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Relativistic Solutions of Dirac Equation with the Molecular Hua Potential in the Spin Symmetry Limit

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Abstract

The study presents solutions of Dirac equation with the Molecular Hua potential energy model using the Formula method. In the non-relativistic limit, the relativistic energy equation becomes the non-relativistic rotation-vibrational energy expression. Numerical results for some molecules are also presented. Interestingly, our results agree with those in literature.

Keywords: Dirac Equation; Molecular Hua Potential; Bound States; Formula Method; Diatomic Molecule

Introduction

The solutions of wave equations are known to be vital in quantum mechanics and related areas of physics. The reason is because the solutions have all the relevant parameters required to evaluate the associated properties of a physical system under consideration. Reports on the nonrelativistic rotational vibrational energies of molecules obtained from solutions of Schrodinger equation in various potential models have been presented [1-5]. It has been established that relativistic interactions are essential for an accurate determination of the rotation-vibration energy spectra of molecules by using quantum mechanical techniques [6]. Recently, by solving Dirac equation with General molecular potential, Improved Tietz potential and Improved Rosen-Morse potential, some authors investigated the relativistic rotation-vibrational energies for $5\,{}^1\Delta_g$ state of Na$_2$ molecule, the $X^2\sum^+$ state of the CP molecule and $3^3\sum_g^+$ state of the Cs$_2$ molecule, and observed that nonrelativistic energies decreases as a result of relativistic effects [7-9].

In this paper, we attempt to investigate the solutions of Dirac equation with the Hua potential energy model. We also explore the relativistic effects of rotational vibrational energies for some molecules.

Recently, Hassanabadi H, et al. [10] studied the Schrodinger equation with Hua potential using the super symmetry quantum mechanics. Also, a similar form of Hua potential has been reported by Hua W, et al. [11], to study the rotation–vibration spectrum of different molecules. The Hua potential can be used in describing the energy levels of diatomic molecules, hence motivation for this work. The Hua potential is expressed as [12,13].

$$U_H = V_0\left(\frac{1-e^{-b_h(r-r_e)}}{1-qe^{-b_h(r-r_e)}}\right)^2, \quad b_h=\beta\left(1-c_h\right), \quad (1)$$

where V_0, r_e, q and β are respectively the potential depth, bond length, deformation parameter and Morse constant. The work is drafted as: The Formula method is presented in Section 5, Section 6 is a review of Dirac equation under spin symmetry [14]. The bound state solutions are given in Section 7. Discussion comes in Section 9. Finally, conclusion is presented in Section 10.

Formula Method

The Formula method is applied by considering the equation.

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

The energy and the wave function are derived respectively, from the equations

$$\left[\frac{\alpha_4^2-\alpha_5^2-\left[\frac{1-2n}{2}-\frac{1}{2\alpha_3^2}\left(\alpha_2-\sqrt{(\alpha_3-\alpha_2)^2-4\xi_1}\right)\right]^2}{2\left[\frac{1-2n}{2}-\frac{1}{2\alpha_3^2}\left(\alpha_2-\sqrt{(\alpha_3-\alpha_2)^2-4\xi_1}\right)\right]}\right]^2-\alpha_5^2=0,\alpha_3\neq 0 \tag{3}$$

$$\psi(s)=N_n s^{\alpha_4}\left(1-\alpha_3 s\right)^{\alpha_5}{}_2F_1\left(-n,n+2(\alpha_4+\alpha_5)+\frac{\alpha_2}{\alpha_3}-1;2\alpha_4+\alpha_1;\alpha_3 s\right), \tag{4}$$

where

$$\left.\begin{aligned}\alpha_4&=\frac{(1-\alpha_1)+\sqrt{(1-\alpha_1)^2-4\xi_3}}{2}\\ \alpha_5&=\frac{1}{2}+\frac{\alpha_1}{2}-\frac{\alpha_2}{2\alpha_3}+\sqrt{\left(\frac{1}{2}+\frac{\alpha_1}{2}-\frac{\alpha_2}{2\alpha_3}\right)^2-\left(\frac{\xi_1}{\alpha_3^2}+\frac{\xi_2}{\alpha_3}+\xi_3\right)}\end{aligned}\right\}, \tag{5}$$

are constants and ${}_2F_1$ is the Hypergeometric function.

