Eigensolution techniques, their applications and Fisher's information entropy of the Tietz–Wei diatomic molecular model

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Abstract

In this study, the approximate analytical solutions of Schrödinger, Klein–Gordon and Dirac equations under the Tietz–Wei (TW) diatomic molecular potential are represented by using an approximation for the centrifugal term. We have applied three types of eigensolution techniques: the functional analysis approach, supersymmetry quantum mechanics and the asymptotic iteration method to solve the Klein–Gordon, Dirac and Schrödinger equations, respectively. The energy eigenvalues and the corresponding eigenfunctions for these three wave equations are obtained, and some numerical results and figures are reported. It has been shown that these techniques yielded exactly the same results. some expectation values of the TW diatomic molecular potential within the framework of the Hellmann–Feynman theorem have been presented. The probability distributions that characterize the quantum mechanical states of TW diatomic molecular potential are analyzed by means of complementary information measures of a probability distribution called Fisher's information entropy. This distribution has been described in terms of Jacobi polynomials, whose characteristics are controlled by quantum numbers.

Keywords: Schrödinger equation, Klein–Gordon equation, Dirac equation, eigensolution techniques, Fisher's information entropy

1. Introduction

In recent decades, solutions of wave equations in relativistic and non-relativistic quantum mechanics have received great attention. Whether in the relativistic or non-relativistic regimes, the exact solutions are only possible for some special cases of interactions due to the inverse square centrifugal term appearing in the realistic three-dimensional space. Therefore, for many potential models one has to use some approximations for the centrifugal term. Among these approximations, the frequently used Pekeris approximation [1, 2] introduces an exponential approximation to the centrifugal barrier. The Tietz–Wei (TW) diatomic molecular potential is one of those

potentials that cannot be exactly solved. This potential was proposed as an intermolecular potential and is one of the best potential models considered to describe the vibrational energy of diatomic molecules [3, 4].

In one of the interesting works of Gordillo-Vizquez and Kunc [5], they derived radial probability distributions of diatomic molecules in excited rotational–vibrational states using the Bohr–Sommerfeld quantization rule and the Hamilton–Jacoby theory. They compared the obtained semi-classical distributions for the rotating Morse and TW oscillators, in a broad range of rotational and vibrational quantum numbers, with one another and with quantum-mechanical distributions obtained from a numerical solution to the

Schrödinger equation (SE) using a Rydberg–Klein–Rees (RKR) potential. In recent years, Hamzavi *et al* [6] have presented energy eigenvalues and corresponding eigenfunctions in closed form. The authors present some remarks and numerical results for some diatomic molecules. Shortly thereafter, the bound state solutions of the relativistic Klein–Gordon equation with the TW diatomic molecular potential have been presented for the s-wave by Sun and Dong [7]. It is shown that the solutions can be expressed by generalized hypergeometric functions.

Apart from the works done on TW diatomic molecular potential, many authors have solved the SE in various potential fields [8–22]. Despite several worthy attempts at solving the SE with several model potentials, the basic information-theoretic quantities remain to be computed. This is because of the lack of knowledge in the information-theoretic properties of special functions. In this paper, our aim is to solve the non-relativisitic SE under the TW diatomic molecular potential via the AIM by considering the Pekeris approximation. We have also calculated some expectation values corresponding to the TW diatomic molecular potential using the Hellmann–Feynman theorem (HFT).

We also study the TW diatomic molecular potential within the framework of relativistic Klein–Gordon and Dirac equations. It is worth noting that the Klein–Gordon equation correctly describes the spinless pion[5]. The Dirac equation provided a description of elementary spin-1/2 particles, such as electrons, consistent with both the principles of quantum mechanics and the theory of special relativity, and made relativistic corrections to quantum mechanics [23, 24]. These relativistic equations have received a lot of interest from several authors in both theoretical physics, nuclear physics and related areas. In this study, these relativistic equations with TW diatomic molecular potential shall be studied extensively.

Furthermore, probability distributions are analyzed by means of complementary information measures of a probability distribution known as Fisher's information entropy. Given a normalized-to-unity (probability) density ρ on $\mathfrak{R}$, we can define several functions of ρ measuring the uncertainty or information content associated with this density. Thus, Fisher's information is a derivative functional of the density, so that it is very sensitive to local rearrangements of ρ. Applications to a large variety of problems in theoretical physics have received a strong impulse when it was realized that the spatial distribution of the single-particle probability density $\rho(\vec{r})$ of a many-particle system, which is the basic variable of the density functional theory [25–28] can be quantitatively measured by its translationally invariant Fisher information in a different and complementary manner as the Shannon entropy. Both quantities characterize the information theoretic content of the density $\rho(\vec{r})$ that describes the physical state under consideration [28]. Fisher information has been used in the current study to analyze probability

distribution of the approximate solution obtained for the TW diatomic molecular potential.

The organization of this paper is as follows: in the next section we briefly introduce FAA, SUSYQM and AIM. In section 3, the non-relativistic solutions of the SE with the TW diatomic molecular potential are presented and some expectation values are reported. We have obtained the energy eigenvalues and the wave functions of the Klein–Gordon and Dirac equations in section 4. Information-theoretic measures for TW diatomic molecular potential are given in section 5. Section 6 present numerical discussions, and finally, our conclusion is given in section 7.

2. Eigensolution techniques

In quantum mechanics, while solving relativistic and non-relativistic wave equations in the presence of some typical central or non-central potential model, we often come across a differential equation of the form

$$
\Psi''(s) + \frac{(k_1 - k_2 s)}{s(1 - k_3 s)} \Psi'(s)
$$
$$
+ \frac{(As^2 + Bs + C)}{s^2(1 - k_3 s)^2} \Psi(s) = 0, \tag{1}
$$

after which an appropriate coordinate transformation of the form $s = s(r)$ has been used. In other to find energy eigenvalues and the wave function (eigensolution) of the second-order homogeneous linear differential equations of the above form, there have been several eigensolution techniques developed to exactly solve the quantum systems. Some of these techniques include the AIM [29, 30, 33–50], the Feynman integral formalism [51–53], FAA [54–59], the exact quantization rule method [60–65], the proper quantization rule [66, 67], the Nikiforov–Uvarov method [68–78], SUS-YQM [79–91, 91–95], the ansatz method [96–99], etc.

The beauty about these techniques is that when they are applied to solve equations of the form (1), they yield exactly the same eigensolution results, despite the fact that the calculation approach varies from one technique to the other. In this work, we focus our attention on three of these techniques: FAA, SUSYQM and AIM. We apply AIM to find the eigensolution of the non-relativistic SE. Furthermore, the eigensolutions of the relativistic Klein–Gordon and Dirac equations are obtained via FAA and SUSYQM, respectively. We have demonstrated that the three techniques yield exactly the same results.

FAA, also called 'the traditional method' by some authors, has been introduced for solving equations of the form (1) ever since the birth of quantum mechanics. In this approach, one transforms the equation of form (1) to the form of a hypergeometric equation $_2F_1(a, b; c; s)$ via an appropriate transformation by considering the singularity points of the differential equation within the framework of the Frebenius theorem. The eigensolutions are obtained from the properties of the hypergeometric functions on the condition

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[5] The pion is a composite particle; no spinless elementary particles have yet been found, although the Higgs boson is theorized to exist as a spin-zero boson, according to the Standard Model.
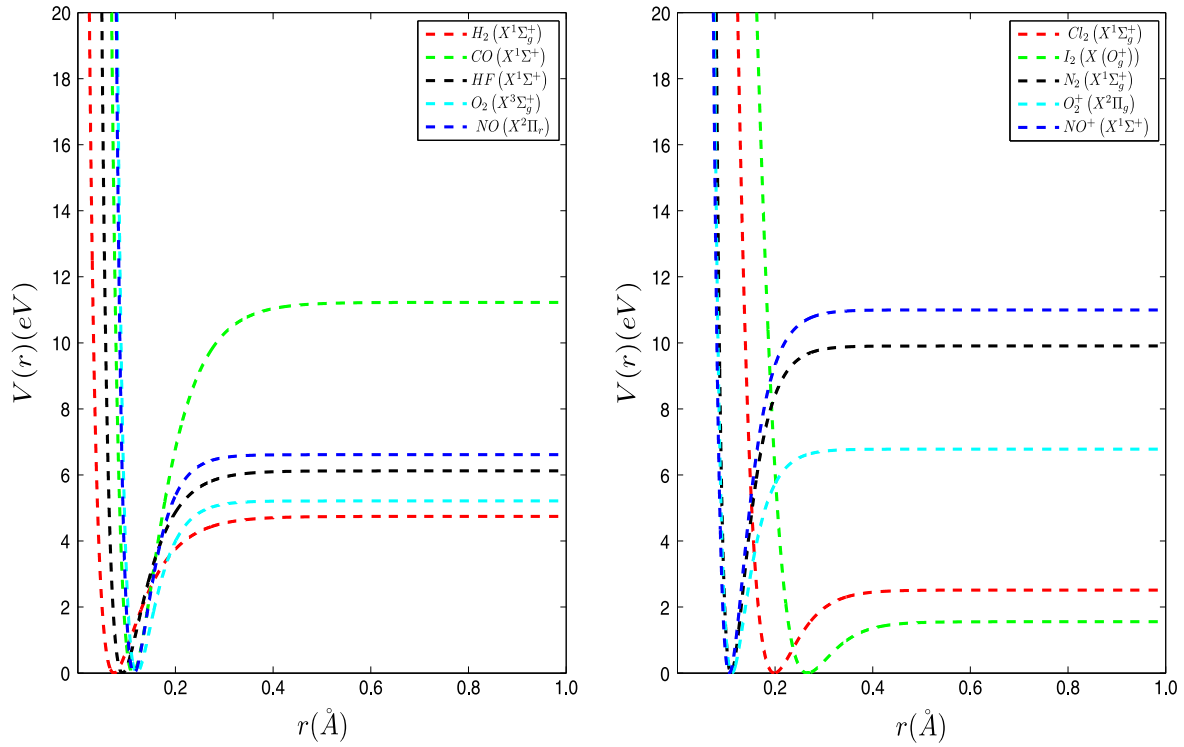
Figure 1. Shape of TW diatomic molecular potential for different diatomic molecules.

that the series $_2F_1(a, b; c; s)$ approaches infinity unless a is a negative integer (i.e. $a = -n$). This method has been employed by many researchers to obtain an eigensolution of quantum mechanical problems in both the relativistic and the non-relativistic case [54–59].

Over the last few decades, the ideas of SUSYQM have been applied to many quantum mechanical problems (both in the non-relativistic and non-relativistic case). In 1982, the path integral formulation of SUSYQM was first given by Salomonson and van Holten [83]. Thereafter, by using SUSY methods, some authors revealed that the tunneling rate through double-well barriers could be accurately determined [100, 101–103]. Recently, there have been many efforts to extend the ideas of SUSYQM to higher-dimensional systems as well as to systems with large numbers of particles, with a motivation of understanding the potential problems of widespread interest in nuclear, atomic, statistical and condensed matter physics [79–94]. The concept of shape-invariant potential was introduced within the framework of SUSYQM in 1983 by Gendenshtein [91].Gendenshtein shows that for any shape-invariant potential, the energy eigenvalue spectra could be obtained algebraically. Very recently, the bound-state spectra for some potentials with unbroken and broken supersymmetry have been investigated by the quantization condition of AIM [104].

The asymptotic iteration method (AIM) to find an eigensolution for an equation of the form (1) was introduced by Ciftci *et al* [31, 32] in 2003 and 2005. Since then, it has been used in many physical systems to obtain the whole spectra [29–50]. The beauty of the method is that it reproduces exact solutions of many exactly solvable quantum

systems and also gives accurate results for the non-solvable potentials such as sextic oscillator, deformed Coulomb potential, etc.

In the subsequent sections, we apply these three techniques to solve various quantum mechanical problems and show that they yield exactly the same results.

