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Vibrational energies of some diatomic molecules for a modified and deformed potential

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Abstract

A molecular potential model is proposed and the solutions of the radial Schrödinger equation in the presence of the proposed potential is obtained. The energy equation and its corresponding radial wave function are calculated using the powerful parametric Nikiforov-Uvarov method. The energies of cesium dimer for different quantum states were numerically obtained for both negative and positive values of the deformed and adjustable parameters. The results for sodium dimer and lithium dimer were calculated numerically using their respective spectroscopic parameters. The calculated values for the three molecules are in excellent agreement with the observed values. Finally, we calculated different expectation values and examined the effects of the deformed and adjustable parameters on the expectation values.

Key words: Eigensolution; Bound state; Wave equation; Schrödinger equation; Diatomic molecules.

1. Introduction

In the recent time, exponential-type potential has been the subject of interest in the quantum mechanics which greatly popularized the relativistic and non-relativistic wave equations such as the Schrödinger equation, Klein-Gordon equation, Dirac equation and others [1-15]. The approximate solutions of these wave equations have been obtained mostly for one-dimensional system with various exponential-type potentials using different approximation methods developed by different authors. The frequently used methods are Nikiforov-Uvarov method [16, 17], asymptotic iteration method [18], supersymmetric approach [19, 20], factorization method [21], exact and proper quantization rule [22, 23]. Recently, Ikot et al. [24, 25] have used a new approach called NU Functional analysis method. The different methods have different approach for the solutions of the wave equations but give results that are approximately the same. For instance, the solutions of the radial Schrödinger equation under the Deng-Fan potential model has been studied by Dong and Gu [26] using factorization method. Zhang et al. [27] and Onate et al. [28] respectively also studied the potential via supersymmetry quantum mechanics and parametric Nikiforov-Uvarov method respectively. The respective result of these authors agreed with one another.

The solutions of the wave equations studied for different potentials, have been applied to the study of several systems such as Theoretic quantities [29-32] and Thermal properties (mean energy, heat capacity, free energy and entropy) [33-38]. In ref. [27], the result was used to study the rotation transition frequency for HF. In ref. [28], the wave function was used to study some theoretic quantities such Shannon entropy and Rényi entropy. In ref. [39], the problem of $so(2,2)$ was studied under the Pöschl-Teller potential. Several authors have also studied the

energy eigenvalues for many diatomic molecules on molecular dynamics and spectroscopy in the field of chemistry and molecular physics [40, 41]. This provides explanations about the dynamics and physical properties of some molecules. The potential energy function involved are used to study the bonding between atoms, hence the predictions to the behaviour of some class of molecules [42]. Some of these potentials can be used to describe some experimental values. Generally, a good empirical internuclear potential function should reproduce the experimental potential energy curves as determined by the RKR method. Considering this, the present study wants to examine an approximate solutions of the Schrödinger equation with a new modified and deformed exponential-type molecular potential model confined on a cesium dimer, sodium dimer and lithium dimer. The study also aim to investigate the potential with two different values for each of the deformed parameter and adjustable parameter under the same cesium dimer. This potential has not been reported for any study yet to the best our understanding.

The cesium dimer is an important molecule that has many applications, e.g. vibrational cooling of molecules, population dynamics, and even coherent control [43-47]. The cesium molecule is an attractive system for examining a possible variation of the electron-to-proton mass ratio and of the fine-structure constant [48]. It is noted that $3^3 \Sigma_g^+$ state of cesium dimer has a strong Fermi contact interaction with the nuclei, and possesses a large hyperfine splitting [49]. The potential energy curve of the cesium dimer for $3^3 \Sigma_g^+$ and $a^3 \Sigma_u^+$ states has been reported in ref. [50, 51]. The modified and deformed exponential-type molecular potential model is given as

$$V(r) = D_e - \frac{D_e}{C e^{-\alpha r} + q_0} \left(e^{\alpha r_e} + q_1 - \frac{(e^{\alpha r_e} + q_1)^2}{C e^{-\alpha r} + q_0} \right), \quad (1)$$