A special case where $\alpha_1=1,\alpha_2=\alpha_3=q$, we put forward a simplified energy equation from Equation (3)

$$\begin{aligned}&q\sqrt{-\xi_3}\left(q+\sqrt{q^2-4\left(\xi_1+q\xi_2+q^2\xi_3\right)}+2qn\right)=q^2\xi_3-\xi_1-q^2n(n+1)\\&-qn\sqrt{q^2-4\left(\xi_1+q\xi_2+q^2\xi_3\right)}-\left(\frac{q}{2}+\frac{1}{2}\sqrt{q^2-4\left(\xi_1+q\xi_2+q^2\xi_3\right)}\right)^2\end{aligned} \tag{6}$$

Dirac Equation

The Dirac equation with scalar, *S(r)* and vector potential, *V(r)* is given as

$$\left.\begin{aligned}&\hat{H}_D\Psi(r)=E_{vk}\Psi(r)\\&\hat{H}_D=c\alpha.\vec{p}+\beta(\mu c^2+S(r))+V(r)\end{aligned}\right\}, \tag{7}$$

where $\mu, E_{vk}, \vec{p}=-i\hbar\vec{\nabla}$ are the reduced mass, relativistic energy, and momentum operator respectively. α,β are the 4×4 Dirac matrices given by

$$\alpha=\begin{pmatrix}0&\sigma_i\\\sigma_i&0\end{pmatrix},\quad \beta=\begin{pmatrix}I&0\\0&-I\end{pmatrix}, \tag{8}$$

Where *I* is the 2×2 matrix and σ_i is the Pauli matrices given as

$$\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix} \tag{9}$$

The spinor, $\Psi(r)$ can be written as

$$\Psi(r)=\frac{1}{r}\begin{pmatrix}F_{n\kappa}(r)&Y_{jm}^{l}(\theta,\phi)\\iG_{n\kappa}(r)&Y_{jm}^{\tilde{l}}(\theta,\phi)\end{pmatrix}, \tag{10}$$

with $F_{n\kappa}(r)$ and $G_{n\kappa}(r)$ as the upper and lower components of the Dirac spinors. $Y_{jm}^{l}(\theta,\phi)$ is the spherical harmonic of the spin component and $Y_{jm}^{\tilde{l}}(\theta,\phi)$ is the spherical harmonic of the pseudo spin component. l and $\tilde{l}$ are the orbital and pseudo-orbital quantum numbers, while κ and *m* are the spin-orbit coupling operator and projection on z-axis. If the spinor in Equation (10) is used, we deduce the following coupled radial differential equations from the Dirac equation

$$\left.\begin{aligned}\left(\frac{d}{dr}-\frac{\kappa}{r}\right)G_{n\kappa}(r)&=\frac{\left(\mu c^2-E_{vk}+\Sigma(r)\right)}{\hbar c}F_{n\kappa}(r)\\\left(\frac{d}{dr}+\frac{\kappa}{r}\right)F_{n\kappa}(r)&=\frac{\left(\mu c^2+E_{vk}-\Delta(r)\right)}{\hbar c}G_{n\kappa}(r)\end{aligned}\right\} \tag{11}$$