3. Non-relativistic solutions of SE with the TW diatomic molecular potential

It is well known that exact solutions play an important role in quantum mechanics since they contain all the necessary information regarding the quantum system under consideration. In this section we obtain the bound-states solution of the SE for the TW diatomic molecular potential. For this purpose, we write the SE in three dimension as

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

where n and ℓ denote the radial and orbital angular momentum quantum numbers, r is the internuclear separation of the diatomic molecules, and $E_{n\ell}$ the bound-state energy eigenvalues. The μ and $V(r)$ represent the reduced mass and interaction potential, respectively. By taking $\psi(r, \theta, \phi) = r^{-1}U_{n\ell}(r)Y_{\ell m}(\theta, \phi)$, we can separate the above SE via the variable separable technique. Thus, we obtain the following

radial SE:

$$\frac{\mathrm{d}^2 U_{n\ell}(r)}{\mathrm{d}r^2} + \frac{2\mu}{\hbar^2}\big(E_{n\ell} - V(r)\big)U_{n\ell}(r) = 0. \tag{3}$$

3.1. Any ℓ–state solution of the radial SE with the TW diatomic molecular potential: asymptotic iteration method

The TW diatomic molecular potential we examine in this study is defined as [5–7, 105]

$$V(r) = D\left[\frac{1 - \mathrm{e}^{-b_h(r - r_e)}}{1 - c_h \mathrm{e}^{-b_h(r - r_e)}}\right]^2, \tag{4}$$

with $b_h = \beta(1 - c_h)$, r_e is the molecular bond length, β is the Morse constant, D is the potential well depth and c_h is an optimization parameter obtained from *ab initio* or RKR intramolecular potentials. When the potential constant approaches zero, i.e. $c_h \to 0$, the TW potential reduces to the Morse potential [106]. The shape of this potential is shown in figure 1 for different molecules. Inserting this potential into the SE, the radial part of the SE takes the following form:

$$\frac{\mathrm{d}^2 U_{n\ell}(r)}{\mathrm{d}r^2} + \frac{2\mu}{\hbar^2}\left[E_{n\ell} - D\left[\frac{1 - \mathrm{e}^{-b_h(r - r_e)}}{1 - c_h \mathrm{e}^{-b_h(r - r_e)}}\right]^2 \right.$$
$$\left. - \frac{\ell(\ell + 1)\hbar^2}{2\mu r^2}\right]U_{n\ell}(r) = 0, \tag{5}$$

in which $U_{n\ell}(0) = 0$ and $\lim_{r \to \infty} U_{n\ell}(r) = 0$. In order to solve the above equation for $\ell \neq 0$ states, we need to apply the following approximation scheme [6] to deal with the centrifugal term:

$$\frac{1}{r^2} \approx \frac{\ell(\ell + 1)}{r_e^2}\left(D_0 + D_1 \frac{\mathrm{e}^{-\alpha x}}{1 - c_h \mathrm{e}^{-\alpha x}}\right.$$
$$\left. + D_2 \frac{\mathrm{e}^{-2\alpha x}}{\left(1 - c_h \mathrm{e}^{-\alpha x}\right)^2}\right), \tag{6}$$

where $\alpha = b_h r_e$, $x = \frac{r - r_e}{r_e}$ and D_i is the parameter of coefficients $i = 0, 1, 2$ and they are obtained as follows:

$$D_0 = \begin{aligned}&1 - \frac{1}{\alpha}(1 - c_h)(3 + c_h)\\ &+ \frac{3}{\alpha^2}(1 - c_h)^2,\end{aligned} \qquad \lim_{c_h \to 0} D_0 = 1 - \frac{3}{\alpha} + \frac{3}{\alpha^2} \tag{7a}$$

$$D_1 = \begin{aligned}&\frac{2}{\alpha}(1 - c_h)^2(2 + c_h)\\ &- \frac{6}{\alpha^2}(1 - c_h)^3,\end{aligned} \qquad \lim_{c_h \to 0} D_1 = \frac{4}{\alpha} - \frac{6}{\alpha^2} \tag{7b}$$

$$D_2 = \begin{aligned}&-\frac{1}{\alpha}(1 - c_h)^3(1 + c_h)\\ &+ \frac{3}{\alpha^2}(1 - c_h)^4,\end{aligned} \qquad \lim_{c_h \to 0} D_2 = -\frac{1}{\alpha} + \frac{3}{\alpha^2}. \tag{7c}$$

By using approximation expression (6), the radial part of the SE with the TW diatomic molecular potential reduces to

$$\frac{\mathrm{d}^2 U_{n\ell}(z)}{\mathrm{d}z^2} + \frac{1}{z}\frac{\mathrm{d}U_{n\ell}(z)}{\mathrm{d}z} + \frac{1}{z^2\left(1 - c_h z\right)^2}$$
$$\times \left\{\left[\frac{2\mu r_e^2}{\hbar^2\alpha^2}\big(E_{n\ell} - D\big) - \frac{\ell(\ell + 1)}{\alpha^2}D_0\right]\right.$$
$$+ \left[-2c_h\left(\frac{2\mu r_e^2 E_{n\ell}}{\alpha^2\hbar^2} - \frac{\ell(\ell + 1)}{\alpha^2}D_0\right)\right.$$
$$\left. + \frac{4\mu r_e^2 D}{\hbar^2\alpha^2} - \frac{\ell(\ell + 1)}{\alpha^2}D_1\right]z$$
$$+ \left[c_h^2\left(\frac{2\mu r_e^2 E_{n\ell}}{\alpha^2\hbar^2} - \frac{\ell(\ell + 1)}{\alpha^2}D_0\right) + \frac{\ell(\ell + 1)}{\alpha^2}\big(D_1 c_h - D_2\big)\right.$$
$$\left.\left. - \frac{2\mu r_e^2 D}{\hbar^2\alpha^2}\right]z^2\right\}U_{n\ell}(z) = 0, \tag{8}$$

where we have introduced a new transformation of the form $z = \mathrm{e}^{-b_h(r - r_e)} \in (\mathrm{e}^\alpha, 0)$ which maintained the finiteness of the transformed wave functions on the boundary conditions. By using the following transformation:

$$U_{n\ell}(z) = z^p\big(1 - c_h z\big)^q R_{n\ell}(z), \tag{9}$$

where

$$p = \sqrt{\left[\frac{2\mu r_e^2}{\hbar^2\alpha^2}\big(D - E_{n\ell}\big) + \frac{\ell(\ell + 1)}{\alpha^2}D_0\right]} \quad \text{and}$$

$$q = \frac{1}{2}\sqrt{1 + \frac{4}{c_h^2}\left[\frac{\ell(\ell + 1)}{\alpha^2}D_2 + \frac{2\mu r_e^2 D}{\hbar^2\alpha^2}\big(1 - c_h\big)^2\right]}, \tag{10}$$

equation (8) is transformed into a more convenient second-order homogeneous linear differential equation, the solution of which can be found by using the asymptotic iteration method [31, 32]

$$R_{n\ell}''(z) + \left[\frac{(2p + 1) - zc_h(2p + 2q + 1)}{z\big(1 - c_h z\big)}\right]R_{n\ell}'(z)$$
$$- \left[\frac{c_h(p + q)^2 + \varsigma/c_h}{z\big(1 - c_h z\big)}\right]R_{n\ell}(z) = 0, \tag{11}$$

where

$$\varsigma = c_h^2\left(\frac{2\mu r_e^2 E_{n\ell}}{\alpha^2\hbar^2} - \frac{\ell(\ell + 1)}{\alpha^2}D_0\right) + \frac{\ell(\ell + 1)}{\alpha^2}\big(D_1 c_h - D_2\big) - \frac{2\mu r_e^2 D}{\hbar^2\alpha^2}$$

has been introduced for mathematical simplicity. The systematic procedure of the asymptotic iteration method begins now by rewriting equation (11) in the following form [31, 32]

$$R_{n\ell}(z) - \lambda_0(z)R'_{n\ell}(z) - s_0(z)R_{n\ell}(z) = 0, \qquad (12)$$

where

$$\lambda_0(z) = \left[\frac{zc_h(2p + 2q + 1) - (2p + 1)}{z(1 - c_hz)} \right] \text{ and}$$

$$s_0(z) = \left[\frac{c_h(p + q)^2 + \varsigma/c_h}{z(1 - c_hz)} \right]. \qquad (13)$$

The primes of $R_{n\ell}(z)$ in equation (12) denotes derivatives with respect to z. The asymptotic aspect of the method for sufficiently large k is given as [31, 32]

$$\frac{s_k(z)}{\lambda_k(z)} = \frac{s_{k-1}(z)}{\lambda_{k-1}(z)} = \eta(z), \qquad (14)$$

where

$$\begin{aligned} \lambda_k(z) &= \lambda'_{k-1}(z) + s_{k-1}(z) + \lambda_0(z)\lambda_{k-1}(z), \\ s_k(z) &= s'_{k-1}(z) + s_0(z)\lambda_{k-1}(z), \end{aligned} \qquad (15)$$

Equation (15) is referred to as the recurrence relations [31, 50]. In accordance with asymptotic iteration method [31, 32], the energy eigenvalues equation are obtained from the roots of the following equation:

$$\delta_k(z) = \begin{vmatrix} \lambda_k(z) & s_k(z) \\ \lambda_{k+1}(z) & s_{k+1}(z) \end{vmatrix} = 0, \quad k = 1, 2, 3\ldots. \qquad (16)$$

Thus, we can easily obtain the following simple arithmetic progressions:

$$\begin{aligned} \delta_0(z) &= \begin{vmatrix} \lambda_0(z) & s_0(z) \\ \lambda_1(z) & s_1(z) \end{vmatrix} = 0 \Leftrightarrow p + q = 0 + \frac{1}{c_h}\sqrt{-\varsigma} \\ \delta_1(z) &= \begin{vmatrix} \lambda_1(z) & s_1(z) \\ \lambda_2(z) & s_2(z) \end{vmatrix} = 0 \Leftrightarrow p + q = -1 + \frac{1}{c_h}\sqrt{-\varsigma} \\ \delta_2(z) &= \begin{vmatrix} \lambda_2(z) & s_2(z) \\ \lambda_3(z) & s_3(z) \end{vmatrix} = 0 \Leftrightarrow p + q = -2 + \frac{1}{c_h}\sqrt{-\varsigma} \\ \delta_3(z) &= \begin{vmatrix} \lambda_3(z) & s_3(z) \\ \lambda_4(z) & s_4(z) \end{vmatrix} = 0 \Leftrightarrow p + q = -3 + \frac{1}{c_h}\sqrt{-\varsigma} \end{aligned}$$

... etc. (17)

By finding the nth term of the above progression and inserting the values of p, q and ς, the energy eigenvalues turn out as

$$\begin{aligned} E_{n\ell} &= \frac{\hbar^2\ell(\ell + 1)D_0}{2\mu r_e^2} + \frac{\hbar^2}{2\mu r_e^2 c_h^2}\left[\ell(\ell + 1) \right. \\ &\quad \times \left. (D_2 - D_1c_h) + \frac{2\mu Dr_e^2}{\hbar^2} \right] \\ &\quad - \frac{\alpha^2\hbar^2}{2\mu r_e^2} \end{aligned}$$

$$\times \left[\frac{(\delta + n)^2 - \frac{\ell(\ell+1)}{\alpha^2 c_h^2}(D_1c_h - D_2) + \frac{2\mu Dr_e^2}{\alpha^2\hbar^2}\left(\frac{1}{c_h^2} - 1\right)}{2(\delta + n)} \right]^2$$

$$= \frac{\hbar^2\ell(\ell + 1)D_0}{2\mu r_e^2} + D - \frac{\alpha^2\hbar^2}{2\mu r_e^2}$$

$$\times \left[\frac{(\delta + n)^2 + \frac{\ell(\ell+1)}{\alpha^2 c_h^2}(D_1c_h - D_2) + \frac{2\mu Dr_e^2}{\alpha^2\hbar^2}\left(1 - \frac{1}{c_h^2}\right)}{2(\delta + n)} \right]^2 \quad (18)$$

with $\delta = \dfrac{1}{2}$

$$+ \frac{1}{2}\sqrt{1 + \frac{4}{c_h^2}\left(\frac{D_2\ell(\ell+1)}{\alpha^2} + \frac{2\mu Dr_e^2}{\alpha^2\hbar^2}(1 - c_h)^2 \right)}.$$

Let us now calculate the eigenfunction solution of this problem. Generally speaking, the differential equation we wish to solve should be transformed to a form that is suitable for applying AIM [31, 32]:

$$\begin{aligned} y''(x) &= 2\left(\frac{\Lambda x^{N+1}}{1 - bx^{N+2}} \right. \\ &\quad - \left. \frac{m+1}{x} \right)y'(x) - \frac{Wx^N}{1 - bx^{N+2}}y(x), \end{aligned} \qquad (19)$$

where Λ, b and m are constants. The general solution of equation (19) is found as [31, 32]

$$\begin{aligned} y_n(x) &= \\ &(-1)^n C_2(N + 2)^n(\sigma)_{n\,2}F_1(-n, t + n; \sigma; bx^{N+2}), \end{aligned} \qquad (20)$$

where

$$\begin{aligned} (\sigma)_n &= \frac{\Gamma(\sigma + n)}{\Gamma(\sigma)}, \quad \sigma = \frac{2m + N + 3}{N + 2} \text{ and} \\ t &= \frac{(2m + 1)b + 2\Lambda}{(N + 2)b}. \end{aligned} \qquad (21)$$

