

Analytical Treatment of the Non-Relativistic System for Diatomic Molecules

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Abstract

The solutions of a radial Schrödinger equation are obtained for an improved generalized Pöschl-Teller potential models. Using the supersymmetric approach, we calculated the non-relativistic energy and its corresponding un-normalized radial wave function for each potential model. Three different expectation values were calculated using Hellmann Feynman Theory (HFT) for the interacting potential model. The energy equation obtained and the various calculated expectation values were used to study NO, CH, H₂ and N₂ molecules. Our results showed that these molecules exhibit some similarities and some differences under the eigenvalues due to the differences in the values of the spectroscopic parameters.

Keywords: Eigensolution; Wave equation; Bound state, Potential model; Schrödinger equation.

1. Introduction

The solutions of the Schrödinger equation for some different physical potential models has drawn much attention in the theoretical sciences over the years due to their importance in both quantum physics and quantum chemistry. The solutions of the Schrödinger equation for these potential terms contain useful information that completely describes a quantum system. These solutions are obtained for any ℓ states using different traditional methodologies such as the asymptotic iteration method [1-3], Nikiforov-Uvarov method including the parametric type [4-8] recently derived by Tezcan and Sever, supersymmetric approach [9-12], exact and proper quantization rule [13, 14], formula method for bound state problem [15, 16] and others. However, there are some special types of potential models that do not admit the solution for due to the inverse squared term. Therefore, to obtain the solutions for any of these type of the potential, an approximation scheme suitable for such potential model must be employed. Generally, the solutions of the radial Schrödinger equation for various potential terms of interest required the use of approximation scheme suitable for them. The frequently used approximation include the Pekeris approximation type [17], Greene-Aldrich approximation type [18] and the recent approximation scheme proposed by Dong et al. [19].

One of the physical potential model that drawn attention in the bound state solutions recently is the Pöschl-Teller potential. The Pöschl-Teller potential model is an important molecular potential that can be use to describe the vibration of polyatomic molecules like ammonia. The Pöschl-Teller potential has been studied for both the relativistic and non-relativistic systems in different forms. For instance, Dong and Gonzalez-Cisneros [13], studied bound state solutions of the Schrödinger equation for a Pöschl-Teller type of potential called the second Pöschl-Teller. Ahmed [20] obtained real and complex discrete eigenvalues of the Schrödinger equation for another form of Pöschl-Teller referred to as the complex PT-invariant potential. In ref. [21], Wei and Dong, studied the pseudospin symmetry of the relativistic Dirac equation for another Pöschl-Teller potential they called modified Pöschl-Teller potential model. Recently, Tang and Jia [22], modified one of the existing Pöschl-Teller potential model to suit their study and named it a simplified Pöschl-Teller potential model. In a similar way, Khordad et al. [23] studied another form of Pöschl-Teller called improved generalized Pöschl-Teller potential model. The improved generalized Pöschl-Teller potential model has not been adequately studied. Motivated by the interest in the Pöschl-Teller form of potential model, the present study wants to examine the non-relativistic solutions of the improved generalized Pöschl-Teller potential model using the elegant supersymmetric approach. The improved generalized Pöschl-Teller potential model is given as [20]

$$V_{IGP}(r) = D_e \left(1 + \frac{1 + \cosh^2(\alpha r_e) - 2\cosh(\alpha r_e)\cosh(\alpha r)}{\sinh^2(\alpha r)} \right). \quad (1)$$

The scheme of our presentation is as follows. In the next section, we present the bound state solution. In section 3, we calculate the expectation values. Section 4 is the results and discussion while the concluding remark is given in the final section.

2. Bound State Solutions

To solve any quantum system in the presence of a given physical potential term of interest, the three-dimensional Schrödinger equation that describes the eigenvalue and eigenfunction can be written as

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

Setting the wave function as $\psi(r) = R_{n,\ell}(r) Y_{m,\ell}(\theta, \phi) r^{-1}$, and consider the radial part of the Schrödinger equation, Eq. (2) turns out to be

$$-\frac{\hbar^2}{2\mu} \frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} R_{n\ell}(r) - E_{n\ell} R_{n\ell}(r) + V(r) R_{n\ell}(r) = 0, \quad (3)$$

where $\frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2}$ has been introduced, $V(r)$ is the interacting potential given in Eq. (1),