If $F_{n\kappa}(r)$ is eliminated in favor of $G_{n\kappa}(r)$, we derive two uncoupled differential equations of the form

$$\frac{d^2F_{n\kappa}(r)}{dr^2}-\frac{\kappa(\kappa+1)}{r^2}F_{n\kappa}(r)-\frac{(\mu c^2-E_{\nu\kappa}+\Sigma(r))(\mu c^2+E_{\nu\kappa}-\Delta(r))}{\hbar^2c^2}F_{n\kappa}(r)$$
$$+\frac{\frac{d\Delta(r)}{dr}\left(\frac{d}{dr}+\frac{\kappa}{r}\right)F_{n\kappa}(r)}{(\mu c^2+E_{\nu\kappa}-\Delta(r))}=0,$$

(12)

$$\frac{d^2G_{n\kappa}(r)}{dr^2}-\frac{\kappa(\kappa-1)}{r^2}G_{n\kappa}(r)-\frac{(\mu c^2-E_{\nu\kappa}+\Sigma(r))(\mu c^2+E_{\nu\kappa}-\Delta(r))}{\hbar^2c^2}G_{n\kappa}(r)$$
$$-\frac{\frac{d\Sigma(r)}{dr}\left(\frac{d}{dr}-\frac{\kappa}{r}\right)G_{n\kappa}(r)}{(\mu c^2-E_{\nu\kappa}+\Sigma(r))}=0,$$

(13)

where $\kappa(\kappa+1)=l(l+1),\kappa(\kappa-1)=\tilde{l}(\tilde{l}+1),\Delta(r)=V(r)-S(r),\Sigma(r)=V(r)+S(r)$.

Bound State Solutions

In spin symmetry, $\frac{d\Delta(r)}{dr}=0;\ \Delta(r)=\text{constant}$. In the non-relativistic limit, Equation (12) reduces to a Schrodinger form with $2V(r)$ in light of the exact symmetry $V(r) = S(r)$. Adopting a proposal by Alhaidari AD, et al. [15], and setting $S(r) = U_H$, $V(r) = C_s + U_H(r)$, expansion of Equation (12) gives

$$\frac{d^2F_{n\kappa}(r)}{dr^2}+\left(-\frac{(\mu c^2+E_{\nu\kappa}-C_s)}{\hbar^2c^2}\left(\frac{C_s}{2}+U_H\right)-\frac{\kappa(\kappa+1)}{r^2}\right)F_{n\kappa}(r)$$
$$=-\frac{\left(E_{\nu\kappa}^2-\mu^2c^4+C_s\left(\mu c^2-E_{\nu\kappa}\right)\right)}{\hbar^2c^2}F_{n\kappa}(r).$$

(14)

To solve Equation (14), we adopt an approximation

$$\frac{1}{r^2}\approx\frac{1}{r_e}\left(D_0+D_1\frac{e^{-b_h(r-r_e)}}{1-qe^{-b_h(r-r_e)}}+D_2\frac{e^{-2b_h(r-r_e)}}{\left(1-qe^{-b_h(r-r_e)}\right)^2}\right)$$

(15)

The approximation is only valid for $qe^{b_hr_e}\geq1$. We can set $\alpha=b_hr_e, x=\frac{r-r_e}{r_e}$ in Equation (14) and expand up to x^2 term, we have

$$\left.\begin{aligned}D_0&=1+\frac{1-q}{\alpha}\left(\frac{3}{\alpha}(1-q)-(3+q)\right)\\D_1&=\frac{2}{\alpha}(1-q)^2\left((2+q)-\frac{3}{\alpha}(1-q)\right)\\D_2&=\frac{(1-q)^3}{\alpha}\left(\frac{3}{\alpha}(1-q)-(1+q)\right)\end{aligned}\right\}$$

(16)

Substituting Equation (15) in Equation (14) and rearranging gives

$$\frac{d^2F_{n\kappa}(r)}{dr^2}+\left(\begin{aligned}&-\varepsilon_1\left(\frac{C_s}{2}+V_0\left(\frac{1-e^{-b_h\left(r-r_e\right)}}{1-qe^{-b_h\left(r-r_e\right)}}\right)^2\right)+\varepsilon_2\\&-\frac{\kappa(\kappa+1)}{r_e^2}\left(D_0+D_1\frac{e^{-b_h\left(r-r_e\right)}}{1-qe^{-b_h\left(r-r_e\right)}}+D_2\frac{e^{-2b_h\left(r-r_e\right)}}{\left(1-qe^{-b_h\left(r-r_e\right)}\right)^2}\right)\end{aligned}\right)F_{n\kappa}(r)=0,$$