By comparing equation (12) with (20), we can deduce that $m = p - \frac{1}{2}$, $t = 2(p + q)$ and $\sigma = 2p + 1$. It is therefore straightforward to show that radial wave functions can be written as

$$\begin{aligned} U_{n\ell}(x) &= (-1)^n C_2\frac{\Gamma(2p + 1 + n)}{\Gamma(2p + 1)}e^{-p\alpha x}(1 - c_he^{-\alpha x})^q \\ &\quad \times {}_2F_1\left(-n, n + 2(p + q); 2p + 1, c_he^{-\alpha x} \right), \\ &= N_{n\ell}e^{-p\alpha x}(1 - c_he^{-\alpha x})^q \\ &\quad \times P_n^{(2p,\ 2q-1)}(1 - 2c_he^{-\alpha x}), \end{aligned} \qquad (22)$$

where $N_{n\ell}$ is a normalization constant to be calculated from the normalization condition

$$\int_0^\infty |U_{n\ell}(r)|^2\,dr = \int_0^{e^\alpha} |U_{n\ell}(z)|^2\frac{dz}{\alpha z} = 1, \quad z = e^{-\alpha x}. (23)$$

By using equation (23) and the following two different forms

of Jacobi polynomials [107, 108]

$$P_n^{(\alpha,\beta)}(s) = \frac{\Gamma(\alpha+n+1)}{n!\Gamma(\alpha+\beta+n+1)}$$

$$\times \sum_{m=0}^{n} \binom{n}{m} \frac{\Gamma(\alpha+\beta+n+m+1)}{\Gamma(\alpha+m+1)} \left(\frac{s-1}{2}\right)^m,$$

$$P_n^{(\alpha,\beta)}(s) = \frac{1}{2^n} \sum_{k=0}^{n} \binom{n+\alpha}{k} \binom{n+\beta}{k}$$

$$\times \binom{n+\beta}{n-k}(s-1)^{n-k}(s+1)^k, \tag{24}$$

then

$$N_{n\ell}^2 \left[\frac{(-c_h)^{m+n-k} W_{m,n,k}}{\alpha n!} \right]$$

$$\int_0^{e^\alpha} z^{m+n-k+2p-1} \left(1 - c_h z\right)^{2q+k} dz = 1, \quad \text{with} \tag{25}$$

$$W_{m,n,k} = \frac{\Gamma(2p+n+1)}{n!\Gamma(2p+2q+n)} \sum_{m=0}^{n} \sum_{k=0}^{n} \binom{n}{m}$$

$$\times \frac{\Gamma(2p+2q+n+m)}{\Gamma(2p+m+1)} \binom{n+2p}{k}$$

$$\times \binom{n+2q-1}{k} \binom{n+2q-1}{n-k}.$$

Thus, the normalization constant can be found as

$$N_{n\ell} =$$

$$\frac{e^{\alpha\left(\frac{k-m-n}{2}\right)-\alpha p}}{\sqrt{\left[\left(\frac{(-c_h)^{m+n-k} W_{m,n,k}}{\alpha n!\,(m+n-k+2p)} \right)_2 F_1(-2q-1, m}{+n-k+2p, m+n-k+2p+1; c_h^2)} \right]}}, \tag{26}$$

where we have utilized the following integral

$$\int_0^w z^y (1-pz)^t dz = \frac{w^{1+y}}{1+y} \,_2F_1(-t, 1+y, 2+y; pw). \tag{27}$$

3.2. Some expectation values for the TW diatomic molecular potential

In this section, we calculate some expectation values of the TW diatomic molecular potential within the framework of the HFT [109–118]. In quantum mechanics, the HFT relates the derivative of the total energy with respect to a parameter and to the expectation value of the derivative of the Hamiltonian with respect to that same parameter. According to the theorem, once the spatial distribution of the electrons has been determined by solving the SE, all forces in the system can be calculated using classical electrostatics. This theorem finds some of its application in the calculation of intramolecular forces in molecules. Assuming that the Hamiltonian H for a particular quantum system is a function of some parameters q, and denoting the eigenvalues and eigenfunctions of H,

respectively, by $E_{n\ell}(q)$ and $U_{n\ell}(q)$ theoretically, we have that

$$\frac{\partial E_{n\ell}(q)}{\partial q} = \left\langle U_{n\ell}(q) \left| \frac{\partial H(q)}{\partial q} \right| U_{n\ell}(q) \right\rangle, \tag{28}$$

provided that the associated normalized eigenfunction $U_{n\ell}(q)$ is continuous with respect to the parameter q. The effective Hamiltonian of the TW diatomic molecular potential radial wave function is given by

$$H = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} + D \left[\frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2. \tag{29}$$

Having determined the effective Hamiltonian of the TW diatomic molecular potential, we can thus find the expectation values of the following parameter.

- The expectation value of V. By setting $q = D$, we can find

$$\langle V \rangle_{n\ell} = \frac{D}{c_h^2} - \frac{\alpha^2 \hbar^2 D}{8\mu r_e^2}$$

$$\times \left[\frac{\left[2\eta\left[(\delta+n)^4 - \zeta^2\right] + \frac{4\mu r_e^2}{\alpha^2 \hbar^2} \right]}{\times \left(\frac{1}{c_h^2} - 1\right)\left[(\delta+n)^2 + \zeta\right](\delta+n)}}{(\delta+n)^3} \right]$$

with $\eta = \frac{2\mu r_e^2}{\alpha^2 \hbar^2} \left(\frac{1}{c_h} - 1\right)^2$

$$\times \left[1 + \frac{4}{c_h^2} \left(\frac{D_2\ell(\ell+1)}{\alpha^2} + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2}\left(1 - c_h\right)^2 \right) \right]^{-\frac{1}{2}} \tag{30}$$

and $\zeta = \frac{\ell(\ell+1)}{\alpha^2 c_h^2}(D_2 - D_1 c_h) - \frac{2\mu D r_e^2}{\alpha^2 \hbar^2}\left(1 - \frac{1}{c_h^2}\right).$

- The expectation value of momentum $\langle p^2 \rangle_{n\ell}$. By setting $q = \mu$, we can find

$$\left\langle p^2 \right\rangle_{n\ell} = \frac{\hbar^2 \ell(\ell+1)}{r_e^2} \left[D_0 - \frac{D_1}{c_h} + \frac{D_2}{c_h^2} \right]$$

$$- \frac{\alpha^2 \hbar^2 \xi}{r_e^2}[\xi - 2\mu\rho],$$

with $\xi = \dfrac{\left[\begin{array}{c} (\delta+n)^2 - \frac{\ell(\ell+1)}{\alpha^2 c_h^2}(D_1 c_h - D_2) \\ + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2}\left(\frac{1}{c_h^2} - 1\right) \end{array} \right]}{2(\delta+n)},$

$$\rho = \frac{4\tau(n+\delta)[\delta+n-\xi] + \frac{4(\delta+n)D r_e^2}{\alpha^2 \hbar^2}\left[\frac{1}{c_h^2} - 1\right]}{4(\delta+n)^2} \quad \text{and} \tag{31}$$

$$\tau = \frac{2Dr_e^2}{\alpha^2\hbar^2c_h^2}\left(1-c_h\right)^2$$

$$\times\left[1+\frac{4}{c_h^2}\left(\frac{D_2\ell(\ell+1)}{\alpha^2}+\frac{2\mu Dr_e^2}{\alpha^2\hbar^2}\left(1-c_h\right)^2\right)\right]^{-\frac{1}{2}}.$$

It is pertinent to note that the expectation of the kinetic energy can simply be obtained from the above result by using the relation $\langle T\rangle_{n\ell}=\frac{1}{2\mu}\left\langle p^2\right\rangle_{n\ell}$ as

$$\langle T\rangle_{n\ell}=\frac{\hbar^2\ell(\ell+1)}{2\mu r_e^2}\left[D_0-\frac{D_1}{c_h}+\frac{D_2}{c_h^2}\right]$$

$$-\frac{\alpha^2\hbar^2\xi}{2\mu r_e^2}[\xi-2\mu\rho].\qquad(32)$$

- The expectation value of r^{-2}.
  By setting $q=\ell$, we can find

$$\left\langle r^{-2}\right\rangle_{n\ell}=\frac{1}{r_e^2}\left[D_0-\frac{D1}{c_h}+\frac{D_2}{c_h}\right]-\frac{2\alpha^2\xi}{(2\ell+1)r_e^2}$$

$$\times\left[\frac{4\varsigma(\delta+n)[\delta+n-\xi]-\frac{2\ell+1}{\alpha^2c_h^2}(D_1c_h-D_2)}{4(\delta+n)^2}\right]$$

with $\varsigma=\frac{D_2(2\ell+1)}{\alpha^2c_h^2}\left[1+\frac{c_h}{4}\left(\frac{D_2\ell(\ell+1)}{\alpha^2}\right.\right.$

$$\left.\left.+\frac{2\mu Dr_e^2}{\alpha^2\hbar^2}\left(1-c_h\right)^2\right)\right]^{-\frac{1}{2}}.\qquad(33)$$

4. Relativistic solutions of the Klein–Gordon equation and the Dirac equation for the TW diatomic molecular potential

The solutions of Klein–Gordon and Dirac equations are very significant in describing the nuclear shell structure. They are used to describe the particle dynamics in relativistic quantum mechanics. We obtain the approximate relativistic solutions of these equations in the presence of TW diatomic molecular potential by two eigensolution approaches.

4.1. Relativistic treatment of the spin-zero particles subject to the TW diatomic molecular potential: functional analysis approach (FAA)

The three-dimensional Klein–Gordon equation with scalar and vector potentials can be written as follows ($\hbar=c=1$) [119]:

$$\left\{\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right.$$

$$\left.+\left(M+V_s\right)^2-\left(E_R-V_v\right)^2\right\}\psi(r,\theta,\phi)=0,\qquad(34)$$

where M and E_R represent the rest mass and energy of the spin-zero particle, respectively. The scalar potential $S(r)$ and vector one $V(r)$ are chosen as equal TW potentials as defined in equation (4). By taking $\psi(r,\theta,\phi)=\frac{R_{n\ell}(r)\Theta(\theta)e^{\pm im\,\phi}}{r}$ and substituting it into equation (34), we obtain the radial part of the Klein–Gordon equation as:

$$\left\{\frac{d^2}{dr^2}+\left(E_R-D\left[\frac{1-e^{-b_h(r-r_e)}}{1-c_he^{-b_h(r-r_e)}}\right]^2\right)^2\right.$$

$$\left.-\left(M+D\left[\frac{1-e^{-b_h(r-r_e)}}{1-c_he^{-b_h(r-r_e)}}\right]^2\right)^2-\frac{\ell(\ell+1)}{r^2}\right\}R_{n\ell}(r)=0.\qquad(35)$$

The above equation is solvable for $\ell=0$ [7], but it is not solvable for $\ell\neq0$. We therefore resort to using an approximation expression (6) to deal with the centrifugal term. Then, we obtain the following equations:

$$\frac{d^2R_{n\ell}(z)}{dz^2}+\frac{1}{z}\frac{dR_{n\ell}(z)}{dz}+\frac{1}{z^2\left(1-c_hz\right)^2}$$

$$\times\left\{\left[\frac{r_e^2}{\alpha^2}\left(\widetilde{E}_{n\ell}-\widetilde{D}\right)-\frac{\ell(\ell+1)}{\alpha^2}D_0\right]\right.$$

$$+\left[-2c_h\left(\frac{r_e^2\widetilde{E}_{n\ell}}{\alpha^2}-\frac{\ell(\ell+1)}{\alpha^2}D_0\right)\right.$$

$$\left.+\frac{2r_e^2\widetilde{D}}{\alpha^2}-\frac{\ell(\ell+1)}{\alpha^2}D_1\right]z$$

$$+\left[c_h^2\left(\frac{r_e^2\widetilde{E}_{n\ell}}{\alpha^2}-\frac{\ell(\ell+1)}{\alpha^2}D_0\right)\right.$$

$$\left.\left.+\frac{\ell(\ell+1)}{\alpha^2}\left(D_1c_h-D_2\right)-\frac{r_e^2\widetilde{D}}{\alpha^2}\right]z^2\right\}R_{n\ell}(z)=0,\qquad(36)$$

where $\widetilde{E}_{n\ell}=E_R^2-M^2$ and $\widetilde{D}=(E_R+M)D$. It is worth noting that only the choice $V_s=+V_v$ produces a non-trivial, non-relativistic limit with a potential function $2V_v(r)$, and not $V_v(r)$. Accordingly, it would be natural to scale the potential terms in equation (35) so that in the non-relativistic limit the interaction potential becomes V, not $2V$ [120]. Thus, we have implement this modifications in equation (36) through which $\widetilde{D}$ becomes $(E_R+M)D$ and not $2(E_R+M)D$. Now, we express the solution to the above second-order differential equation in terms of the hypergeometric function as

$$R_{n\ell}(z)$$

$$=\frac{[(\zeta+n)(\zeta+n-1)....][(\beta+n)(\beta+n-1).....][\Gamma(\gamma)]}{[\Gamma(\zeta)][\Gamma(\beta)][(\gamma+n)(\gamma+n-1)(\gamma+n-2).....]}$$

$$\times\frac{(c_h)^n}{n!}z^u\left(1-c_hz\right)^v\qquad(37)$$

$$=z^u\left(1-c_hz\right)^v+z^u\left(1-c_hz\right)^v\sum_{n=1}^{\infty}\frac{(\alpha)_n\left(\beta_n\right)(c_hz)^n}{n!(\gamma)_n}$$

$$=z^u\left(1-c_hz\right)^v\,{}_2F_1\left(\zeta,\beta;\gamma;c_hz\right),$$

where we have introduced the following notations to avoid

mathematical complexity:

$$u = \sqrt{\left[\frac{r_e^2}{\alpha^2}\left(\widetilde{D} - \widetilde{E}_{n\ell}\right) + \frac{\ell(\ell+1)}{\alpha^2}D_0\right]} \quad \text{and}$$

$$v = \frac{1}{2}\left[\sqrt{1 + \frac{4}{c_h^2}\left[\frac{\ell(\ell+1)}{\alpha^2}D_2 + \frac{r_e^2\widetilde{D}}{\alpha^2}(1-c_h)^2\right]}\right], \quad (38)$$

