=e^{-\alpha r}$ and substituting into Equation (8) gives

$$\frac{d^2U_{n,\ell}(\mathrm{y})}{dy^2}+\frac{1-y}{y(1-y)}\frac{dU_{n,\ell}(y)}{dr}+\frac{-A_1y^2+A_2y-A_3}{\left(y(1-y)\right)^2}U_{n,\ell}(y)=0, \tag{9}$$

where

$$A_1=\ell(\ell+1)(C_0+1)+\frac{2\mu\left[D_e\left(1+2b+b^2\right)-E_{n,\ell}\right]}{\alpha^2\hbar^2}, \tag{10}$$

$$A_2=2\ell(\ell+1)C_0+\frac{4\mu\left[D_e(1+b)-E_{n,\ell}\right]}{\alpha^2\hbar^2}, \tag{11}$$

$$A_3=\ell(\ell+1)C_0+\frac{2\mu\left[D_e-E_{n,\ell}\right]}{\alpha^2\hbar^2}. \tag{12}$$

Comparing Equation (9) with Equation (3), the values of the parametric constants are obtain as

$$\left.\begin{aligned}
&\theta_1=\theta_2=\theta_3=1,\theta_4=0,\theta_5=-\frac{1}{2},\theta_6=\frac{1}{4}+A_1,\theta_7=-A_2,\theta_8=A_3,\\
&\theta_9=\frac{1}{4}\left[(1+2\ell)^2+\frac{8\mu D_e b^2}{\alpha^2\hbar^2}\right],\theta_{10}=1+2\sqrt{\ell(\ell+1)C_0+\frac{2\mu D_e b}{\alpha^2\hbar^2}-\frac{2\mu E_{n,\ell}}{\alpha^2\hbar^2}},\\
&\theta_{11}=4\theta_9+2\left(1+\sqrt{\ell(\ell+1)C_0+\frac{2\mu D_e b}{\alpha^2\hbar^2}-\frac{2\mu E_{n,\ell}}{\alpha^2\hbar^2}}\right),\\
&\theta_{12}=\sqrt{\ell(\ell+1)C_0+\frac{2\mu D_e b}{\alpha^2\hbar^2}-\frac{2\mu E_{n,\ell}}{\alpha^2\hbar^2}},\theta_{13}=-\theta_{12}-\frac{1}{2}-\frac{1}{2}\sqrt{(1+2\ell)^2+\frac{8\mu D_e b^2}{\alpha^2\hbar^2}}.
\end{aligned}\right\} \tag{13}$$

Now substituting the appropriate parametric constants in Equation (13) into Equation (4) and Equation (5) gives the wave function in Equation (14) and the energy equation in Equation (17)

$$U_{n,\ell}(y) = N_{n,\ell} y^{\eta} (1-y)^{\upsilon} P_n^{(2\eta,2\upsilon-1)}(1-2y), \tag{14}$$

where

$$\eta = \sqrt{\ell(\ell+1)C_0 + \frac{2\mu D_e b}{\alpha^2\hbar^2} - \frac{2\mu E_{n,\ell}}{\alpha^2\hbar^2}}, \tag{15}$$

$$\upsilon = \frac{1}{2} + \frac{1}{2}\sqrt{(1+2\ell)^2 + \frac{8\mu D_e b^2}{\alpha^2\hbar^2}}. \tag{16}$$

$$E_{n,\ell} = D_e + \frac{\ell(\ell+1)C_0\alpha^2\hbar^2}{2\mu} - \frac{\alpha^2\hbar^2}{2\mu}\left[\frac{\frac{4\mu D_e b}{\alpha^2\hbar^2} - \frac{1}{2}\left[(2n+1)\sqrt{(1+2\ell)^2 + \frac{4\mu D_e b^2}{\alpha^2\hbar^2}} - 1\right] - n(n+1)}{2n+1+\sqrt{(1+2\ell)^2 + \frac{4\mu D_e b^2}{\alpha^2\hbar^2}}}\right]^2. \tag{17}$$

Table 1: Comparision of bound state energy eigen values in eV for various *n* and ℓ quantum numbers of the generalized Morse potential for 2*p*, 3*p*, 3*d*, 4*p*, 4*d* and 4*f* states with $\hbar = \mu = 1$ and $D_e = 15cm^{-1}$