(17)

where

$$\left.\begin{aligned}\varepsilon_1&=\frac{(\mu c^2+E_{\nu\kappa}-C_s)}{\hbar^2c^2}\\\varepsilon_2&=\frac{\left(E_{\nu\kappa}^2-\mu^2c^4+C_s\left(\mu c^2-E_{\nu\kappa}\right)\right)}{\hbar^2c^2}\end{aligned}\right\}$$

(18)

To solve Equation (17), we use the transformation $s=e^{-b_h(r-r_e)}$, which gives

$$\frac{d^2F_{n\kappa}(s)}{ds^2}+\frac{(1-qs)}{s(1-qs)}\frac{dF_{n\kappa}(s)}{ds}+\frac{Ps^2+Qs+R}{s^2(1-qs)^2}F_{n\kappa}=0,$$

(19)

where,

$$\left.\begin{aligned} P &= \frac{-1}{b_h}\left(q^2\varepsilon_2 + \frac{q\kappa(\kappa+1)D_1}{r_e^2} - \frac{\kappa(\kappa+1)D_2}{r_e^2} - \frac{q^2\varepsilon_1 C_s}{2} - \varepsilon_1 V_0 - \frac{q^2\kappa(\kappa+1)D_0}{r_e^2}\right) \\ Q &= \frac{1}{b_h}\left(q\varepsilon_1 C_s + 2\varepsilon_1 V_0 - 2q\varepsilon_2 + \frac{2q\kappa(\kappa+1)D_0}{r_e^2} - \frac{\kappa(\kappa+1)D_1}{r_e^2}\right) \\ R &= \frac{-1}{b_h}\left(\varepsilon_2 - \frac{\varepsilon_1 C_s}{2} - \varepsilon_1 V_0 - \frac{\kappa(\kappa+1)D_0}{r_e^2}\right) \end{aligned}\right\}.$$

(20)

The constants are calculated from Equation (5) as

$$\left.\begin{aligned} &\alpha_1 = 1, \alpha_2 = \alpha_3 = q, \alpha_4 = \sqrt{-R}, \\ &\alpha_5 = \frac{1}{2} + \frac{1}{2q}\sqrt{\frac{4}{b_h^2}\left(\varepsilon_1 V_0 (q-1)^2 + \frac{\kappa(\kappa+1)D_2}{r_e^2}\right) + q^2}, \end{aligned}\right\}.$$

(21)

Using Eqs. (6) and (4), the relativistic energy and unnormalized eigen function are derived as

$$\left.\begin{aligned} &\frac{\left(E_{\nu\kappa}^2 - \mu^2c^4 + C_s\left(\mu c^2 - E_{\nu\kappa}\right)\right)}{\hbar^2c^2} = \frac{(\mu c^2 + E_{\nu\kappa} - C_s)}{\hbar^2c^2}\left(\frac{C_s}{2} + V_0\right) + \frac{\kappa(\kappa+1)D_0}{r_e^2} \\ &-b_h^2\left[\frac{\frac{1}{b_h^2}\left(\frac{\kappa(\kappa+1)D_1}{r_e^2} + \frac{2V_0(\mu c^2 + E_{\nu\kappa} - C_s)}{\hbar^2c^2}(q-1)\right) + \frac{q}{2} + qn(n+1) + \left(n+\frac{1}{2}\right)\sqrt{\frac{4}{b_h^2}\left(V_0\frac{(\mu c^2 + E_{\nu\kappa} - C_s)}{\hbar^2c^2}(q-1)^2 + \frac{\kappa(\kappa+1)D_2}{r_e^2}\right) + q^2}}{q + 2qn + \sqrt{\frac{4}{b_h^2}\left(V_0\frac{(\mu c^2 + E_{\nu\kappa} - C_s)}{\hbar^2c^2}(q-1)^2 + \frac{\kappa(\kappa+1)D_2}{r_e^2}\right) + q^2}}\right]^2 \end{aligned}\right\}$$