ζ, β and γ are given by

$$\zeta = u + v$$
$$- \sqrt{\left[\frac{r_e^2\widetilde{D}}{\alpha^2} - c_h^2\left(\frac{r_e^2\widetilde{E}_{n\ell}}{\alpha^2} - \frac{\ell(\ell+1)}{\alpha^2}D_0\right) - \frac{\ell(\ell+1)}{\alpha^2}\left(D_1c_h - D_2\right)\right]} \tag{39}$$

$$\beta = u + v$$
$$+ \sqrt{\left[\frac{r_e^2\widetilde{D}}{\alpha^2} - c_h^2\left(\frac{r_e^2\widetilde{E}_{n\ell}}{\alpha^2} - \frac{\ell(\ell+1)}{\alpha^2}D_0\right) - \frac{\ell(\ell+1)}{\alpha^2}\left(D_1c_h - D_2\right)\right]}$$
$$\text{and} \quad \gamma = 2u + 1.$$

Now, by considering the finiteness of the solutions, it can be readily seen from equation (37) that $R_{n\ell}(z)$ approaches infinity unless ζ is a negative integer. This implies that the wave function $R_{n\ell}(z)$ will not be finite everywhere unless we take

$$u + v$$
$$- \sqrt{\left[\frac{r_e^2\widetilde{D}}{\alpha^2} - c_h^2\left(\frac{r_e^2\widetilde{E}_{n\ell}}{\alpha^2} - \frac{\ell(\ell+1)}{\alpha^2}D_0\right) - \frac{\ell(\ell+1)}{\alpha^2}\left(D_1c_h - D_2\right)\right]}$$
$$= -n. \tag{40}$$

Thus, the relativistic energy spectrum can be found by utilizing equation (40) as:

$$E_R^2 - M^2 - \frac{\ell(\ell+1)D_0}{r_e^2}$$
$$- \left[\frac{\ell(\ell+1)\left(D_2 - D_1c_h\right) + \widetilde{D}r_e^2}{r_e^2 c_h^2}\right]$$
$$+ \frac{\alpha^2}{r_e^2}\left[\frac{(\delta_c + n)^2 - \frac{\ell(\ell+1)}{\alpha^2 c_h^2}(D_1c_h - D_2) + \frac{\widetilde{D}r_e^2}{\alpha^2}\left(\frac{1}{c_h^2}-1\right)}{2(\delta_c + n)}\right]^2$$
$$= 0 \tag{41}$$

$$\text{with} \quad \delta_c = \frac{1}{2} + \frac{1}{2}$$
$$\times \sqrt{1 + \frac{4}{c_h^2}\left(\frac{D_2\ell(\ell+1)}{\alpha^2} + \frac{\widetilde{D}r_e^2}{\alpha^2}(1-c_h)^2\right)}.$$

Hence, with equation (40), the expression for β given by equation (39) can be rewritten as

$$\beta = 2(v + u) + n, \tag{42}$$

and the total radial wave functions can be written as

$$R_{n\ell}(r) = e^{-ub_h(r-r_e)}\left(1 - c_h e^{-b_h(r-r_e)}\right)^v {}_2F_1(-n, n$$
$$+ 2(v+u); 2u+1, c_h e^{-b_h(r-r_e)}),$$
$$= N_{n\ell}e^{-ub_h(r-r_e)}\left(1 - c_h e^{-b_h(r-r_e)}\right)^v$$
$$\times P_n^{(2v, \ 2v-1)}\left(1 - 2c_h e^{-b_h(r-r_e)}\right). \tag{43}$$

Before we proceed, let us first obtain the non-relativistic limit of equation (41) and eigenfunctions (43) of the TW diatomic molecular potential. de Souza Dutra *et al* [121] noted that there is the possibility of obtaining approximate non-relativistic (NR) solutions from relativistic (R) ones. Very recently, Sun [121] proposed a meaningful approach for deriving the bound-state solutions of the NR SE from the bound state of R equations. The essence of the approach was that, within the NR limit, the SE may be derived from the R equation when the energies of the potential $V(r)$ are small compared to the rest mass mc^2, then the NR energy approximated as $E^{NR} \to E - mc^2$ and the NR wave function is the $\psi^{NR}(r) \to \psi(r)$. That is, for its NR energies, E^{NR} can be determined by taking the NR limit values of the R eigen-energies E. For this purpose, we apply the following appropriate transformations

$$M + E_R \to \frac{2\mu}{\hbar^2} \qquad \text{and} \qquad M - E_R \to -E_{n\ell}. \quad (44)$$

Then we can have the energy equation as

$$E_{n\ell} = \frac{\hbar^2\ell(\ell+1)D_0}{2\mu r_e^2} + \frac{\hbar^2}{2\mu r_e^2 c_h^2}$$
$$\times \left[\ell(\ell+1)\left(D_2 - D_1c_h\right) + \frac{2\mu D r_e^2}{\hbar^2}\right]$$
$$- \frac{\alpha^2\hbar^2}{2\mu r_e^2}$$
$$\times \left[\frac{(\delta + n)^2 - \frac{\ell(\ell+1)}{\alpha^2 c_h^2}(D_1c_h - D_2) + \frac{2\mu D r_e^2}{\alpha^2\hbar^2}\left(\frac{1}{c_h^2}-1\right)}{2(\delta + n)}\right]^2 \tag{45}$$

$$\text{with} \quad \delta = \frac{1}{2} + \frac{1}{2}$$
$$\times \sqrt{1 + \frac{4}{c_h^2}\left(\frac{D_2\ell(\ell+1)}{\alpha^2} + \frac{2\mu D r_e^2}{\alpha^2\hbar^2}(1-c_h)^2\right)},$$

and the eigenfunction as

$$R_{n\ell}(r) = N_{n\ell}e^{-pb_h(r-r_e)}\left(1 - c_h e^{-b_h(r-r_e)}\right)^q$$
$$\times P_n^{(2p, \ 2q-1)}\left(1 - 2c_h e^{-b_h(r-r_e)}\right), \tag{46}$$

where $N_{n\ell}$ is the normalization constant. It is pertinent to note that the results we obtain in equations (45) and (46) as non-relativistic limit solutions are exactly the same with the ones we obtained previously for the Schrödinger system.

4.2. Fermionic massive spin-$\frac{1}{2}$ particles interacting with TW diatomic molecular potential: supersymmetry approach

In spherical coordinates, the Dirac equation for fermionic massive spin $-\frac{1}{2}$ particles interacting with arbitrary scalar potential S(r), the time-component $V(r)$ of a four-vector potential and the tensor potential $U(r)$ can be expressed as [122, 123]

$$\left[\vec{\alpha} \cdot \vec{p} + \beta(M + S(r)) - i\beta\vec{\alpha} \cdot \hat{r} U(r) \right] \psi(\vec{r})$$
$$= \left[E_r - V(r) \right] \psi(\vec{r}), \tag{47}$$

where E_r, $\vec{p}$ and M denote the relativistic energy of the system, the momentum operator and mass of the particle respectively. α and β are 4×4 Dirac matrices. The eigenvalues of the spin–orbit coupling operator are $\kappa = \left(j + \frac{1}{2}\right) > 0$ and $\kappa = -\left(j + \frac{1}{2}\right) < 0$ for unaligned spin $j = \ell - \frac{1}{2}$ and the aligned spin $j = \ell + \frac{1}{2}$, respectively. The set (H^2, K, J^2, J_Z) can be taken as the complete set of conservative quantities, with $\vec{J}$ being the total angular momentum operator and $K = (\vec{\sigma} \cdot \vec{L} + 1)$ being the spin–orbit, where $\vec{L}$ is the orbital angular momentum of the spherical nucleons that commutes with the Dirac Hamiltonian. Thus, the spinor wave functions can be classified according to their angular momentum j, the spin–orbit quantum number κ and the radial quantum number n. Hence, they can be written as follows:

$$\psi_{n\kappa}(\vec{r}) = \begin{pmatrix} f_{n\kappa}(\vec{r}) \\ g_{n\kappa}(\vec{r}) \end{pmatrix} = \begin{pmatrix} \dfrac{F_{n\kappa}(r)}{r} Y_{jm}^{\ell}(\theta, \phi) \\ \dfrac{iG_{n\kappa}(r)}{r} Y_{jm}^{\tilde{\ell}}(\theta, \phi), \end{pmatrix}, \tag{48}$$

where $F_{n\kappa}(\vec{r})$ and $G_{n\kappa}(\vec{r})$ are the radial wave functions of the upper- and lower-spinor components, respectively and $Y_{jm}^{\ell}(\theta, \phi)$ and $Y_{jm}^{\tilde{\ell}}(\theta, \phi)$ are the spherical harmonic functions coupled to the total angular momentum j and its projection m on the z axis. The orbital angular momentum quantum numbers ℓ and $\tilde{\ell}$ refer to the upper and lower components, respectively. The quasi-degenerate doublet structure can be expressed in terms of pseudospin angular momentum $s = 1/2$ and pseudo-orbital angular momentum $\tilde{\ell}$, which is defined as $\tilde{\ell} = \ell + 1$ for the aligned spin $j = \tilde{\ell} - 1/2$ and $\tilde{\ell} = \ell - 1$, and for the unaligned spin $j = \tilde{\ell} + 1/2$. Substitution of equation (48) into equation (47) yields the following coupled differential equations:

$$\left(\frac{d}{dr} + \frac{\kappa}{r} \right) F_{n\kappa}(r) = \left(M + E_{n\kappa} - \Delta(r) \right) G_{n\kappa}(r)$$
$$\left(\frac{d}{dr} - \frac{\kappa}{r} \right) G_{n\kappa}(r) = \left(M - E_{n\kappa} + \sum(r) \right) F_{n\kappa}(r), \tag{49}$$

where $\Delta(r) = V(r) - S(r)$ and $\sum(r) = V(r) + S(r)$ are the difference and sum potentials, respectively. On solving equation (49), we obtain the following Schrödinger-like differential equation with coupling to the r^{-2} singular term and

satisfying $F_{n\kappa}(r)$ and $F_{n\kappa}(r)$ respectively as:

$$\left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa + 1)}{r^2} + \frac{\dfrac{d\Delta(r)}{dr}\left(\dfrac{d}{dr} + \dfrac{\kappa}{r} \right)}{M + E_{n\kappa} - \Delta(r)} \right] F_{n\kappa}(r)$$
$$= \left[\left(M + E_{n\kappa} - \Delta(r) \right)\left(M - E_{n\kappa} + \sum(r) \right) \right] F_{n\kappa}(r), \tag{50}$$

$$\left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa - 1)}{r^2} + \frac{\dfrac{d\sum(r)}{dr}\left(\dfrac{d}{dr} - \dfrac{\kappa}{r} \right)}{M - E_{n\kappa} + \sum(r)} \right] G_{n\kappa}(r)$$
$$= \left[\left(M + E_{n\kappa} - \Delta(r) \right)\left(M - E_{n\kappa} + \sum(r) \right) \right] G_{n\kappa}(r). \tag{51}$$

The spin–orbit quantum number κ is related to the orbital angular momentum quantum number ℓ via $\kappa(\kappa - 1) = \tilde{\ell}(\tilde{\ell} + 1)$ and $\kappa(\kappa + 1) = \ell(\ell + 1)$.