$E_{n\ell}$ is the non-relativistic energy of the system, \hbar is the reduced Planck's constant, μ is the reduced mass of the particle, n is the quantum number, $R_{n\ell}(r)$ is the wave function. The centrifugal term in Eq. (3) can be approximated using the formula

$$\frac{1}{r^2} \approx \frac{\alpha^2}{\sinh^2(\alpha r)}. \quad (4)$$

Substitute Eq. (1) and Eq. (4) into Eq. (3), we have a second-order differential equation of the form

$$\frac{d^2 R_{n,\ell}(r)}{dr^2} = \frac{2\mu(D_e - E_{n,\ell})}{\hbar^2} + \frac{\ell(\ell+1)\alpha^2 + \frac{2\mu D_e(1 - 2\cosh(\alpha r_e)\cosh(\alpha r) + \cosh^2(\alpha r_e))}{\hbar^2}}{\sinh^2(\alpha r)}. \quad (5)$$

To proceed to the next level under the methodology of the powerful supersymmetric quantum mechanics, we write out the ground state wave function in the following form

$$R_{0,\ell}(r) = \exp\left(-\int W(r)dr\right), \quad (6)$$

where $W(r)$ is the called the superpotential function in supersymmetric quantum mechanics. The superpotential function plays a key role in the deduction of energy eigenvalue equation. It gives a solution to Eq. (5) through a non-linear Riccati equation. For each potential model, a specific superpotential function is suitable for it. Considering the interacting potential in this case, we propose a superpotential function of the form

$$W(r) = \rho_0 + \frac{\rho_1 + \rho_2 \cosh(\alpha r)}{\sinh(\alpha r)}, \quad (7)$$

The parameters ρ_0 , ρ_1 and ρ_2 in the above equation are known to be superpotential parameters. Substituting the superpotential function in Eq. (7) into the ground state wave function in Eq. (6) leads to another equation of the form

$$W^2(r) - \frac{dW(r)}{dr} = \rho_0^2 + V_{T_0} + \frac{2\rho_0(\rho_1 + \rho_2 \cosh(\alpha r))}{\sinh(\alpha r)}, \quad (8)$$

where

$$V_{T_0} = \frac{\rho_1(\rho_1 + \alpha \cosh(\alpha r)) + \rho_2 [\cosh(\alpha r)(2\rho_1 + \cosh(\alpha r)(\rho_2 + \alpha)) - \alpha]}{\sinh^2(\alpha r)}. \quad (9)$$

To proceed towards the deduction of the energy equation of the system, we must obtain different equations for the parameters ρ_0 , ρ_1 and ρ_2 which will enhance a concrete establishment relationship and formula for a residual term. Using Eq. (5) and Eq. (8) with some mathematical manipulations and simplifications, the three superpotential constants are deduce as follows

$$\rho_0^2 = \frac{2\mu(D_e - E_{n,\ell})}{\hbar^2}, \quad (10)$$

$$\rho_1 = \frac{\alpha}{2} \left(-1 \pm \sqrt{(1+2\ell)^2 + \frac{8\mu D_e(1+2\cosh(\alpha r) + \cosh^2(\alpha r))}{\alpha^2 \hbar^2}} \right), \quad (11)$$

$$\rho_2 = \frac{\alpha}{2} \left(-1 \pm \sqrt{(1+2\ell)^2 + \frac{8\mu D_e(1+2\cosh(\alpha r) - \cosh^2(\alpha r))}{\alpha^2 \hbar^2}} \right), \quad (12)$$

$$\rho_0 = \frac{-(\rho_1 - \rho_2)}{2}. \quad (13)$$

To deduce the energy equation using supersymmetric approach, we examine the shape invariance system via the proposed superpotential function. This is only achieved via the construction of partner potentials $V_{\pm}(r) = W^2(r) \pm \frac{dW(r)}{dr}$. Hence

$$V_+(r) = \rho_0^2 + \rho_2(\rho_2 - \alpha) + \frac{2\rho_0(\rho_1 + \rho_2 \cosh(\alpha r))}{\sinh(\alpha r)} + \frac{\rho_1(\rho_1 - \alpha \cosh(\alpha r)) + \rho_2(\rho_2 + 2\rho_1 \cosh(\alpha r))}{\sinh^2(\alpha r)}, \quad (14)$$

and

$$V_-(r) = \rho_0^2 + \rho_2(\rho_2 + \alpha) + \frac{2\rho_0(\rho_1 + \rho_2 \cosh(\alpha r))}{\sinh(\alpha r)} + \frac{\rho_1(\rho_1 + \alpha \cosh(\alpha r)) + \rho_2(\rho_2 + 2\rho_1 \cosh(\alpha r))}{\sinh^2(\alpha r)}. \quad (15)$$