(22)

$$F_{n\kappa}(r) = N_{n\kappa}s^{\sqrt{-R}}(1-qs)^{\alpha_5}\,{}_2F_1\left(-n, n+2\left(\sqrt{-R}+\alpha_5\right); 2\sqrt{-R}+1, qs\right), \quad (23)$$

$N_{n\kappa}$ is a normalization condition.

Non-Relativistic Limit

The non-relativistic limit is obtained in the exact symmetry condition (C_s = 0) by using the mapping $\mu c^2 + E_{vk} \to 2\mu c^2, E_{vk} - \mu c^2 \to E_{vJ}$ on Equation (22) to obtain the non-relativistic rotational-vibrational energy of the molecular Hua potential for the case of the unaligned spin ($\kappa = J$) in the form

$$E_{\nu J} = V_0 + \frac{J(J+1)D_0\hbar^2}{2\mu r_e^2} - \frac{b_h^2\hbar^2}{2\mu}\left[\frac{\frac{J(J+1)D_1}{b_h^2r_e^2} + \frac{4\mu V_0}{b_h^2\hbar^2}(q-1) + \frac{q}{2} + q\nu(\nu+1) + \left(\nu+\frac{1}{2}\right)\sqrt{q^2 + \frac{8\mu V_0}{b_h^2\hbar^2}(q-1)^2 + \frac{4J(J+1)D_2}{b_h^2r_e^2}}}{q + 2q\nu + \sqrt{q^2 + \frac{8\mu V_0}{b_h^2\hbar^2}(q-1)^2 + \frac{4J(J+1)D_2}{b_h^2r_e^2}}}\right]^2.$$

(24)

Equation (24) is the same as Equation (14) in Falaye BJ [13].

Discussions

In the present work, we have considered $Cl_2(X^1\Sigma_g^+)$, $I_2(X(O_g^+))$ and HF($X^1\Sigma^+$) molecules. The parameters for the molecules were taken from Pekeris CL [18], Khodja A, et al. [19] and presented in (Table 1). The relativistic and the non-relativistic energy expressions are given in Equations (22) and (24), respectively (Table 2) contains values of the constants associated with the Pekeris approximation from Equation (16). (Tables 3-5) show the numerical results of the non-relativistic energies of the $Cl_2(X^1\Sigma_g^+)$, $I_2(X(O_g^+))$ and HF($X^1\Sigma^+$) molecules, respectively. These results appear to agree with those in literature.

Molecule	$^a q$	$^b b_h(Å^{-1})$	$^b r_e(Å)$	$^b V_0(cm^{-1})$	$^b \mu/10^{23}(g)$
$Cl_2(X^1\Sigma_g^+)$	0.012624658	2.200354	1.987	20276.44	2.924
$I_2(X(O_g^+))$	0.003478812	2.12343	2.666	12547.3	63.4522(amu)
HF($X^1\Sigma^+$)	0.168490116	1.94207	0.917	49382	0.16

Table 1: Spectroscopic parameters used in this study.

^{a}Minimum values calculated from $q = e^{-b_h r_e}$

^{b}Taken from Tezcan C, Alhaidari AD, Ikot AN, et al. [14-16].