State	α	Present result (NU)	Dong and Gu (numerical) [17]	Zhang *et al.* (SUSY) [33]
2*p*	0.05	7.77122	7.86280	7.86080
	0.10	7.77577	7.95537	7.95330
	0.15	7.78125	8.04724	8.04510
	0.20	7.78768	8.13842	8.13620
3*p*	0.05	10.9468	10.9998	10.9978
	0.10	11.0628	11.1647	11.1626
	0.15	11.1779	11.3265	11.3262
	0.20	11.2921	11.4851	11.4828
3*d*	0.05	10.0723	10.2165	10.2160
	0.10	10.1725	10.3541	10.3535
	0.15	10.2734	10.4899	10.4894
	0.20	10.4739	10.6240	10.6235
4*p*	0.05	12.4651	12.4992	12.4976
	0.10	12.6344	12.6985	12.6968
	0.15	12.7986	12.8901	12.8884
	0.20	12.9579	13.0740	13.0722
4*d*	0.05	12.0105	12.0981	12.0983
	0.10	12.1143	12.2857	12.2850
	0.15	12.2176	12.4672	12.4664
	0.20	12.3204	12.6432	12.6426
4*f*	0.05	11.6417	11.8209	11.8208
	0.10	11.6456	11.9981	11.9980
	0.15	11.6518	12.1718	12.1717
	0.20	11.6603	12.3421	12.0421

Table 2: Comparative analysis of rotational-transition frequencies for HF with the generalized Morse potential

$\ell\left(\rightarrow \ell-1\right)$	Present result (NU) (cm^{-1})	SUSY method [33] (cm^{-1})	Experimental Result [36] (cm^{-1})
1	40.92	41.56	41.11
2	81.85	83.07	82.07
3	121.46	124.48	122.92
4	162.08	165.74	163.54
5	202.10	206.80	203.93
6	242.57	247.62	243.93
7	282.06	288.15	283.57
8	321.44	328.33	322.85
9	360.56	368.13	361.74
10	399.14	407.49	400.05

4.0 Discussion

In order to verify how well the approximation scheme performed, bound state eigen values of the obtained energy equation (18) for the generalized Morse potential for various n and ℓ quantum numbers in the 2*p*, 3*p*, 3*d*, 4p, 4*d* and 4*f* states were computed. The computed eigen values obtained from this study were compared with those from other methods (Table 1). It was observed that the eigen values obtained for the different states compared well with eigen values from other methods.

The rotational-transition frequencies for HF was computed and the experimental data of molecular constants for the computation was obtained from literature [36]: $\alpha = 1.440_{cm^{-1}}$, $r_e = 1.2746\ \overset{0}{A}$ and $D_e/_{hc} = 62{,}773_{cm^{-1}}$. Table 2 shows a comparative analysis of the results of the rotational-vibrational frequencies obtained from this study with the results of Zhang *et al*. [33] who used the super-symmetric approach and experimental results by Lonardo and Douglas [36]. It can be observed from Table 2 that the results from this study obtained from the paramertric Nikiforov-Uvarov technique alligned better well with experimental results when compared with the results of Zhang *et al*. [33].

Conclusion

In this paper, the bound state solution of the Schrödinger equation with the generalized Morse potential model using the parametric Nikiforov-Uvarov method was studied. The improved approximation scheme was employed to deal with the centrifugal term, eigen values and rotational-vibration energy for diatomic molecules represented by the generalized Morse potential were obtained analytically. The eigen values obtained from this study, compare favourably well with those obtained from other methods and the computed rotational-transition frequencies for the HF diatomic molecule are in better agreement with those obtained using the SUSY method. This shows that the parametric Nikiforov-Uvarov method is a more efficient and reliable method than the SUSY method.

Acknowledgement

The Authors wish to appreciate Dr. M. Onyeaju of the Department of Physics, University of Port Harcourt for his immense contribution that led to significant improvement of this paper.

References

[1] Singh, R.M., Chand, F. and Mishra, S.C. (2009). The Solutions of the Schrödinger Equation for Coupled Quadratic and Quartic Potentials in Two Dimensions. PRAMANA Journal of Physics, Vol. 72, pp. 647-654.
[2] Miranda, M.G., Sun, G.H and Dong, S.H. (2010). The Solution of the Second Pösch-Teller like Potential by Nikiforov-Uvarov Method. International Journal of Modern Physics, Vol. E 19, pp. 123-151.
[3] Arda, A. and Sever, R. (2012). Non-Central Potentials, Exact Solutions and Laplace Transforms Method. Journal of Mathematical Chemistry, Vol. 50, pp. 1484-1494.