Eq. (14) and Eq. (15) are connected via a simple formula/relation that satisfied the partner potentials V_{\pm} :

$$V_+(r, a_0) = V_-(r, a_1) + R(a_1), \quad (16)$$

where a_1 is a new set of parameters uniquely determined from a_0 an old set of parameter via mapping of the form $a_1 = h(a_0) = a_0 + \alpha$, and the remainder or residual $R(a_1)$ is independent of the variable r . From the mapping, it can be deduce that $a_2 = a_0 + 2\alpha$, $a_3 = a_0 + 3\alpha$, $a_4 = a_0 + 4\alpha$ and subsequently, $a_n = a_0 + n\alpha$. Taking then Eq. (14) and Eq. (15) satisfied the shape invariance concept as shown by Eq. (16). Hence

$$R(a_1) = \left(\frac{a_0 - \rho_1}{2} \right)^2 - \left(\frac{a_1 - \rho_1}{2} \right)^2, \quad (17)$$

$$R(a_2) = \left(\frac{a_1 - \rho_1}{2} \right)^2 - \left(\frac{a_2 - \rho_1}{2} \right)^2, \quad (18)$$

$$R(a_3) = \left(\frac{a_2 - \rho_1}{2} \right)^2 - \left(\frac{a_3 - \rho_1}{2} \right)^2, \quad (19)$$

$$R(a_n) = \left(\frac{a_{n-1} - \rho_1}{2} \right)^2 - \left(\frac{a_n - \rho_1}{2} \right)^2, \quad (20)$$

The energy spectrum can be exactly be determined following

$$\sum_{i=1}^n R(a_i) = R(a_1) + R(a_2) + R(a_3) + \dots + R(a_n), \quad (21)$$

from which we actually determine the real energy equation of the system as

$$E_{n,\ell}^{IGP} = D_e - \frac{\alpha^2 \hbar^2}{32\mu} \left(2n+1 - \sqrt{V_{T_2} + \frac{V_{T_3} (\cosh(\alpha r_e) + 2)}{\alpha^2 \hbar^2}} + \sqrt{V_{T_2} + \frac{V_{T_3} (\cosh(\alpha r_e) - 2)}{\alpha^2 \hbar^2}} \right)^2, \quad (22)$$

$$V_{T_2} = (1+2\ell)^2 + \frac{8\mu D_e}{\alpha^2 \hbar^2}, \quad V_{T_3} = 8\mu D_e \cosh(\alpha r_e). \quad (23)$$

3. Expectation Values

In this section, we calculate some expectation values using Hellmann-Feynman Theorem (HFT) [23, 24]. Given a Hamiltonian H for a quantum system as a function of some parameter say v , the energy-eigenvalue $E_{n,\ell}$ and the eigenfunction $R_{n,\ell}(v)$ of H are given by

$$\frac{\partial E_{n,\ell}(v)}{\partial v} = \left\langle R_{n,\ell}(v) \left| \frac{\partial H(v)}{\partial v} \right| R_{n,\ell}(v) \right\rangle, \quad (24)$$

with the effective Hamiltonian as

$$H = -\frac{\hbar^2}{2\mu} \frac{d^2 R_{n,\ell}(r)}{dr^2} + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} + D_e + \frac{D_e \sinh^4(\alpha r_e)}{\sinh^2(\alpha r)} - \frac{D_e \cosh^4(\alpha r_e)}{\cosh^2(\alpha r)}. \quad (25)$$