Molecule	D_0	D_1	D_2
Cl2($X^1\Sigma_g^+$)	0.4726477323	0.5954208116	-0.07378279326
I2($X(O_g^+)$)	0.5642559227	0.5176197442	-0.08310143541
HF($X^I\Sigma^+$)	0.1746151145	0.5961507758	-0.07755614766

Table 2: Calculated values of the approximation constants.

v	*J*	Present	Okorie US, et al. [16]
0	0	-2.489532120	-2.548719684
	1	-2.488972028	
	2	-2.487851970	
	3	-2.486172200	
	4	-2.483933104	
1	0	-2.452017290	-2.618990605
	1	-2.451523262	
	2	-2.450535582	
	3	-2.449055005	
	4	-2.447082687	
2	0	-2.429420043	-2.690130852
	1	-2.428991768	-2.689566057
	2	-2.428135839	
	3	-2.426853509	
	4	-2.425146688	
3	0	-2.421580695	-2.762137335
	1	-2.421217671	-2.761572143
	2	-2.420492485	-2.760441727
	3	-2.419406874	
	4	-2.417963488	
4	0	-2.428342382	-2.835006978
	1	-2.428043924	-2.834441374
	2	-2.427448103	-2.833310161
	3	-2.426557126	-2.831613265
	4	-2.425374358	

Table 3: Ro-Vibrational energies in *eV* for Cl_2 molecule.

N	*J*	Present	Oluwadare OJ, et al. [2]
0	0	-1.547325482	−1.542189775
	1	-1.547285176	−1.542169077
	2	-1.547204637	−1.542127681
	3	-1.547084012	−1.542065587
	4	-1.546923521	−1.541982794
1	0	-1.532622202	−1.515545095
	1	-1.532580947	−1.515524411
	2	-1.532498497	−1.515483043
	3	-1.532374975	−1.515420991
	4	-1.532210565	−1.515338255
2	0	-1.520551523	−1.489134196
	1	-1.520509328	−1.489113527
	2	-1.520424988	−1.489072187
	3	-1.5201303161	−1.489010177
	4	-1.520130316	−1.488927498
3	0	-1.511109275	−1.462957037
	1	-1.511066150	−1.462936382
	2	-1.510979937	−1.462895070
	3	-1.510850711	−1.462833103
	4	-1.510678586	−1.462750480
4	0	-1.504291302	
	1	-1.504247253	
	2	-1.504159181	
	3	-1.504027137	
	4	-1.503851199	

Table 4: Ro-Vibrational energies for I_2 molecule.

v	*J*	Present	Roy AK, et al. [17]
0	0	-5.996097728	−5.8687195228
	1	-5.996097728	−5.8636625262
	2	-5.917092019	−5.8535547327
	3	-5.861617074	
	4	-5.818770714	
1	0	-5.898378354	
	1	-5.889684644	
	2	-5.878348924	
	3	-5.875112697	
	4	-5.893229709	
2	0	-5.950763660	
	1	-5.957329774	
	2	-5.974864982	
	3	-6.011233988	
	4	-6.011233988	
3	0	-6.117534046	
	1	-6.135982061	
	2	-6.176129874	
	3	-6.243814806	
	4	-6.346374801	
4	0	-6.375922588	
	1	-6.403980106	
	2	-6.462510722	
	3	-6.555867128	
	4	-6.689554994	

Table 5: Ro-Vibrational energies in *eV* for HF molecule.

In (Figure 1), we plot the shape of molecular Hua potential for the selected diatomic molecules. The figure gives an insight of the characteristics of the the Hua potential. (Figures 2-7) are various plots showing variation of rotational-vibrational energy against various parameters for the diatomic molecules. A monotonic increase in the energy is seen In (Figure 2) for the molecules as the quantum number, *v*, and increases. In (Figure 3) the energy is seen to increase with rotational quantum number, ***J***. For Cl_2 molecule, the increase is more visible than in I_2 and HF molecules. The Cl_2 atom appears to shift to higher values than the I_2 and HF molecules. (Figure 4) indicates a progressive increase in energy as the deformation parameter, *q*, and increases. In (Figure 5), the energy of the diatomic molecules is observed to increase as the potential depth, V_0, increases. In (Figure 6), we observe an increase in energy of the Hua potential as the parameter, b_h, increases for the molecules. In (Figure 7), the energy of the diatomic molecules first decreases as the molecular bond length increases between 0 to 0.04 for the I_2 and HF molecules; it then maintains a constant value with increase in the molecular bond length. For the Cl_2 molecule, the energy first decreases as the molecular bond length increases between 0 to 0.14.