where C is a modified parameter, q_0 is a deformed parameter and q_1 is an adjustable parameters whose value can be taken as ± 1 . When the value of the adjustable parameter equals the value of the deformed parameter within ± 1 , the results of potential (1) gives other useful results. D_e is the dissociation energy r_e is the equilibrium bond separation and α is the screening parameter. Its numerical value can be obtain using the formula

$$\alpha = \pi c \omega_e \sqrt{\frac{2\mu}{D_e}} + \frac{1}{r_e} W \left(-\pi c \omega_e \sqrt{\frac{2\mu}{D_e}} e^{-\pi c \omega_e \sqrt{\frac{2\mu}{D_e}}} \right), \quad (2)$$

where W is the Lambert function, μ is the reduced mass, c is the speed of light and ω_e is the vibrational frequency.

2. Parametric Nikiforov-Uvarov Method.

The parametric Nikiforov-Uvarov method is one of the shortest and accurate traditional techniques to solve bound state problems. This method was derived from the conventional Nikiforov-Uvarov method by Tezcan and Sever [17]. According to the authors, the reference equation for the parametric Nikiforov-Uvarov is given as

$$\left(\frac{d^2}{ds^2} + \frac{\alpha_1 - \alpha_2}{s(1 - \alpha_3 s)} \frac{d}{ds} + \frac{-\xi_1 s^2 + \xi_2 s - \xi_3}{s^2(1 - \alpha_3 s)^2} \right) \psi(s) = 0. \quad (3)$$

Following the work of these authors, the condition for eigenvalues equation and wave function are respectively given by [17, 52]

$$n\alpha_2 - (2n+1)\alpha_5 + \alpha_7 + 2\alpha_3\alpha_8 + n(n-1)\alpha_3 + (2n+1)\sqrt{\alpha_9} + (2\sqrt{\alpha_9} + \alpha_3(2n+1))\sqrt{\alpha_8} = 0, \quad (4)$$

$$\psi_{n,1}(s) = N_{n,1} s^{\alpha_{12}} (1 - \alpha_3 s)^{-\alpha_{12} - \frac{\alpha_{13}}{\alpha_3}} \times P_n^{\left(\alpha_{10}-1, \frac{\alpha_{11}-\alpha_{10}-1}{\alpha_3}\right)} (1 - 2\alpha_3 s), \quad (5)$$

The parametric constants in equations (3) and (4) are deduced as follows

$$\left. \begin{aligned} \alpha_4 &= \frac{1 - \alpha_1}{2}, \alpha_5 = \frac{\alpha_2 - 2\alpha_3}{2}, \alpha_6 = \alpha_5^2 + \xi_1, \alpha_7 = 2\alpha_4\alpha_5 - \xi_2, \alpha_8 = \alpha_4^2 + \xi_3, \\ \alpha_9 &= \alpha_3(\alpha_7 + \alpha_3\alpha_8) + \alpha_6, \alpha_{10} = \alpha_1 + 2\alpha_4 + 2\sqrt{\alpha_8}, \alpha_{11} = \alpha_2 - 2\alpha_5 + 2(\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}), \\ \alpha_{12} &= \alpha_4 + \sqrt{\alpha_8}, \alpha_{13} = \alpha_5 - (\sqrt{\alpha_9} + \alpha_3\sqrt{\alpha_8}) \end{aligned} \right\}. \quad (6)$$

3. The radial Schrödinger equation and the interacting potential.

To obtain the energy eigenvalues of the Schrödinger equation with potential (1), we consider the original Schrödinger equation given by

$$\left[-\frac{\hbar^2}{2m} \left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right) + V(r) - E \right] \psi(r) = 0. \quad (7)$$