4.2.1. Spin symmetry solutions of the Dirac equation with TW diatomic molecular potential.

In the spin symmetry limit, $\frac{d\Delta(r)}{dr} = 0$ or $\Delta(r) = C_s =$ constant. We take

$$\sum(r) = D\left[\frac{1 - e^{-b_h(r - r_e)}}{1 - c_h e^{-b_h(r - r_e)}} \right]^2, \tag{52}$$

and as a consequence, we can rewrite equation (50) as

$$\frac{d^2 F_{n\kappa}(x)}{dx^2} = \left[V_{\text{eff}}(x) - \widetilde{E}^s \right] F_{n\kappa}(x), \tag{53}$$

where we have approximated the centrifugal term by approximation (6) and have also introduced the following parameters for convenience:

$$V_{\text{eff}}(x) = \frac{D_1\kappa(\kappa + 1) + 2E_a r_e^2(c_h - 1)}{(e^{\alpha x} - c_h)}$$
$$+ \frac{D_2\kappa(\kappa + 1) + 2E_a r_e^2(c_h - 1)^2}{(e^{\alpha x} - c_h)^2} \quad \text{and}$$
$$\widetilde{E}^s = -D_0\kappa(\kappa + 1) - (M + E_r - C_s)(M - E_r + D)r_e^2$$
$$E_a = D(M + E_r - C_s). \tag{54}$$

Now, let us apply the basic concepts of the supersymmetric quantum mechanics formalism and shape invariance technique to obtain an approximate relativistic solution to the above equation (54). For a good SUSY, the ground-state function for the upper component $F_{nk}(r)$ can be written in the form of

$$F_{0k}(r) = \exp\left(\int W(r) dr \right), \tag{55}$$

where $W(r)$ is named as a superpotential in supersymmetric quantum mechanics [92–94]. Now, by substituting equation (55) into equation (53), we obtain the following

equation for $W(r)$:

$$
W^2(r) - W'(r) = \frac{D_1\kappa(\kappa+1) + 2E_a r_e^2(c_h - 1)}{(e^{\alpha x} - c_h)}
$$

$$
+ \frac{D_2\kappa(\kappa+1) + 2E_a r_e^2(c_h - 1)^2}{(e^{\alpha x} - c_h)^2} - \widetilde{E}_0^s, \tag{56}
$$

where the $\widetilde{E}_0^s$ denotes the ground-state energy. Since it is required that the superpotential should be made compatible with the right-hand side of the nonlinear Riccati equation (56), therefore, we take the superpotential $W(r)$ as

$$
W(r) = \mathcal{M}_a + \frac{\mathcal{M}_b}{e^{\alpha x} - c_h}, \tag{57}
$$

where $\mathcal{M}_a$ and $\mathcal{M}_b$ are two parametric constants to be determine later. We now construct a pair of supersymmetric partner potentials $V_-(r)$ and $V_+(r)$ as follows

$$
V_-(r) = W^2(r) - W'(r) = \mathcal{M}_a^2
$$

$$
+ \frac{2\mathcal{M}_a\mathcal{M}_b + \alpha\mathcal{M}_b}{e^{\alpha x} - c_h}e^{\alpha x} - \frac{(2\mathcal{M}_b\mathcal{M}_a - \mathcal{M}_b^2)}{(e^{\alpha x} - c_h)^2} \tag{58}
$$

$$
V_+(r) = W^2(r) + W'(r) = \mathcal{M}_a^2
$$

$$
+ \frac{2\mathcal{M}_a\mathcal{M}_b - \alpha\mathcal{M}_b}{e^{\alpha x} - c_h}e^{\alpha x} - \frac{(2\mathcal{M}_b\mathcal{M}_a - \mathcal{M}_b^2)}{(e^{\alpha x} - c_h)^2}. \tag{59}
$$

On comparing equation (58) with (56), we can establish the following relationship between the parametric constants and other variables:

$$
e^{2\alpha x}: \quad \mathcal{M}_a^2 = -\widetilde{E}_0^s, \tag{60a}
$$

$$
e^{\alpha x}: \quad \alpha\mathcal{M}_b - 2\mathcal{M}_a^2 c_h + 2\mathcal{M}_a\mathcal{M}_b = M + 2\widetilde{E}_0^s c_h, \tag{60b}
$$

$$
\text{constant}: \quad \mathcal{M}_a^2 c_h^2 - 2\mathcal{M}_a\mathcal{M}_b c_h + \mathcal{M}_b^2
$$

$$
= \kappa(\kappa+1)(D_2 - D_1 c_h) + E_a r_e^2(1 - c_h^2). \tag{60c}
$$

Our interest lies only in the bound-state solutions, which demand that the radial part of the wave function $F_{n\kappa}$ must satisfy the boundary conditions

$$
\frac{F_{n\kappa}(r)}{r} = \begin{cases} 0, & r \to \infty \\ \infty, & r \to 0 \end{cases}. \tag{61}
$$

By considering these regularity conditions and their consequences (i.e. the restriction conditions $\mathcal{M}_a > 0$, $\mathcal{M}_b > 0$), we can solve equations (60b) and (60c) to have

$$
\mathcal{M}_b = \alpha c_h\left[-\frac{1}{2} \right.
$$

$$
\left. \pm \sqrt{1 + \frac{4}{\alpha^2 c_h^2}\left(D_2\kappa(\kappa+1) + E_a r_e^2(c_h - 1)^2\right)} \right] \tag{62a}
$$

$$
\mathcal{M}_a =
$$

$$
\frac{\kappa(\kappa+1)\left(D_1 - \frac{D_2}{c_h}\right) + E_a r_e^2\left(c_h - \frac{1}{c_h}\right) + \frac{\mathcal{M}_b^2}{c_h}}{2\mathcal{M}_b}. \tag{62b}
$$

From these relations, we can obtain the supersymmetric partner potentials $V_-(r)$ and $V_+(r)$ as

$$
V_-(r) = \left[\frac{\kappa(\kappa+1)\left(D_1 - \frac{D_2}{c_h}\right) + E_a r_e^2\left(c_h - \frac{1}{c_h}\right) + \frac{\mathcal{M}_b^2}{c_h}}{2\mathcal{M}_b} \right]^2
$$

$$
+ \frac{2\mathcal{M}_a\mathcal{M}_b + \alpha\mathcal{M}_b}{e^{\alpha x} - c_h}e^{\alpha x} - \frac{(2\mathcal{M}_b\mathcal{M}_a - \mathcal{M}_b^2)}{(e^{\alpha x} - c_h)^2}, \tag{63}
$$

$$
V_+(r) = \left[\frac{\kappa(\kappa+1)\left(D_1 - \frac{D_2}{c_h}\right) + E_a r_e^2\left(c_h - \frac{1}{c_h}\right) + \frac{\mathcal{M}_b^2}{c_h}}{2\mathcal{M}_b} \right]^2
$$

$$
+ \frac{2\mathcal{M}_a\mathcal{M}_b - \alpha\mathcal{M}_b}{e^{\alpha x} - c_h}e^{\alpha x} - \frac{(2\mathcal{M}_b\mathcal{M}_a - \mathcal{M}_b^2)}{(e^{\alpha x} - c_h)^2}. \tag{64}
$$

With the help of equations (63) and (64), we get the following relationship, which is satisfied by the partner potentials $V_-(r)$ and $V_+(r)$

$$
V_+(r, a_0) = V_-(r, a_1) + R(a_1), \tag{65}
$$

where $a_0 = \mathcal{M}_b$, a_1 is a function of a_0, i.e. $a_1 = h(a_0) = a_0 c_h \alpha$, and the reminder $R(a_1)$ is independent of r, $R(a_1) = \left[\frac{\chi_m + \frac{a_0^2}{c_h}}{2a_0}\right]^2 - \left[\frac{\chi_m + \frac{a_1^2}{c_h}}{2a_1}\right]^2$. Consequently, $a_n = f(a_0) = a_0 - nc_h\alpha$, with the remainder $R(a_n) = \left[\frac{\chi_m + \frac{a_{n-1}^2}{c_h}}{2a_{n-1}}\right]^2 - \left[\frac{\chi_m + \frac{a_n^2}{c_h}}{2a_n}\right]^2$. We see that the shape invariance holds via a mapping of the form $\mathcal{M}_b \to \mathcal{M}_b - \alpha$. Thus, the energy spectra of the potential $V_-(r)$ can be determined by using the shape invariance approach and the following results can be obtained

$$
\widetilde{E}_0^{s(-)} = 0, \tag{66a}
$$

$$
\widetilde{E}_n^{s(-)} = \sum_{k=1}^n R(a_k) = R(a_1) + R(a_2)
$$

$$
+ R(a_3) + \dots + R(a_n)
$$

$$
= \left[\frac{\chi_m c_h + a_0^2}{2a_0 c_h}\right]^2 - \left[\frac{\chi_m c_h + a_1^2}{2a_1 c_h}\right]^2 + \dots
$$

$$
+ \left[\frac{\chi_m c_h + a_{n-1}^2}{2a_{n-1} c_h}\right]^2 - \left[\frac{\chi_m c_h + a_n^2}{2a_n c_h}\right]^2 \tag{66b}
$$

$$= \left[\frac{\chi_m c_h + a_0^2}{2a_0 c_h} \right]^2 - \left[\frac{\chi_m c_h + a_n^2}{2a_n c_h} \right]^2$$

$$= \left[\frac{\chi_m c_h + \mathcal{M}_b^2}{2\mathcal{M}_b c_h} \right]^2 - \left[\frac{\chi_m c_h + \left(\mathcal{M}_b - nc_h\alpha\right)^2}{2\left(\mathcal{M}_b - nc_h\alpha\right)c_h} \right]^2$$

$$\text{with } \chi_m = \kappa(\kappa+1)\left(D_1 - \frac{D_2}{c_h} \right)$$

$$+ E_a r_e^2 \left(c_h - \frac{1}{c_h} \right),$$

where $n = 0, 1, 2, 3,...$ denotes the quantum numbers. We can obtain the energy levels of the system as

$$\widetilde{E}^s = \widetilde{E}_n^{s(-)} + \widetilde{E}_0^s = -\left[\frac{\chi_m c_h + \left(\mathcal{M}_b - nc_h\alpha\right)^2}{2\left(\mathcal{M}_b - nc_h\alpha\right)c_h} \right]^2 \quad (67)$$

Thus, the relativistic energy spectrum can be obtain directly from equation (67) as follows:

$$(M + E - C_s)(M - E + D)r_e^2 + \kappa(\kappa+1)D_0 - \alpha^2$$

$$\left[\frac{\frac{\kappa(\kappa+1)}{\alpha^2 c_h^2}\left(D_1 c_h - D_2 \right) + \frac{D\left(M + E - C_s\right)r_e^2}{\alpha^2}\left(1 - \frac{1}{c_h^2} \right) + \delta_s^2}{2\delta_s} \right]^2 = 0, \quad (68)$$

with

$$\delta_s =$$

$$n + \frac{1}{2} + \frac{1}{2}\sqrt{\left[1 + \frac{4}{\alpha^2 c_h^2}\left[D_2\kappa(\kappa+1) + D\left(M + E - C_s\right)r_e^2\left(c_h - 1\right)^2 \right] \right]}. \quad (69)$$

4.2.2. Pseudospin symmetry solutions of the Dirac equation with the TW diatomic molecular potential.
In the pseudospin symmetry limit, $\frac{d\sum(r)}{dr} = 0$ or $\sum(r) = C_{ps}=$ constant. By taking

$$\Delta(r) = D\left[\frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2, \quad (70)$$

and then substituting it into equation (51), we can find:

$$\frac{d^2 G_{n\kappa}(x)}{dx^2} = \left[\bar{V}_{\text{eff}}(x) - \widetilde{E}^{ps} \right] G_{n\kappa}(x), \quad (71)$$

where we have introduced the following parameters for mathematical simplicity

$$\bar{V}_{\text{eff}}(x) = \frac{D_1\kappa(\kappa-1) + 2E_b r_e^2\left(c_h - 1\right)}{\left(e^{\alpha x} - c_h\right)}$$

$$+ \frac{D_2\kappa(\kappa+1) + 2E_b r_e^2\left(c_h - 1\right)^2}{\left(e^{\alpha x} - c_h\right)^2} \text{ and}$$

$$\widetilde{E}^{ps} = -D_0\kappa(\kappa-1) - \left(M - E_r + C_{ps}\right)\left(M - E_r + D\right)r_e^2$$

$$E_b = D\left(E_r - M + C_s\right). \quad (72)$$

By employing the same procedure of solving equation (50), we obtain the relativistic energy spectrum equation for the TW potential with pseudospin symmetry within the framework of Dirac theory as

$$\left(M - E_r + C_{ps}\right)\left(M + E_r - D\right)r_e^2 + \kappa(\kappa-1)D_0 - \alpha^2$$

$$\left[\frac{\frac{\kappa(\kappa-1)}{\alpha^2 c_h^2}(D_1 c_h - D_2) + \frac{D\left(E_r - M - C_{ps}\right)r_e^2}{\alpha^2}\left(1 - \frac{1}{c_h^2} \right) + \delta_{ps}^2}{2\delta_{ps}} \right]^2$$

$$= 0 \quad (73)$$

with

$$\delta_{ps}$$

$$= n + \frac{1}{2} + \frac{1}{2}\sqrt{\left[1 + \frac{4}{\alpha^2 c_h^2}\left[D_2\kappa(\kappa-1) + D\left(E - M + C_{ps}\right)r_e^2\left(c_h - 1\right)^2 \right] \right]}. \quad (74)$$

Let us remark that a careful inspection to our present spin-symmetric solution shows that it can be easily recovered by knowing the relationship between the present set of parameters $(\bar{V}_{\text{eff}}, \widetilde{E}^{ps})$ and the previous set of parameters $(V_{\text{eff}}, \widetilde{E}^s)$. This tells us that the positive energy solution for spin symmetry (the negative energy solution for pseudospin symmetry) can be obtained directly from those of the negative energy solution for pseudospin symmetry (the positive energy solution for spin symmetry) by performing the following parametric mappings:

$$\kappa \to \kappa - 1, \ V(r) \to -V(r), \ E_r \to -E_r \quad (75)$$

4.2.3. Non-relativistic limit.
Let us now present the non-relativistic limit. This can be achieved when we set $C_s = 0$ and by using the mapping $E_{n\kappa} - M = E_{n_r\ell}$ and $E_{n\kappa} + M = \frac{2\mu}{\hbar^2}$ in equation (68) and (69); then the resulting energy eigenvalues

are:

$$E_{n\ell} = \frac{\hbar^2 \ell(\ell+1)D_0}{2\mu r_e^2} + D - \frac{\alpha^2 \hbar^2}{2\mu r_e^2}$$

$$\times \left[\frac{(\delta+n)^2 + \frac{\ell(\ell+1)}{\alpha^2 c_h^2}(D_1 c_h - D_2) + \frac{2\mu D r_e^2}{\alpha^2 \hbar^2}\left(1 - \frac{1}{c_h^2}\right)}{2(\delta+n)} \right]^2. \quad (76)$$

It is worth noting that despite variation in calculations, equation (76) which is the non-relativistic limit of the spin Dirac–TW problem and equation (45) which happen to be the non-relativistic limit of Klein–Gordon–TW problem are exactly the same as the one we obtain for the Schrödinger system in equation (18). We have completed the first fold of this work; however, this investigation is not complete without computing the information-theoretic quantity.