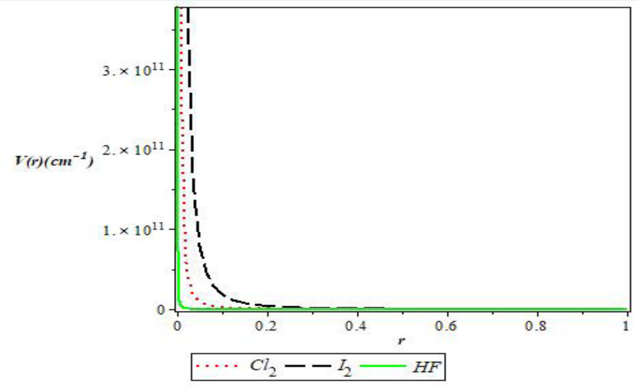

Figure 1: Variation of the Molecular Hua potential with internuclear distance.

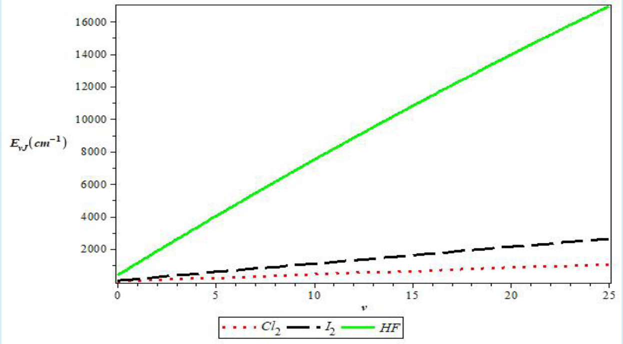

Figure 2: Variation of non-relativistic energy of the Molecular Hua potential with the vibrational quantum number for the selected diatomic molecules with J=1.

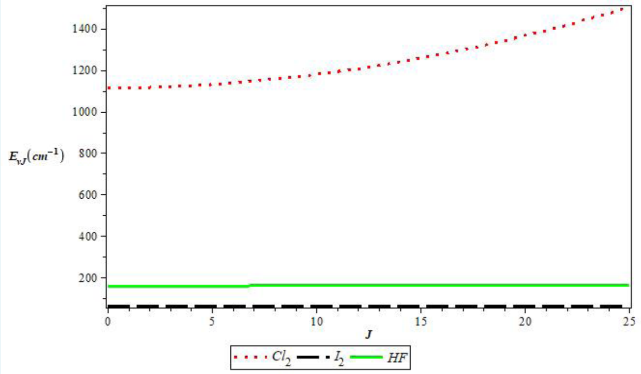

Figure 3: Variation of non-relativistic energy of the Molecular Hua potential with the rotational quantum number for the selected diatomic molecules with ν=1.

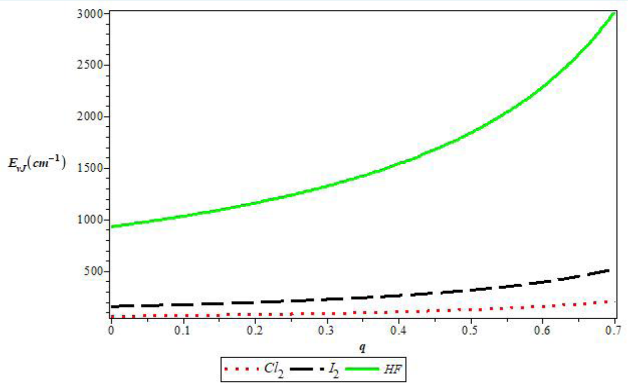

Figure 4: Variation of non-relativistic energy of the Molecular Hua potential with the deformation parameter for the selected diatomic molecules with J=1 and ν=1.