Setting the wave function $\psi(r) = U_{n,1}(r) Y_{m,1}(\theta, \phi) r^{-1}$, and consider the radial part of the Schrödinger equation, Eq. (7) becomes

$$-\frac{\hbar^2}{2\mu} \frac{d^2 U_{n,1}(r)}{dr^2} + \frac{\hbar^2}{2\mu} \frac{1(1+1)}{r^2} U_{n,1}(r) = E_{n,1} U_{n,1}(r) - V(r) U_{n,1}(r), \quad (8)$$

where $\frac{\hbar^2}{2\mu} \frac{1(1+1)}{r^2}$ has been introduced, $V(r)$ is the interacting potential given in Eq. (1), $E_{n,1}$ is the non-relativistic energy of the system, $\hbar$ is the reduced Planck's constant, m is the mass, n is the quantum number, $U_{n,1}(r)$ is the wave function. To overcome the centrifugal term in Eq. (7), the following approximation scheme is employed

$$\frac{1}{r^2} \approx \alpha^2 \left(C_0 + \frac{e^{\alpha r}}{(1 + q_0 e^{\alpha r})^2} \right). \quad (9)$$

For the approximation scheme to suit the interacting potential, the modified parameter is taken to be unity. Substituting Eq. (1) and Eq. (9) into (8), and by defining $y = \frac{1}{e^{-\alpha r}}$, the radial Schrödinger equation with the deformed exponential-type potential turns to be

$$\frac{d^2 U_{nl}(y)}{dy^2} + \frac{1+y}{y(1+q_0 y)} \frac{dU_{nl}(y)}{dy} + \frac{-Py^2 + Qy - R}{y^2(1+q_0 y)^2} U_{nl}(y) = 0, \quad (10)$$

where

$$P = \frac{2\mu D_e}{\alpha^2 \hbar^2} \left(q_0^2 - \frac{E_{n,l} q_0^2}{D_e} - 2q_0(e^{\alpha r_e} + q_1)(1 + e^{\alpha r_e} + q_1) \right) + 1(1+1)C_0 q_0^2, \quad (11)$$

$$Q = \frac{4\mu D_e}{\alpha^2 \hbar^2} \left(\frac{E_{n,l} q_0}{D_e} - q_0 + e^{\alpha r_e} + q_1 \right) - 1(1+1)(1+2q_0 C_0), \quad (12)$$

$$R = \frac{2\mu(D_e - E_{n,l})}{\alpha^2 \hbar^2} + 1(1+1)C_0. \quad (13)$$

Comparing Eq. (10) with Eq. (3), the parametric constants in Eq. (6) are obtain as follows

$$\left. \begin{aligned} \alpha_1 &= 1, \alpha_2 = \alpha_3 = -q_0, \alpha_4 = 0, \alpha_5 = \frac{q_0}{2}, \\ \alpha_6 &= q_0^2 \left(\frac{1}{4} + 1(1+1)C_0 \right) + \frac{2\mu D_e}{\alpha^2 \hbar^2} \left(q_0^2 - 2q_0(e^{\alpha r_e} + q_1) - \frac{E_{n,l} q_0^2}{D_e} + e^{\alpha r_e} + q_1 \right), \\ \alpha_7 &= \frac{4\mu D_e}{\alpha^2 \hbar^2} \left(q_0 - \frac{E_{n,l} q_0}{D_e} - e^{\alpha r_e} - q_1 \right) + 1(1+1)(1+2q_0 C_0), \\ \alpha_8 &= \frac{2\mu(D_e - E_{n,l})}{\alpha^2 \hbar^2} + 1(1+1)C_0, \alpha_9 = \frac{1}{4} \left(q_0^2 + \frac{8\mu D_e (e^{\alpha r_e} + q_1)^2}{\alpha^2 \hbar^2} \right) - 4l(1+1)q_0, \\ \alpha_{10} &= 1 + 2T_{V_1}, \alpha_{11} = -2q_0 \left[1 + T_{V_1} \right] + T_{V_2}, \alpha_{12} = T_{V_1}, \alpha_{13} = \frac{q_0}{2} - \frac{1}{2} T_{V_2} + q_0 T_{V_1}, \\ T_{V_1} &= \sqrt{\frac{2\mu(D_e - E_{n,l})}{\alpha^2 \hbar^2} + 1(1+1)C_0}, T_{V_2} = \sqrt{q_0^2 - 4l(1+1)q_0 + \frac{8\mu D_e (e^{\alpha r_e} + q_1)^2}{\alpha^2 \hbar^2}} \end{aligned} \right\}. \quad (14)$$