5. Information-theoretic measures for TW diatomic molecular potential

Recently, the information theory of quantum-mechanical systems have aroused the interest of many theoretical physicists [28, 124–135]. This is due to the following facts:

- It provides a deeper insight into the internal structure of the systems [128].
- It is the strongest support of the modern quantum computation and information, which has been basic for numerous technological developments [129, 130].

In this section, the probability distributions that characterize the quantum-mechanical states of TW diatomic molecular potential are analyzed by means of a complementary information measurement of a probability distribution called Fisher's information entropy.

This information measurement was originally introduced in 1925 by Fisher in the theory of statistical estimation [131, 132]. This provides the main theoretic tool of the extreme physical information principle and a general variational principle that allows one to derive numerous fundamental equations of physics such as the Maxwell equations, the Einstein field equations, the Dirac and Klein–Gordon equations, various laws of statistical physics and some laws governing nearly incompressible turbulent fluid flows [28, 133–135]. This probability distribution is defined as

$$I(\rho) := \int \frac{\left[\bar{\nabla}\rho(\bar{\mathbf{r}})\right]^2}{\rho(\bar{\mathbf{r}})}d\bar{\mathbf{r}}, \quad (77)$$

where $\bar{\nabla}$ is the gradient operator in polar coordinates. Since equation (3) was obtained from the original SE via the variable separable method using the wave function $\Psi(r, \theta, \varphi) = G(r)Y_{\ell m}(\theta, \varphi)$ with $G(r) = r^{-1}U_{n\ell}(r)$, we can therefore obtain the radial probability distribution function

for this problem as

$$\rho(r) = \aleph e^{-2pb_h(r-r_e)}\left(1 - c_h e^{-b_h(r-r_e)}\right)^{2q}$$

$$\times \left[P_n^{(2p,\ 2q-1)}\left(1 - 2c_h e^{-b_h(r-r_e)}\right)\right]^2, \quad (78)$$

where $\aleph = N_{n\ell}^2$. The Fisher information entropy of the radial probability distribution function can be calculated by using

$$I(\rho) = \int_0^\infty \frac{1}{\rho(r)}\left[\frac{d\rho(r)}{dr}\right]^2 dr$$

$$= \int_0^{c_h e^{b_h r_e}} \frac{1}{\rho(z)}\left[\frac{d\rho(z)}{dz}\right]^2 \frac{dz}{b_h z},$$

$$z = c_h e^{-b_h(r-r_e)}. \quad (79)$$

It should be noted that the present calculation becomes rather difficult and too cumbersome due to the interval of the variable $[0, c_h e^\alpha]$. To overcome this difficulty, as shown in [4, 7], Wei considered it by weakening the limit of the integral from $[0, c_h e^\alpha]$ to $[0, 1]$ since the solution solved by the modified condition is consistent with the original condition (and shows a high degree of accuracy) because of the quickly decreasing factor $(1-z)^q$. If we consider this approximation, we can therefore calculate $I(\rho)$ as

$$I(\rho) = \int_0^\infty \frac{1}{\rho(r)}\left[\frac{d\rho(r)}{dr}\right]^2 dr$$

$$= \frac{1}{2b_h}\int_{-1}^1 \frac{1}{\rho(s)}\left[\frac{d\rho(s)}{ds}\right]^2\left(\frac{2}{1-s}\right)ds,$$

$$s = 1 - 2z. \quad (80)$$

In order to calculate the integral (80), first we obtain the first derivative of the radial probability distribution function as

$$\frac{d\rho(r)}{dr} = \aleph b_h \left\{ 2\left(\frac{1-s}{2}\right)^{\tilde{u}}\left(\frac{1+s}{2}\right)^{\tilde{v}+1} \right.$$

$$\times \left[P_n^{(\tilde{u},\tilde{v})}(s)\right]^2\left[\frac{q(1-s)}{1+s} - p\right]$$

$$+ \frac{1}{2}\left(\frac{1-s}{2}\right)^{\tilde{u}}\left(\frac{1+s}{2}\right)^{\tilde{v}} P_n^{(\tilde{u},\tilde{v})}(s)$$

$$\times \left[\frac{n\left[(\tilde{u}-\tilde{v}) - (2n+\tilde{u}+\tilde{v})s\right]}{2n+\tilde{u}+\tilde{v}}P_n^{(\tilde{u},\tilde{v})}(s)\right.$$

$$\left.\left. + \frac{2(n+\tilde{u})(n+\tilde{v})}{(2n+\tilde{v}+\tilde{u})}P_{n-1}^{(\tilde{u},\tilde{v})}(s)\right]\right\}, \quad (81)$$

where we have used the parameters $\tilde{u} = 2p$, $\tilde{v} = 2q-1$ for simplicity and then utilized the following properties of

Jacobi polynomials [108]

$$\left(1 - x^2\right)\frac{d}{ds}P_n^{(\tilde{u}, \tilde{v})}(s)$$

$$= \left[\frac{n\left[\left(\tilde{u} - \tilde{v}\right) - \left(2n + \tilde{u} + \tilde{v}\right)s\right]}{2n + \tilde{u} + \tilde{v}}P_n^{(\tilde{u}, \tilde{v})}(s)\right.$$

$$\left.+ \frac{2\left(n + \tilde{u}\right)\left(n + \tilde{v}\right)}{\left(2n + \tilde{v} + \tilde{u}\right)}P_{n-1}^{(\tilde{u}, \tilde{v})}(s)\right]. \tag{82}$$

It is a very straightforward calculation to show that

$$\frac{1}{\rho(r)}\left[\frac{d\rho(r)}{dr}\right]^2 =$$

$$4b_h^2 \aleph \begin{cases} \left(\frac{1-s}{2}\right)^{\tilde{u}}\left(\frac{1+s}{2}\right)^{\tilde{v}+1}\left[P_n^{(\tilde{u}, \tilde{v})}(s)\right]^2 \\ \times\left[\left(\frac{n(n + \tilde{u})}{2n + \tilde{u} + \tilde{v}} + 2q\right)\frac{1}{1 + s} - \left(p + q + \frac{n}{2}\right)\right]^2 \\ +\left[\frac{(n + \tilde{u})(n + \tilde{v})}{(2n + \tilde{u} + \tilde{v})}\right]\left[\left(\frac{n(n + \tilde{u})}{2n + \tilde{u} + \tilde{v}} + 2q\right)\frac{1}{1 - s} - \left(p + q + \frac{n}{2}\right)\right] \\ \times\left(\frac{1-s}{2}\right)^{\tilde{u}}\left(\frac{1+s}{2}\right)^{\tilde{v}}P_n^{(\tilde{u}, \tilde{v})}(s)P_{n-1}^{(\tilde{u}, \tilde{v})}(s) \\ +\left[\frac{(n + \tilde{u})(n + \tilde{v})}{(2n + \tilde{u} + \tilde{v})}\right]^2\left(\frac{1-s}{2}\right)^{\tilde{u}} \\ \left(\frac{1+s}{\tilde{v} - 1}\right)^{\tilde{v}+1}\left[P_{n-1}^{(\tilde{u}, \tilde{v})}(s)\right]^2. \end{cases} \tag{83}$$

Thus, the Fisher information entropy can be calculated by substituting equation (83) into equation (80) and then decomposing them into a sum of three integrals to have

$$I(\rho) = 2b_h \aleph \left(I_1 + I_2 + I_3\right) \tag{84}$$

with

$$I_1 = \left[\frac{n\left(n + \tilde{u}\right)}{2n + \tilde{u} + \tilde{v}} + 2q\right]^2 I_a + 2\left(p + q + \frac{n}{2}\right)\left[\left(p + q + \frac{n}{2}\right)\right.$$

$$\left.+ \left(\frac{n\left(n + \tilde{u}\right)}{2n + \tilde{u} + \tilde{v}} + 2q\right)\right]I_b - \left(p + q + \frac{n}{2}\right)^2 I_c$$

$$I_2 = \left[\frac{(n + \tilde{u})(n + \tilde{v})}{(2n + \tilde{u} + \tilde{v})}\right]^2 I_d$$

and $I_3 = \left(n + \tilde{v}\right)\left[\frac{n\left(n + \tilde{u}\right)}{2n + \tilde{u} + \tilde{v}} + 2q\right]$

$$\times I_e - \left(n + \tilde{v}\right)\left(p + q + \frac{n}{2}\right)I_f$$

$$+ \left[\frac{n\left(n + u + \tilde{v}\right)}{2n + \tilde{u} + \tilde{v}} + 2q\right]\left(p + q + \frac{n}{2}\right)I_b$$

$$- \left[\frac{(n + \tilde{u} + \tilde{v})(n + \tilde{v})}{(2n + \tilde{u} + \tilde{v})}\right]\left[\frac{n\left(n + \tilde{u}\right)}{2n + \tilde{u} + \tilde{v}} + 2q\right]I_a,$$

where we have utilized the relation $(n + \tilde{u})P_{n-1}^{\tilde{u}, \tilde{v}}(s) + (n + u + v)P_n^{\tilde{u}, \tilde{v}}(s) - (2n + \tilde{u} + \tilde{v})P_n^{\tilde{u}, \tilde{v} - 1}(s)$ in the calculation of I_3 and $I_a, I_b \ldots \ldots I_f$ are integrals to be obtain in the next subsection.

5.1. Evaluation of integrals I_a, I_b, I_c, I_e and I_f

In this section, we calculate the above integrals as follows:

•

$$I_a = \int_{-1}^1 \left(\frac{1-s}{2}\right)^{\tilde{u}-1}\left(\frac{1+s}{2}\right)^{\tilde{v}-1}\left[P_n^{(\tilde{u}, \tilde{v})}(s)\right]^2 ds. \tag{85}$$

By using the standard integral[6] (A.1), we can find I_a as

$$I_a = \frac{n!2^{2n+1}\Gamma\left(n + 2q + 2p - 1\right)}{[\Gamma\left(2n + 2p + 2q\right)]^2}\Gamma\left(n + 2q\right)\Gamma\left(n + 2p + 1\right)$$

$$\times\left(\frac{n + 2q - 1}{2p} + 2 + \frac{n + 2p}{2q - 1}\right). \tag{86}$$

•

$$I_b = \int_{-1}^1 \left(\frac{1-s}{2}\right)^{\tilde{u}-1}\left(\frac{1+s}{2}\right)^{\tilde{v}}\left[P_n^{(\tilde{u}, \tilde{v})}(s)\right]^2 ds. \tag{87}$$

By using the standard integral [108] of the (A.2), I_b can be calculated as

$$I_b = \frac{\Gamma\left(2p + n + 1\right)\Gamma\left(2q + n\right)}{n!\left(p + q + n\right)\Gamma\left(2p + 2q + n\right)} \tag{88}$$

•

$$I_c = \int_{-1}^1 \left(\frac{1-s}{2}\right)^{\tilde{u}}\left(\frac{1+s}{2}\right)^{\tilde{v}}\left[P_n^{(\tilde{u}, \tilde{v})}(s)\right]^2 ds. \tag{89}$$

Also, by using the standard integral [108] of the (A.2), I_b can be calculated as

$$I_c = \frac{\Gamma\left(2p + n + 1\right)\Gamma\left(2q + n\right)}{n!p\Gamma\left(2p + 2q + n\right)} \tag{90}$$

•

$$I_d = \int_{-1}^1 \left(\frac{1-s}{2}\right)^{\tilde{u}-1}\left(\frac{1+s}{2}\right)^{\tilde{v}-1}\left[P_{n-1}^{(\tilde{u}, \tilde{v})}(s)\right]^2 ds. \tag{91}$$

The above integral can be calculated in a similar fashion as I_a. Thus we find

$$I_d = \frac{(n - 1)!2^{2n-1}\Gamma\left(n + 2q + 2p - 2\right)}{[\Gamma\left(2n + 2p + 2q - 2\right)]^2}\Gamma\left(n + 2q - 1\right)$$

$$\times\Gamma\left(n + 2p\right)\left(\frac{n + 2q - 2}{2p} + 2 + \frac{n + 2p - 1}{2q - 1}\right) \tag{92}$$

•

$$I_e = \int_{-1}^1 \left(\frac{1-s}{2}\right)^{\tilde{u}-1}\left(\frac{1+s}{2}\right)^{\tilde{v}-1}$$

$$\times\left[P_n^{(\tilde{u}, \tilde{v})}(s)\right]\left[P_n^{(\tilde{u}, \tilde{v} - 1)}(s)\right]ds. \tag{93}$$

Since there are no available standard integrals in the literature to calculate I_e, we therefore resort to splitting the

---

[6] This integral was first derived and used by Ruiz and Dehesa in an attempt to find the Fisher information of orthogonal hypergeometric polynomials [127].