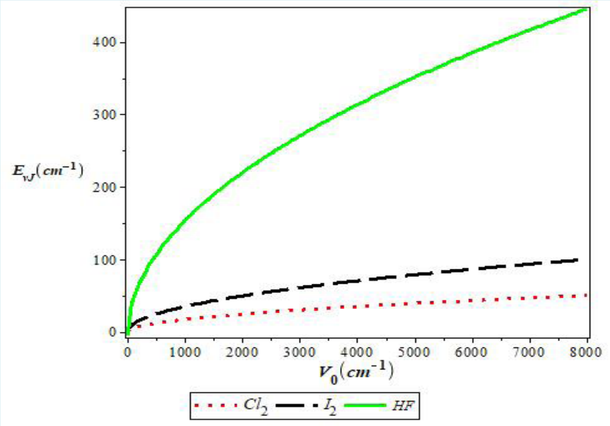

Figure 5: Variation of non-relativistic energy of the Molecular Hua potential with the potential depth for the selected diatomic molecules with J=1, ν=1.

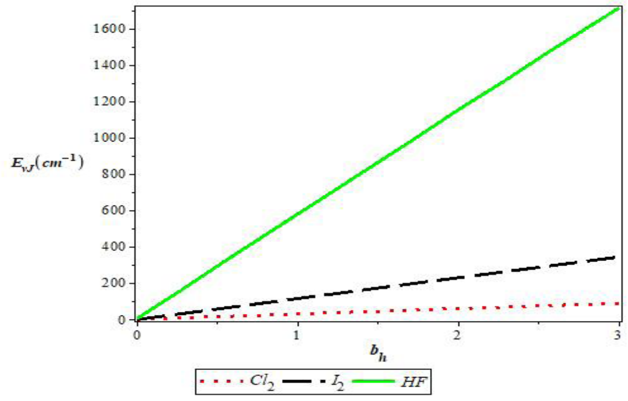

Figure 6: Variation of non-relativistic energy of the Molecular Hua potential with bh for the selected diatomic molecules with J=1, ν=1.

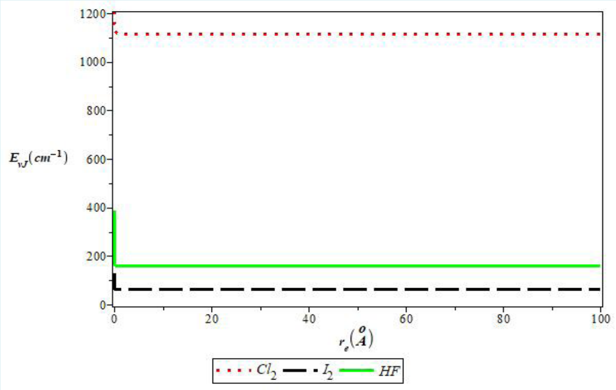

Figure 7: Variation of non-relativistic energy of the Molecular Hua potential with molecular bond length for the selected diatomic molecules with J=1, ν=1.

Conclusion

In this work, we present solutions of Dirac equations with Hua potential energy model using the Formula method. Using the spin symmetry and the Pekeris form of approximation, we evaluated the relativistic rotation-vibrational energy equation for diatomic molecules under the Hua potential. In the nonrelativistic limit, the relativistic energy expression becomes the nonrelativistic rotation-vibrational energy equation. Numerical results are also computed for the selected molecules. The results show considerable agreement with reports in literature. This study can be applied in molecular physics, spectroscopy and other fields of science.

Declaration of Interest

The authors declare that they have no known conflict of interest.

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