To obtain the expectation value $\langle p^2 \rangle_{n,\ell}$, $\langle V \rangle_n$ and $\langle r^{-2} \rangle_n$ we set $v = \mu$, $v = D_e$ and $v = \ell$ respectively to have

$$\langle p^2 \rangle_{n,\ell}^{IGP} = \left(\frac{2n+1+V_{T_4}}{4\mu} \right) \left[\frac{\alpha^2 \hbar^2 \left(\frac{2n+1+V_{T_4}}{4} \right)}{2\mu} + \frac{D_e (1+\cosh(\alpha r_e))^2}{\sqrt{V_{T_2} + \frac{V_{T_3} (\cosh(\alpha r_e) + 2)}{\alpha^2 \hbar^2}}} - \frac{D_e (1-\cosh(\alpha r_e))^2}{\sqrt{V_{T_2} + \frac{V_{T_3} (\cosh(\alpha r_e) - 2)}{\alpha^2 \hbar^2}}} \right], \quad (26)$$

$$\langle V \rangle_{n,\ell}^{IGP} = 1 - \frac{1}{\mu} \left[\left(\frac{2n+1+V_{T_4}}{4} \right) \left(\frac{\mu (1+\cosh^2(\alpha r) - 2\cosh(\alpha r))}{\alpha^2 \hbar^2 \sqrt{V_{T_2} + \frac{V_{T_3} (\cosh(\alpha r) - 2)}{\alpha^2 \hbar^2}}} - \frac{\mu (1+\cosh^2(\alpha r) + 2\cosh(\alpha r))}{\alpha^2 \hbar^2 \sqrt{V_{T_2} + \frac{V_{T_3} (\cosh(\alpha r) + 2)}{\alpha^2 \hbar^2}}} \right) \right], \quad (27)$$

$$\langle r^{-2} \rangle_{n,\ell}^{IGP} = \frac{-\alpha^2}{2(2\ell+1)} \left[\frac{(n+1+V_{T_5})}{\sqrt{V_{T_2} + \frac{V_{T_3}(\cosh(\alpha r) - 2)}{\alpha^2 \hbar^2}}} - \frac{(n+1+V_{T_5})}{\sqrt{V_{T_2} + \frac{V_{T_3}(\cosh(\alpha r) + 2)}{\alpha^2 \hbar^2}}} \right], \quad (28)$$

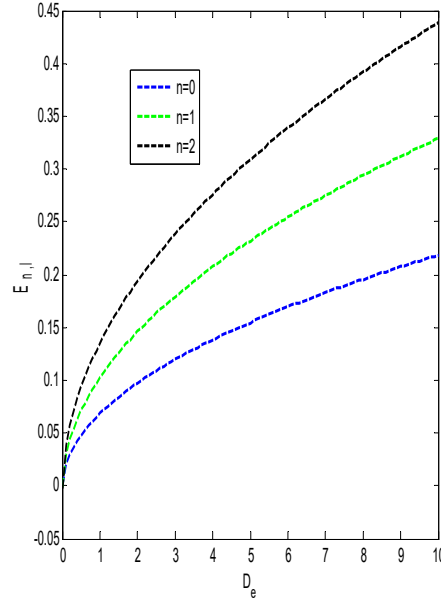


Figure1. Variation of energy against the dissociation energy with $\ell = \mu = \hbar = 1$, $\alpha = 0.05$, $r_e = 0.5$ for the three first quantum states.

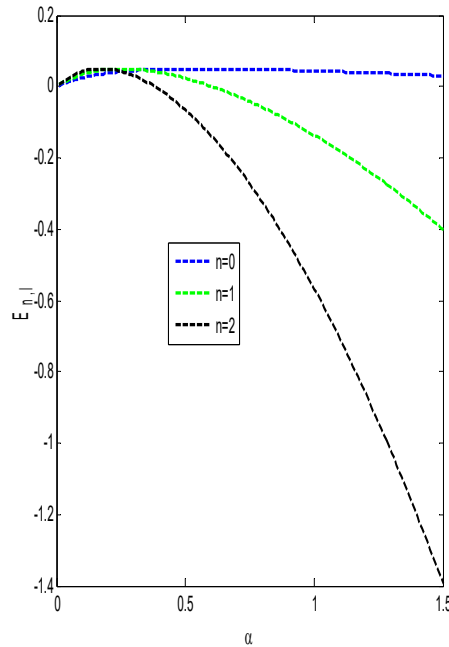


Figure 2: Variation of energy against the screening parameter with $\ell = \mu = \hbar = 1$, $D_e = 0.05$, $r_e = 0.5$ for the first three quantum state.