Table 1. Model parameters of the diatomic molecules studied in the current work.

Molecules (states)	c_h	$\mu/10^{-23}$(g)	$b_h(\text{Å}^{-1})$	$r_e(\text{Å})$	$D\,(\text{cm}^{-1})$
$H_2\left(X^1\Sigma_g^+\right)$	0.170 066	0.084	1.618 90	0.741	38 318
$CO\left(X^1\Sigma^+\right)$	0.149 936	1.146	2.204 81	1.128	90 531
$HF\left(X^1\Sigma^+\right)$	0.127 772	0.160	1.942 07	0.917	493 82
$O_2\left(X^3\Sigma_g^+\right)$	0.027 262	1.337	2.591 03	1.207	42 041
$NO\left(X^2\Pi_r\right)$	0.013727	1.249	2.715 59	1.151	53 341
$Cl_2\left(X^1\Sigma_g^+\right)$	−0.096 988	2.924	2.203 54	1.987	20 276
$I_2\left(X\left(O_g^+\right)\right)$	−0.139 013	10.612	2.123 43	2.666	12 547
$N_2\left(X^1\Sigma_g^+\right)$	−0.032 325	1.171	2.785 85	1.097	79 885
$O_2^+\left(X^2\Pi_g\right)$	−0.019 445	1.337	2.869 87	1.116	54 688
$NO^+\left(X^1\Sigma^+\right)$	−0.029 000	1.239	2.733 49	1.063	88 694

integral into two as

$$I_e = (n+v)\left[\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}}+2q\right]\left[I_a+\int_{-1}^{1}\left(\frac{1-s}{2}\right)^{n+\tilde{u}-1}\right.$$

$$\left.\times\left(\frac{1+s}{2}\right)^{\tilde{v}-1}\left[P_n^{(\tilde{u},\tilde{v})}(s)\right]\mathrm{d}s\right],\qquad(94)$$

where we have used the following notations of the Jacobi polynomial [108]:

$$P_n^{(\tilde{u},\tilde{v}-1)}(s)=P_n^{(\tilde{u},\tilde{v})}(s)+\left(\frac{1-s}{2}\right)^n.\qquad(95)$$

Now, by using the integral relation [108] given by (A.4), we can now calculate I_e as

$$I_e=(n+\tilde{v})\left(\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}}+2q\right)I_a+I_{\tilde{e}},\qquad(96)$$

with

$$I_{\tilde{e}}=\left[(n+v)\left(\frac{n(n+\tilde{u})}{2n+\tilde{u}+\tilde{v}}+2q\right)\right]$$

$$\times\frac{(-1)^n\Gamma(n+2q)\Gamma(2p+n)}{n!q\Gamma(2p+2q-1+n)}$$

$$\times\,_3F_2\left(\begin{matrix}-n,2+2p+2q,2p+n\\2p+1,2p+2q+n-1\end{matrix}\middle|1\right).\qquad(97)$$

•

$$I_f=\int_{-1}^{1}\left(\frac{1-s}{2}\right)^{\tilde{u}-1}\left(\frac{1+s}{2}\right)^{\tilde{v}}$$

$$\times\left[P_n^{(\tilde{u},\tilde{v})}(s)\right]\left[P_n^{(\tilde{u},\tilde{v}-1)}(s)\right]\mathrm{d}s$$

$$I_f=(n+\tilde{v})\left(p+q+\frac{n}{2}\right)\left[I_b+\int_{-1}^{1}\left(\frac{1-s}{2}\right)^{n+\tilde{u}-1}\right.$$

$$\left.\times\left(\frac{1+s}{2}\right)^{\tilde{v}}\left[P_n^{(\tilde{u},\tilde{v})}(s)\right]^2\mathrm{d}s\right],\qquad(98)$$

where we have also used the relation (95). Finally, by using

the integral [108] of (A.5)

$$I_f=(n+\tilde{v})\left(p+q+\frac{n}{2}\right)I_b+I_{\tilde{f}},\qquad(99)$$

with

$$I_{\tilde{f}}=2(-1)^n$$

$$\times\frac{\Gamma(n+2q)\Gamma(2p+1)\Gamma(n+2p)}{n!\Gamma(n+2p+2q)\Gamma(2p+n+1)\Gamma(1-n)}$$

$$\times(n+\tilde{v})\left(p+q+\frac{n}{2}\right).\qquad(100)$$

5.2. Main result

The Fisher information entropy embedded by the radial probability distribution function can be calculated from equations (84)–(100) as

$$I(R)=$$

$$2b_h\aleph\left\{\begin{matrix}(n+2q)I_a+\left(p+q+\dfrac{n}{2}\right)\\[2mm]\left[\dfrac{3n(n+2p)}{2n+2p+2q-1}-2+p+9q+\dfrac{3n}{2}\right]I_b\\[2mm]-\left(p+q+\dfrac{n}{2}\right)^2I_c\\[2mm]+\left[\dfrac{(n+2p)(n+2q-1)}{(2n+2p+2q-1)}\right]I_d+I_{\tilde{e}}+I_{\tilde{f}}.\end{matrix}\right.\qquad(101)$$

6. Numerical results

In table 1, we present spectroscopic parameters for some diatomic molecules that are taken from the interesting work of Gordillo-Vizquez and Kunc [5]. In the case of the non-relativistic limit, we have calculated the bound-state energy eigenvalues of $H_2\left(X^1\Sigma_g^+\right)$ and $CO\left(X^1\Sigma^+\right)$ for different values of n and ℓ in table 2 by using the values in table 1. In order to test the accuracy of our results, we compared

Table 2. Comparison of the bound-state energy eigenvalues $-(E_{n\ell} - D)(eV)$ of H$_2$ and CO molecules for various n and rotational ℓ quantum numbers in TW diatomic molecular potential.

n	ℓ	Present	N-U [6]	Present	N-U [6]
0	0	4.481 442 828	4.481 571 8267	11.073 782 707	11.073 709 64
	5	4.266 910 238	4.265 822 0403	11.066 682 384	11.066 596 06
	10	3.737 244 885	3.733 630 4360	11.047 753 377	11.047 631 73
5	0	2.280 571 333	2.266 965 0930	9.632 316 0070	9.629 868 985
	5	2.120 961 179	2.107 007 2990	9.625 607 4980	9.623 148 913
	10	1.725 024 443	1.710 502 6080	9.607 723 2750	9.084 920 084
7	0	1.628 985 073	1.613 091 1000	9.088 167 4810	9.084 920 084
	5	1.488 262 184	1.472 279 9590	9.081 612 5880	9.078 354 525
	10	1.138 505 495	1.122 535 6530	9.064 137 9900	9.060 851 440

Table 3. Bound-state energy eigenvalues for H$_2\left(X^1\Sigma_g^+\right)$, CO$\left(X^1\Sigma^+\right)$, HF$\left(X^1\Sigma^+\right)$, O$_2\left(X^3\Sigma_g^+\right)$ and NO$\left(X^2\Pi_r\right)$ molecules for various n and rotational ℓ quantum numbers in TW diatomic molecular potential.

n	ℓ	H$_2\left(X^1\Sigma_g^+\right)$	CO$\left(X^1\Sigma^+\right)$	HF$\left(X^1\Sigma^+\right)$	O$_2\left(X^3\Sigma_g^+\right)$	NO$\left(X^2\Pi_r\right)$
0	0	0.269 255 177	0.150 703 328	0.253 867 064	0.097 520 341	0.117 508 622
1	0	0.778 774 368	0.448 390 501	0.742 676 288	0.289 698 792	0.349 308 434
	1	0.792 535 216	0.448 858 605	0.747 534 657	0.290 048 441	0.349 720 567
2	0	1.252 418 022	0.741 348 914	1.207 523 735	0.478 099 389	0.576 841 245
	1	1.265 398 618	0.741 811 764	1.212 186 887	0.478 444 568	0.577 248 398
	2	1.291 246 200	0.742 737 445	1.221 507 324	0.479 134 962	0.578 062 645
3	0	1.691 333 219	1.029 610 568	1.648 826 110	0.662 728 172	0.800 110 112
	1	1.703 567 986	1.030 068 193	1.653 297 607	0.663 068 932	0.800 512 223
	2	1.727 931 688	1.030 983 431	1.662 234 886	0.663 750 364	0.801 316 967
	3	1.764 215 767	1.032 356 253	1.675 626 521	0.664 772 574	0.802 523 312
4	0	2.096 613 542	1.313 207 150	2.066 989 237	0.843 591 024	1.019 118 256
	1	2.108 134 592	1.313 659 582	2.071 272 547	0.843 927 335	1.019 515 545
	2	2.131 078 206	1.314 564 429	2.079 833 592	0.844 599 847	1.020 309 967
	3	2.165 250 313	1.315 921 667	2.092 661 234	0.845 608 699	1.021 501 665
	4	2.210 366 885	1.317 731 254	2.109 738 804	0.846 953 691	1.023 090 734
5	0	2.469 302 053	1.592 170 028	2.462 408 428	1.020 693 823	1.233 868 623
	1	2.480 139 341	1.592 617 287	2.466 506 913	1.021 025 634	1.234 261 023
	2	2.501 722 377	1.593 511 812	2.474 698 450	1.021 689 355	1.235 045 656
	3	2.533 870 783	1.594 853 558	2.486 972 183	1.022 684 786	1.236 222 354
	4	2.576 320 598	1.596 642 482	2.503 311 852	1.024 012 093	1.237 791 733
	5	2.628 731 798	1.598 878 537	2.523 695 846	1.025 671 003	1.239 753 045
6	0	2.810 394 062	1.866 530 245	2.835 468 783	1.194 042 501	1.444 364 456
	1	2.820 575 527	1.866 972 369	2.839 385 715	1.194 369 905	1.444 751 656
	2	2.840 853 493	1.867 856 625	2.847 214 278	1.195 024 707	1.445 526 678
	3	2.871 060 545	1.869 182 965	2.858 943 887	1.196 006 859	1.446 688 856
	4	2.910 951 716	1.870 951 346	2.874 558 705	1.197 316 355	1.448 238 358
	5	2.960 211 497	1.873 161 728	2.894 037 651	1.198 953 074	1.450 175 034
	6	3.018 462 601	1.875 814 019	2.917 354 461	1.200 917 082	1.452 498 823
7	0	3.120 839 735	2.136 318 554	3.186 545 521	1.363 642 945	1.650 608 943
	1	3.130 391 433	2.136 755 573	3.190 284 072	1.363 965 886	1.650 991 545
	2	3.149 416 096	2.137 629 616	3.197 756 011	1.364 611 822	1.651 756 445
	3	3.177 758 594	2.138 940 639	3.208 951 016	1.365 580 727	1.652 903 645
	4	3.215 191 967	2.140 688 596	3.223 853 651	1.366 872 458	1.654 433 256
	5	3.261 423 932	2.142 873 447	3.242 443 361	1.368 487 069	1.656 345 856
	6	3.316 105 073	2.145 495 102	3.264 694 547	1.370 424 434	1.658 639 934
	7	3.378 838 214	2.148 553 507	3.290 576 601	1.372 684 523	1.661 316 623

our obtained energy spectrum with the ones obtained pre-viously in the literature. It is obvious that the present results are in agreement with those obtained by other authors and via other approaches. In tables 3 and 4, we have reported some numerical results for different molecules and states. These molecules are H$_2\left(X^1\Sigma_g^+\right)$, CO$\left(X^1\Sigma^+\right)$, HF$\left(X^1\Sigma^+\right)$, O$_2\left(X^3\Sigma_g^+\right)$, NO$\left(X^2\Pi_r\right)$ in table 3 and Cl$_2\left(X^1\Sigma_g^+\right)$,