Substituting the parameters in Eq. (14) into Eq. (4), we have the energy equation for the system as

$$E_{n,l} = D_e + \frac{1(1+1)C_0 \alpha^2 \hbar^2}{2\mu} - \frac{\alpha^2 \hbar^2}{2\mu} \left[\frac{\frac{4\mu D_e (e^{\alpha r_e} + q_1)}{\alpha^2 \hbar^2} - 1(1+1) - \frac{n(n+1)}{q_0^{-1}} + \frac{q_0}{2} - \left(n + \frac{1}{2} \right) \lambda_T}{\lambda_T - q_0(2n+1)} \right]^2, \quad (15)$$

$$\lambda_T = \sqrt{q_0^2 - 4l(1+1)q_0 + \frac{8\mu D_e (e^{\alpha r_e} + q_1)^2}{\alpha^2 \hbar^2}}, \quad (16)$$

and the corresponding wave function is obtain when the values of α_{10} to α_{13} in Eq. (6) are substituted into Eq. (5),

$$U_{n,l}(y) = N_{n,l} y^{T_{V_1}} (1 + q_0 y)^{T_{V_1}(q_0-1) + \frac{1}{2}(T_{V_2}-q_0)} \left[P_n \left(\frac{2T_{V_1} - T_{V_2}}{q_0} \right) (1 + 2q_0 y) \right]. \quad (17)$$

4. Expectation Values

In this section, we calculated some expectation values using Hellmann-Faynman Theorey (HFT) [53-57]. When a Hamiltonian H for a given quantum system is a function of some parameter v , the energy-eigenvalue $E_{n,l}$ and the eigenfunction $U_{n,l}(v)$ of H are given by

$$\frac{\partial E_{n,l}(v)}{\partial v} = \left\langle U_{n,l}(v) \left| \frac{\partial H(v)}{\partial v} \right| U_{n,l}(v) \right\rangle, \quad (18)$$

with the effective Hamiltonian as

$$H = -\frac{\hbar^2}{2\mu} \frac{d^2 U_{n,l}(r)}{dr^2} + \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} + D_e - \frac{D_e}{e^{-\alpha r} + q_0} \left(e^{\alpha r_e} + q_1 - \frac{(e^{\alpha r_e} + q_1)^2}{e^{-\alpha r} + q_0} \right). \quad (19)$$

Setting $v = D_e$, $v = 1$ and $v = \mu$, we have the expectation values of p^2 , r^{-2} and V respectively are

$$\langle p^2 \rangle_{n,l} = 1 - \frac{4\alpha^2 \hbar^2 A_2 (e^{\alpha r_e} + q_1) \left(\frac{\mu \lambda_T - (n+1/2)(e^{\alpha r_e} + q_1) \mu}{\alpha^2 \hbar^2 \lambda_T} \right)}{\mu A_1^2}, \quad (20)$$

$$\langle r^{-2} \rangle_{n,l} = \frac{\mu B}{\hbar^2 (2l+1)} + \frac{2\alpha^2 \lambda_T (2l+1+B_0)}{(2l+1)A_1^2} - \frac{4q_0 \alpha^2}{\lambda_T A_1}, \quad (21)$$

$$\langle V \rangle_{n,l} = \frac{\alpha^2 \hbar^2 A_2^2}{2\mu^2 A_1^2} + \frac{4D_e A_2^2 (e^{\alpha r_e} + q_1)^2}{\mu \lambda_T A_1^2} - \frac{l(l+1)C_0 \alpha^2 \hbar^2}{2\mu^2} - \frac{4D_e A_2 (e^{\alpha r_e} + q_1)^2 \left(\frac{1 - (n+1/2)(e^{\alpha r_e} + q_1)}{\lambda_T} \right)}{\mu A_1^2}, \quad (22)$$

$$A_0 = \lambda_T (n+1/2), \quad (23)$$

$$A_1 = \lambda_T - q_0 (1+2n), \quad (24)$$

$$A_2 = \frac{4\mu D_e (e^{\alpha r_e} + q_1)}{\alpha^2 \hbar^2} + \frac{q_0}{2} - \frac{n(n+1)}{q_0} - (n+1/2)\lambda_T - 1(1+1), \quad (25)$$