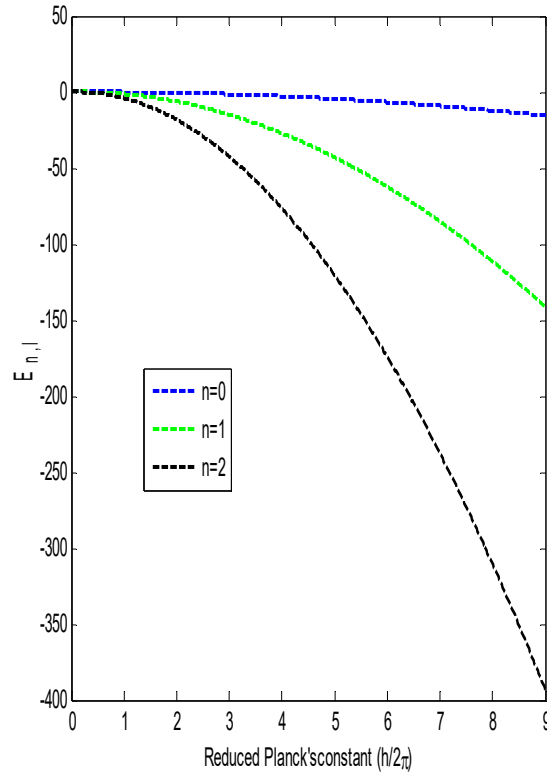


Figure 3: Variation of energy against the reduced Planck's constant with $\ell = \mu = 1$, $D_e = 0.05 r_e = 1.5$ $\alpha = 2.5$ and for the first three quantum state.

Table 1. Spectroscopic parameters for NO, CH, H₂ and N₂.

Parameter	NO	CH	H ₂	N ₂
D_e (eV)	8.043729855	3.947418665	4.7446	11.938193820
r_e (Å)	1.1508	1.1198	0.7416	1.0940
μ (amu)	7.46844100	0.929931	0.50391	7.00335

Table 2. Ro-vibrational energy of the improved generalized Pöschl-Teller potential for various states with $\mu = \hbar = 1$, $D_e = 5$ and $\alpha = 0.15$ for three values of the bond length.

state	$r_e = 0.25$	$r_e = 0.75$	$r_e = 1.50$
2p	0.453730168	0.428186644	0.356430157
3p	0.677071456	0.652162371	0.582178722
3d	0.666614232	0.641186376	0.563690088
4p	0.894787744	0.870513099	0.802302288
4d	0.884597089	0.859816088	0.784279662
4f	0.869315598	0.844314225	0.765511804

Table 3. The ro-vibrational energy spectra of improved generalized Pöschl-Teller potential for NO, CH, H₂ and N₂ molecules for various n and ℓ with $\alpha = 1.25$.

n	ℓ	<i>NO</i>	<i>CH</i>	<i>H₂</i>	<i>N₂</i>
0	0	0.066811645	0.173443495	0.292658796	0.083245290
1	0	0.176052295	0.384092456	0.602341516	0.220841820
	1	0.246411150	0.575103909	0.889270254	0.306602810
2	0	0.284539780	0.588692580	0.900861529	0.357635160
	1	0.354410770	0.774062553	1.177068923	0.442893160
	2	0.446605120	0.954909985	1.434893930	0.557790060
3	0	0.392274095	0.787243870	1.188218834	0.493625320
	1	0.461657220	0.966972359	1.453704885	0.578380320
	2	0.553204425	1.142154817	1.701140761	0.692596400
	3	0.650399120	1.308027722	1.930594194	0.815049810
4	0	0.499255240	0.979746323	1.464413431	0.628812290
	1	0.568150495	1.153833331	1.719178137	0.713064290
	2	0.659050565	1.323350815	1.956224886	0.826599560
	3	0.755553850	1.483694337	2.175659698	0.948319200
	4	0.853408985	1.634726411	2.378465710	1.072414820
5	0	0.605483220	1.166199940	1.729445318	0.763196070
	1	0.673890605	1.334645467	1.973488684	0.846945080
	2	0.764143535	1.498497975	2.200146303	0.959799530
	3	0.859955410	1.653312117	2.409562496	1.080785380
	4	0.957104770	1.798968821	2.602721103	1.204128730
	5	1.054183705	1.935777081	2.780656681	1.327853920

Table 4. Expectation value $\langle p \rangle_n$ of improved generalized Pöschl-Teller for NO, CH, H₂ and N₂ for various quantum states with $\alpha = 1.25$ and $\ell = 0$.