[4] Ikot, A.N., Awoga, A.O. and Ita, B.I. (2012). Bound State Solutions of Exponential-Coshine Screened Coulomb Plus Morse Potential. Journal of Atomic and Molecular Sciences, Vol. 3, pp. 285-296.
[5] Rajabi, A.A. (2007). A Method to Solve the Schrödinger Equation for any Hypercentral Potentials. Communications in Theoretical Physics, Vol. 48, pp. 151-158.
[6] Aktas, M. and Sever, R. (2004). Exact Super-Symmetric Solution of Schrödinger Equation for Central Confining Potentials by using the Nikiforov-Uvarov Method. Journal of Molecular Structure in Theoretical Chemistry, Vol. 710, pp. 223-228.
[7] Bayrak, O. and Boztosun, I. (2007). Bound State Solutions of the Hulthén Potential by using the Asymptotic Iteration Method. Journal of Molecular Structure in Theoretical Chemistry, Vol. 802, pp. 17-21.
[8] Marales, D.A. (2004). Supersymmetric Improvement of the Pekeris Approximation for the Rotating Morse Potential. Chemical Physics Letters, Vol. 394, pp. 68-75.
[9] Asgarifar, S. and Goudarzi, H. (2013). Exact Solutions of the Manning-Rosen Potential Plus a Ring-Shaped like Potential for the Dirac Equation: Spin and Pseudospin Symmetry. Physica Scripta, Vol. 87, pp. 1-10.
[10] Castro, E., Paz, J. L. and Martin, P. (2006). Analytical Approximations to the Eigen Values of the Morse Potential with Centrifugal Terms. Journal of Molecular Structure in Theoretical Chemistry, Vol. 769, pp. 15-18.
[11] Greene, R.L. and Aldrich, C.C. (1976). Variational Wave Functions for a Screened Coulomb Potential. Physical Review, Vol. A 14, pp. 2363-2366.
[12] Bayrak, O., Kocak, G. and Boztosun, O. (2006). Any *l*–State Solutions of the Hulthén Potential by the Asymptotic Iteration Method. Journal of Physics A: Mathematical and General, Vol. 39, pp. 11521-11529.
[13] Ikhdair, S.M. and Sever, R. (2007). Approximate Eigen value and Eigen function Solutions for the Generalized Hulthén Potential with any Angular Momentum. Journal of Mathematical Chemistry, Vol. 42, pp. 461-471.
[14] Qiang, W.C. and Dong, S.H. (2007). Analytical Approximation to the Solution of the Manning-Rosen Potential with Centrifugal Term. Physics Letters A, Vol. 368, No. 1, pp. 13-17.
[15] Ikhdair, S.M. and Sever, R. (2008). Approximate l – State Solutions of the D-Dimension Schrödinger Equation for the Manning-Rosen Potential. Annals of Physics, Vol. 17, pp. 897-910.
[16] Dong, S.H., Qiang, W.C., Sun, G.H. and Bezerrz, V.B. (2007). Analytical Approximations to the l – Wave Solutions of the Schrödinger Equation with the Eckart Potential. Journal of Physics A: Mathematical and Theoretical, Vol. 40, No. 34, pp. 10535-10540.
[17] Dong, S.H.S and Gu, X.Y. (2008). Arbitrary l – State Solutions of the Schrödinger Equation with the Deng-Fan Molecular Potential. Journal of Physics: Conference Series, Vol. 96, pp. 1-7.
[18] Bayrak, O. and Boztosun, I. (2007). Bound State Solutions of the Hulthén Potential by using the Asymptotic Iteration Method. Physica Scripta, Vol. 76, pp. 92-96.
[19] Soylu, A., Bayrak, O. and Boztosun, I. (2008). *K* State Solutions of the Dirac Equation for the Eckart Potential with Pseudospin and Spin Symmetry. Journal of Physics A: Mathematical and Theoretical, Vol. 41, pp. 1-8.
[20] Bayrak, O. and Boztosun, I. (2007). The Pseudospin Symmetric Solution of the Morse Potential for only *K* State. Journal of Physics A: Mathematical and Theoretical, Vol. 40, pp. 11119-11127.
[21] Soylu, A., Bayrak, O. and Boztosun, I. (2007). An Approximate Solution of Dirac-Hulthén Problem with Pseudospin and Spin Symmetry for any *K* State. Journal of Mathematical Physics, Vol. 48, pp. 1-9.
[22] Oyewumi, K.J., Falaye, B.J. Onate, C.A., Oluwadare, O.J. and Yahya, W.A. (2014). Thermodynamic Properties and the Approximate Solutions of the Schrödinger Equation with the Shifted Deng-Fan Potential Model. Journal of Molecular Physics, Vol. 112, No. 1, pp. 127-141.
[23] Oyewumi, K.J., Falaye, B.J. Onate, C.A., Oluwadare, O.J. and Yahya, W.A. (2014). *K* State Solutions for the Fermionic Massive Spin-$1/2$ Particles Interacting with Double Ring-Shaped Kratzer and Oscillator Potentials. International Journal of Modern Physics, Vol. E 23, pp. 1-26.
[24] Wei, G.F. and Dong, S.H. (2010). Pseudospin Symmetry in the Relativistic Manning-Rosen Potential Including a Pekeris-Type Approximation to the Pseudo-Centrifugal Term. Physics Letters, Vol. B 686, pp. 288-292.
[25] Hassanabadi, H., Zarrinkamar, S. and Rahimov, H. (2011). Approximate Solution of D-Dimensional Klein-Gordon Equation with Hulthén-Type Potential via SUSYQM. Communications in Theoretical Physics, Vol. 56, pp. 423-428.
[26] Hassanabi, H., Maghsoodi, E., Zarrinkamar, S. and Rahimov, H. (2012). Actual and General Manning-Rosen Potentials under Spin and Pseudospin Symmetries of the Dirac Equation. Canadian Journal of Physics, Vol. 90, pp. 633-646.
[27] Onate, C.A. (2013). Relativistic and Non-Relativistic Solutions of the Inversely Quadratic Yukawa Potential. African Review of Physics, Vol. 8, pp. 325-329.
[28] Ebomwonyi, O., Onate, C.A., Onyeaju, M.C. and Ikot, A.N. (2017). Any l – State Solutions of the Schrödinger Equation Interacting with Hellmann-Generalized Morse Potential Model. Karbala International Journal of Modern Science, Vol. 3, pp. 59-68.