$$B = \frac{\alpha^2 \hbar^2 (2l+1)C_0}{2\mu}, \quad (26)$$

$$B_0 = -\frac{q_0(2n+1)(2l+1)}{\lambda_T}. \quad (27)$$

Table 1: Comparison of theoretical values with experimental values for the vibrational energy levels of the modified deformed exponential-type molecular potential for $3^3 \Sigma_g^+$ state of cesium dimer.

n	RKR [58] cm^{-1}	$q_1 = 1$ cm^{-1}	RKR [51] cm^{-1}	$q_1 = -1$ cm^{-1}
0	14.4248	14.42647874	19,477.5507	19,477.55769
1	43.1680	43.17554991	19,506.2939	19,506.29999
2	71.7657	71.77608344	19,534.8916	19,534.90041
3	100.2211	100.2450879	19,563.3470	19,563.35986
4	128.5375	128.5580953	19,591.6634	19,591.68592
5	156.7182	156.7410068	19,619.8441	19,620.43756
6	184.7663	184.7735524	19,647.8922	19,648.55903
7	212.6851	212.6619860	19,675.8110	19,677.08704
8	240.4778	240.4268832	19,703.6037	19,704.38389
9	268.1477	268.2399412	19,731.2736	19,732.74500
10	295.6980	296.0578830	19,758.8239	19,759.62187
11	323.1320	323.3428999	19,786.2579	19,786.99999
12	350.4529	351.0106935	19,813.5788	19,814.29857

Table 2: Comparison of theoretical values with experimental (in cm^{-1}) values for the vibrational energy levels of the modified deformed exponential-type molecular potential for $5^1 \Delta_g$ state sodium dimer and $a^3 \Sigma_u^+$ state of lithium dimer

n	Na_2 [18]	$q_0 = q_1 = 1$ present results	Li_2 [18]	$q_0 = q_1 = -1$ present results
0	60.333	60.31364676	31.8570	31.80143202
1	180.373	180.2577331	90.4530	90.39261096
2	299.555	299.3324068	142.523	142.4220678
3	417.871	417.3016667	188.240	188.1901675
4	535.313	534.5243524	227.679	227.4621906
5	651.872	650.4688333	260.837	260.5360334
6	767.539	765.3824841	287.665	287.3995111
7	882.305	879.7021966	308.098	307.9601021

8	996.162	993.6386433	322.155	322.2963805
9	1109.100	1104.753548	330.170	330.7599572
10	1221.113	1215.707839	333.269	333.5586499

Table 3: Expectation values at various quantum states with $l = h = \mu = 1$, $r_e = 0.4$, $\alpha = 0.25$,

$D_e = 5$ and $q_0 = q_1 = -1$.

n	$\langle p^2 \rangle_{n,l}$	$\langle r^{-2} \rangle_{n,l}$	$\langle V \rangle_{n,l}$
0	1.069858799	0.039999669	0.368447529
1	1.051727481	0.029330271	0.260041512
2	1.030363793	0.023397637	0.133941612
3	1.013262325	0.019620392	0.043515090
4	1.000377469	0.017004496	-0.004319914
5	0.990813897	0.015085714	-0.010405957
6	0.983773583	0.013618148	0.023299645
7	0.978655270	0.012459383	0.095013696
8	0.975020088	0.011521231	0.203320911
9	0.972547147	0.010746167	0.347136241
10	0.970998984	0.010095063	0.525631819

Table 4: Expectation values at various quantum states with $l = h = \mu = 1$, $r_e = 0.4$, $\alpha = 0.25$,

$D_e = 5$ and $q_0 = q_1 = 1$.