n	<i>NO</i>	<i>CH</i>	<i>H₂</i>	<i>N₂</i>
0	-6.764512182	-0.287558072	2.122543234	-9.985587504
1	-6.351217766	-0.875042212	-0.261014848	-9.479203968
2	-5.927838651	-0.812065632	-0.429354412	-8.961351820
3	-5.494374845	-0.098628330	1.617524541	-8.432031056
4	-5.050826346	1.265269691	5.879622010	-7.891241688
5	-4.597193159	3.279628433	12.35693799	-7.338983702
6	-4.133475278	5.944447895	21.04947250	-6.775257108

Table 5. Expectation value $\langle V \rangle_n$ of improved generalized Pöschl-Teller for NO, CH, H₂ and N₂ for various quantum states with $\alpha = 1.25$ and $\ell = 0$.

n	<i>NO</i>	<i>CH</i>	<i>H₂</i>	<i>N₂</i>
0	0.034222788	0.139312551	0.180800185	0.029007980
1	0.102667459	0.417645942	0.532498685	0.087023247
2	0.171112131	0.695979332	0.884197186	0.145038514
3	0.239556802	0.974312723	1.235895686	0.203053782
4	0.308001474	1.252646113	1.587594187	0.261069050
5	0.376446145	1.530979504	1.939292687	0.319084317
6	0.444890817	1.809312894	2.290991188	0.377099585

Table 6. Expectation value $\langle r^{-2} \rangle_n$ of improved generalized Pöschl-Teller potential for NO, CH, H₂ and N₂ for various quantum states with $\alpha = 1.25$ and $\ell = 0$.

n	NO	CH	H ₂	N ₂
0	-1.781567677	-1.927348488	-4.016970651	-1.973269644
1	-1.802343278	-2.018406647	-4.377990010	-1.994410690
2	-1.823118879	-2.109464806	-4.739009374	-2.015551736
3	-1.843894480	-2.200522964	-5.100028735	-2.036692783
4	-1.864670080	-2.291581124	-5.461048090	-2.057833830
5	-1.885445682	-2.382639282	-5.822067450	-2.078974876
6	-1.906221282	-2.473697441	-6.183086810	-2.100115922

4. Discussion

Figure 1 showed the effect of dissociation energy on energy eigenvalue for the improved generalized Pöschl-Teller potentials. There is a direct variation between the energy and the dissociation energy for the ground state and the first two excited states studied. It is also seen that the more the excited state, the more the energy of the system. In Figure 2, we plotted energy against the screening parameter for the ground state and the first two excited states. The energy is seen to have inverse variation with the screening parameter. As the screening parameter increases, the ground state energy is seen to be greater than the excited states. The variation of the energy against the reduced Planck's constant are shown in Figure 3. The energy of the system and the reduced Planck's constant has inverse variation with each other. We presented the spectroscopic parameters for NO, CH, H₂ and N₂ in Table 1. For all computations in this work, the screening parameter has a constant value $\alpha = 1.25$ except where stated. The energy eigenvalues for 2p, 3p, 3d, 4p, 4d and 4f with three different values of r_e are presented in Table 2. There is an inverse variation between energy and the equilibrium bond length for the improved generalized Pöschl-Teller potential. However, there is a turning point at 4d state. Using Eq. (18) and the spectroscopic parameters in Table 1, we computed numerical results for four molecules (NO, CH, H₂ and N₂) as presented in Tables 3. The variation of energy with the quantum states and angular momentum quantum state is the same for all the molecules. At the ground state, H₂ with the least value of the equilibrium bond length has the highest energy value while NO with the highest reduced mass has the least energy. The momentum expectation value for NO, CH, H₂ and N₂ molecules for different quantum states are presented in Table 4. The momentum expectation value and the quantum state have a direct variation. However, the ground state expectation value for NO and N₂ are higher than the expectation value of the first excited state for CH and H₂. In Table 5, we presented the numerical values of $\langle V \rangle_n$. The expectation value $\langle V \rangle_n$ varies linearly with the quantum states for all the four molecules. In Table 6, there is an inverse variation between the expectation value $\langle r^{-2} \rangle_n$ and the quantum state for all the molecules. However, the expectation value presented for the four molecules are bounded below zero.

5. Conclusion

The solutions of the non-relativistic improved generalized Pöschl-Teller potential models were obtained by applying a suitable approximation scheme to the centrifugal term. The energy equations obtained were used to calculate the expectation values via Hellmann Feynman Theory. Our studies reviews that the behaviour of the molecules interacting in a system are subject to the values of the various spectroscopic parameter of the molecules.

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