[29] Ita, B.I. (2009). Arbitrary Angular Momentum Solutions of the Schrödinger Equation for Hellmann Potential Energy Function using Maclaurin's Expansion and Nikiforov-Uvarov Method. Ultra Science, Vol. 21, pp. 573-578.
[30] Kocak, G., Bayrak, O. and Boztosun, I. (2007). Arbitrary l – State Solution of the Hellmann Potential. Journal of Theoretical Chemistry, Vol. 6, pp. 893-903.
[31] Mesa, A.D., Quesne, C. and Smirnov, Y.F. (1998). Generalized Morse Potential: Symmetry and Satellite Potentials. Journal of Physics A: Mathematical and General, Vol. 31, pp. 321-335.
[32] Arda, A. and Sever, R. (2011). Bound State Solutions of Schrödinger Equation for Generalized Morse Potential with Position-Dependent Mass. Communications in Theoretical Physics, Vol. 56, No. 1, pp. 51-54.
[33] Zhang, L.H., Li, X.P. and Jia, C.S. (2009). Approximate Solutions of the Schrödinger Equation with the Generalized Morse Potential Model Including the Centrifugal Term. International Journal of Quantum Chemistry, Vol. 111, pp. 1870-1878.
[34] Nikiforov, A.F. and Uvarov, V.B. (1988). Special Functions of Mathematical Physics, Birkhauser, Basel.
[35] Tezcan, C. and Server, R. (2009). A General Approach for the Exact Solution of the Schrödinger Equation. International Journal of Theoretical Physics, Vol. 48, pp. 337-350.
[36] Lonardo, G.D. and Douglas, A.E. (1972). The Electronic Spectrum of HF.I. The $B^1\sum^+ - X^1\sum^+$ Band System. Canadian Journal of Physics, Vol. 51, pp. 434-445.