n	$\langle p^2 \rangle_{n,l}$	$\langle r^{-2} \rangle_{n,l}$	$\langle V \rangle_{n,l}$
0	12.54126260	0.004909147	261.9950729
1	14.07512966	0.005000995	285.8523651
2	15.80688031	0.005100467	312.2648238
3	17.77133204	0.005208552	341.6413784
4	20.01151893	0.005326420	374.4812757
5	22.58116336	0.005455464	411.3997764
6	25.54806604	0.005597350	453.1629487
7	28.99882749	0.005754097	500.7354772
8	33.04553492	0.005928168	555.3474242
9	37.83541012	0.006122603	618.5891346
10	43.56501898	0.006341198	692.5488475

The average deviation of the calculated results from the experimental results is obtained using the formula

$$\sigma_{av} = \frac{100}{N} \sum_n \left| \frac{E_{ER} - E_{CR}}{E_{ER}} \right|, \quad (28)$$

where E_{ER} is the sum of the experimental data, E_{CR} is the sum of the calculated values and N is the total number of the experimental data.

Figure 1: Variation of energy $E_{n,l}$ against the screening parameter α , with $C=1 = \hbar = \mu = 1$, $r_e = 0.4$ and $D_e = 10$.

5. Discussion of Result

The comparison of the observed values of RKR and calculated values for $3^3\Sigma_g^+$ state of cesium dimer with $q_0 = q_1 = 1$, $q_0 = q_1 = -1$, $D_e = 2722.28 \text{ cm}^{-1}$, $r_e = 5.3474208 \text{ \AA}$, and $\omega_e = 28.891 \text{ cm}^{-1}$ is reported in Table 1. The results for two values for each of the deformed parameter and adjustable parameter agreed with the observed values of the cesium dimer. In Table 2, the comparison of vibrational energies of sodium dimer and lithium dimer respectively are reported. When the deformed parameter and the adjustable parameter are taken as one with $D_e = 79885 \text{ cm}^{-1}$, $r_e = 1.097 \text{ \AA}$, $\omega_e = 2358.6 \text{ cm}^{-1}$, the results agreed with the observed values of $5^1\Delta_g$ state of

sodium dimer. Taken the deformed parameter and adjustable parameter respectively as minus one, with $D_e = 2722.28\text{cm}^{-1}$, $r_e = 4.173\text{\AA}$ and $\omega_e = 65.130\text{cm}^{-1}$, the results obtained correspond to the observed values of lithium dimer.

To deduce the effect of the deformed and adjustable parameters on the numerical values and discrepancy of the calculated results from the experimental data, we used the formula given in Eq. (28). For cesium dimer, the average percentage deviation for $q_0 = q_1 = 1$ is 0.0038% while the average percentage deviation for $q_0 = q_1 = -1$ is 0.0002%. For sodium dimer with $q_0 = q_1 = 1$, the average percentage deviation is 0.0283% while the average percentage deviation for lithium dimer with $q_0 = q_1 = -1$, is 0.0010%. In Table 3 and Table 4, we presented the numerical results for the three different expectation values calculated in Eq. (20), Eq. (21) and Eq. (22) respectively. The results obtained with $q_0 = q_1 = 1$ are higher than their counterpart obtained with $q_0 = q_1 = -1$.

The effect of the screening parameter on the energy eigenvalues with two values each of the deformed parameter and adjustable parameter is shown in Figure 1. For $q_0 = q_1 = 1$, the energy of the system rises as the screening parameter increases from zero but the reverse is the case for $q_0 = q_1 = -1$.

6. Conclusion

The solutions of a one-dimensional Schrödinger equation is obtained for a molecular potential model using parametric Nikiforov-Uvarov method. By changing the numerical values of the deformed parameter and adjustable parameter, the results different obtained for different molecules agreed with experimental values. However, the results obtained with $q_0 = q_1 = -1$ are closer to the experimental values compared with the results obtained with $q_0 = q_1 = 1$. In the computation of numerical values for the expectation values, it is noted that the results obtained with $q_0 = q_1 = 1$ are higher than their counterpart obtained with $q_0 = q_1 = -1$.

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Authors' contributions: C.A. Onate; Formulate the work, solved the calculations

I.B. Okon; Wrote the introduction

M.C. Onyeaju; Makes all the plots and discussed the results

O. Ebomwonyi; Solved the calculations and typeset the paper

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