Table 4. Bound-state energy eigenvalues for $Cl_2\left(X^1\Sigma_g^+\right)$, $I_2\left(X\left(O_g^+\right)\right)$, $N_2\left(X^1\Sigma_g^+\right)$, $O_2^+\left(X^2\Pi_g\right)$ and $NO^+\left(X^1\Sigma^+\right)$ molecules for various n and rotational ℓ quantum numbers in TW diatomic molecular potential.

n	ℓ	$Cl_2\left(X^1\Sigma_g^+\right)$	$I_2\left(X\left(O_g^+\right)\right)$	$N_2\left(X^1\Sigma_g^+\right)$	$O_2^+\left(X^2\Pi_g\right)$	$NO^+\left(X^1\Sigma^+\right)$
0	0	−0.034 819 832	−0.013 326 639	−0.146 754 672	−0.118 620 934	−0.147 932 212
1	0	−0.105 090 197	−0.040 121 814	−0.443 362 676	−0.358 867 912	−0.446 647 624
	1	−0.105 029 462	−0.040 112 565	−0.442 863 155	−0.358 444 223	−0.446 145 438
2	0	−0.176 229 866	−0.067 116 219	−0.744 144 013	−0.603 144 924	−0.749 198 864
	1	−0.176 168 730	−0.067 106 939	−0.743 639 828	−0.602 716 512	−0.748 692 050
	2	−0.176 046 445	−0.067 088 376	−0.742 631 522	−0.601 859 914	−0.747 678 995
3	0	−0.248 235 753	−0.094 309 263	−1.049 092 718	−0.851 448 145	−1.055 581 449
	1	−0.248 174 213	−0.094 299 951	−1.048 583 979	−0.851 015 224	−1.055 070 323
	2	−0.248 051 126	−0.094 281 326	−1.047 566 427	−0.850 149 446	−1.054 048 112
	3	−0.247 866 497	−0.094 253 391	−1.046 040 089	−0.848 850 667	−1.052 515 317
4	0	−0.321 104 777	−0.121 700 354	−1.358 203 204	−1.103 773 145	−1.365 790 735
	1	−0.321 042 835	−0.121 691 011	−1.357 689 794	−1.103 335 534	−1.365 275 425
	2	−0.320 918 943	−0.121 672 325	−1.356 663 018	−1.102 460 745	−1.364 244 756
	3	−0.320 733 113	−0.121 644 296	−1.355 122 889	−1.101 148 245	−1.362 698 698
	4	−0.320 485 340	−0.121 606 922	−1.353 069 424	−1.099 398 515	−1.360 637 524
5	0	−0.394 833 886	−0.149 288 907	−1.671 469 715	−1.360 116 144	−1.679 822 917
	1	−0.394 771 542	−0.149 279 532	−1.670 951 742	−1.359 674 023	−1.679 303 323
	2	−0.394 646 854	−0.149 260 783	−1.669 915 721	−1.358 789 934	−1.678 263 938
	3	−0.394 459 821	−0.149 232 663	−1.668 361 692	−1.357 463 945	−1.676 705 078
	4	−0.394 210 451	−0.149 195 166	−1.666 289 908	−1.355 695 956	−1.674 626 437
	5	−0.393 898 743	−0.149 148 297	−1.663 700 136	−1.353 485 989	−1.672 028 338
6	0	−0.469 420 044	−0.177 074 336	−1.988 886 468	−1.620 473 134	−1.997 673 567
	1	−0.469 357 301	−0.177 064 931	−1.988 363 928	−1.620 026 744	−1.997 149 548
	2	−0.469 231 814	−0.177 046 120	−1.987 318 690	−1.619 133 434	−1.996 101 546
	3	−0.469 043 594	−0.177 017 907	−1.985 750 985	−1.617 793 611	−1.994 529 545
	4	−0.468 792 626	−0.176 980 288	−1.983 660 639	−1.616 007 412	−1.992 433 758
	5	−0.468 478 925	−0.176 933 265	−1.981 047 963	−1.613 774 723	−1.989 814 254
	6	−0.468 102 492	−0.176 876 837	−1.977 912 901	−1.611 095 634	−1.986 670 600
7	0	−0.544 860 232	−0.205 056 063	−2.310 447 874	−1.884 840 245	−2.319 338 467
	1	−0.544 797 097	−0.205 046 628	−2.309 920 665	−1.884 389 145	−2.318 809 929
	2	−0.544 670 819	−0.205 027 756	−2.308 866 326	−1.883 486 923	−2.317 753 276
	3	−0.544 481 405	−0.204 999 450	−2.307 284 746	−1.882 133 323	−2.316 168 345
	4	−0.544 228 850	−0.204 961 709	−2.305 176 089	−1.880 328 918	−2.314 055 274
	5	−0.543 913 166	−0.204 914 532	−2.302 540 413	−1.878 073 478	−2.311 414 009
	6	−0.543 534 355	−0.204 857 921	−2.299 377 826	−1.875 366 92	−2.308 244 687
	7	−0.543 092 414	−0.204 791 875	−2.295 688 306	−1.872 209 698	−2.304 547 249

$I_2\left(X\left(O_g^+\right)\right)$, $N_2\left(X^1\Sigma_g^+\right)$, $O_2^+\left(X^2\Pi_g\right)$ and $NO^+\left(X^1\Sigma^+\right)$ in table 4. For the mentioned diatomic molecules, expectation values of $\langle V\rangle_{n\ell}$, $\left\langle p^2\right\rangle_{n\ell}$, $\langle T\rangle_{n\ell}$, $\langle T/V\rangle_{n\ell}$, $\langle r^{-2}\rangle_{n\ell}$ are represented in tables 5 and 6. We have shown the behavior of the energy of the non-relativistic limit of TW potential as a function of b_h, μ, c_h, r_e and D in figures 2–6. We have also represented the behavior of the energy of TW potential for different values of n and ℓ in figures 7–11.

The energy of the Dirac equation in the case of the spin symmetry limit and pseudospin symmetry limit under the TW diatomic molecular potential is represented in tables 7 and 8, respectively, for different values of n and κ. From table 7, we can deduce that there are degeneracies between the eigenstates $(np_{1/2}, np_{3/2})$, $(nd_{3/2}, nd_{5/2})$, $(nf_{5/2}, nf_{7/2})$, $(ng_{7/2}, ng_{9/2})$, etc. It is worth mentioning that each of these eigenstates form a spin doublet. For example, for any specific value of n,

where $n = 0, 1, 2,...,$ $np_{1/2}$ with $\kappa = 1$ is considered as the partner of $np_{3/2}$ with $\kappa = 2$. Again, from table 8, we can deduce that there are degeneracies between the eigenstates $(ns_{1/2}, (n-1)d_{3/2})$, $(np_{3/2}, (n1)f_{5/2})$, $(nd_{5/2}, (n-1)g_{7/2})$, $(nf_{7/2}, (n-1)h_{9/2})$, etc. It is worth noting that, each of these eigenstates form a pseudospin doublet. For example, for specific value of $n = 1$, $1s_{1/2}$ with $\kappa = -1$ is considered as the partner of $0d_{3/2}$ with $\kappa = 2$. Thus, states that have pseudo orbital-angular momentum $\tilde{\ell}$ quantum numbers, radial n and $n - 1$ with $j = \tilde{\ell} - 1/2$ and $j = \tilde{\ell} + 1/2$, respectively, are degenerate.

7. Conclusions

In this paper, we have shown the beauty of eigensolution techniques via approximate bound-state solutions of the

Table 5. Expectation values of $\langle V\rangle_{n\ell}\,(eV)$, $\langle p^2\rangle_{n\ell}\,(eV)$, $\langle T\rangle_{n\ell}\,(eV\,\text{Å}^{-1})$, $\langle T/V\rangle_{n\ell}\,(eV\,\text{Å}^{-1})$, $\langle r^{-2}\rangle_{n\ell}\,(eV\,\text{Å}^{-1})$, $\langle V\rangle_{n\ell}\,(eV)$, $\langle p^2\rangle_{n\ell}\,(eV)$, $\langle T\rangle_{n\ell}\,(eV\,\text{Å}^{-1})$, $\langle T/V\rangle_{n\ell}\,(eV\,\text{Å}^{-1})$, $\langle r^{-2}\rangle_{n\ell}\,(eV\,\text{Å}^{-1})$ corresponding to TW potential with various n and ℓ quantum numbers for $H_2(X^1\Sigma_g^+)$, $CO(X^1\Sigma^+)$, $HF(X^1\Sigma^+)$, $O_2(X^3\Sigma_g^+)$, $NO(X^2\Pi_r)$ and $Cl_2(X^1\Sigma_g^+)$ diatomic molecules.

$H_2(X^1\Sigma_g^+)$ Diatomic molecule / $CO(X^1\Sigma^+)$ Diatomic molecule

n	ℓ	$\langle V\rangle_{n\ell}$	$\langle p^2\rangle_{n\ell}$	$\langle T\rangle_{n\ell}$	$\langle T/V\rangle_{n\ell}$	$\langle r^{-2}\rangle_{n\ell}$	$\langle V\rangle_{n\ell}$	$\langle p^2\rangle_{n\ell}$	$\langle T\rangle_{n\ell}$	$\langle T/V\rangle_{n\ell}$	$\langle r^{-2}\rangle_{n\ell}$
0	0	0.136 646 347	11 761 824 963.6	112 325 124.629	822 013 373.171	17 696 441 386	0.075 611 988	4076 474 146.97	2853 524.185 76	37 739 044.5780	7815 433 017.7
	5	0.144 410 929	11 652 913 581.6	111 285 023.743	770 613 585.229	16 930 544 843	0.075 632 410	4076 661 983.18	2853 655.670 75	37 730 592.8867	7814 265 945.0
	10	0.201 431 069	11 372 661 386.7	108 608 622.520	539 185 057.495	15 181 051 187	0.075 692 046	4077 162 943.39	2854 006.341 95	37 705 498.6986	7811 153 289.6
5	0	2.774 220 723	11 744 033 916.5	112 155 220.588	40 427 648.6215	13 156 799 314	1.584 869 235	4076 193 491.98	2853 327.727 80	18 003 553.0048	7384 185 493.1
	5	2.818 977 983	11 630 287 679.9	111 068 946.966	39 400 430.8071	12 620 296 343	1.585 263 957	4076 378 680.13	2853 457.359 16	17 999 887.9465	7383 030 423.9
	10	2.946 710 003	11 339 677 399.5	108 293 626.294	36 750 690.1540	11 396 406 805	1.586 321 554	4076 872 577.36	2853 803.086 28	17 990 066.8883	7379 949 787.1
7	0	4.494 731 690	11 729 814 715.1	112 019 427.582	24 922 383.6500	11 597 034 082	1.881 625 750	4075 954 419.26	2853 160.377 35	1516 327.238 48	7215 106 777.5
	5	3.785 165 467	11 614 622 325.2	110 919 343.234	29 303 697.3419	11 135 810 214	2.185 570 465	4076 138 565.08	2853 289.279 08	1305 512.370 69	7213 956 498.7
	10	3.928 165 719	11 320 959 571.8	108 114 871.523	27 522 991.4563	10 085 139 484	2.186 995 973	4076 629 682.30	2853 633.060 20	1304 818.616 69	7210 888 638.4

$HF(X^1\Sigma^+)$ Diatomic molecule / $O_2(X^3\Sigma_g^+)$ Diatomic molecule

n	ℓ	$\langle V\rangle_{n\ell}$	$\langle p^2\rangle_{n\ell}$	$\langle T\rangle_{n\ell}$	$\langle T/V\rangle_{n\ell}$	$\langle r^{-2}\rangle_{n\ell}$	$\langle V\rangle_{n\ell}$	$\langle p^2\rangle_{n\ell}$	$\langle T\rangle_{n\ell}$	$\langle T/V\rangle_{n\ell}$	$\langle r^{-2}\rangle_{n\ell}$
0	0	0.128 298 808	10 734 402 400.0	53 819 464.4828	419 485 304.047	11 659 305 959	0.048 990 53	12 036 391 366.8	7221 815.289 29	14 741 247.5213	6821 023 698
	5	0.129 283 327	10 731 490 713.3	53 804 866.0531	416 177 919.471	11 588 335 479	0.049 007 87	12 036 676 718.3	7221 986.499 73	14 736 381.1154	6819 660 995
	10	0.134 115 260	10 723 642 492.3	53 765 517.1415	400 890 376.990	11 401 257 947	0.049 059 22	12 037 437 741.7	7222 443.112 53	14 721 887.3690	6816 026 510
5	0	2.657 367 932	10 729 489 031.8	53 794 830.1496	20 243 651.4349	94 490 582 249	1.028 234 10	12 036 342 934.0	7221 786.229 69	7023 484.466 90	6391 758 894
	5	2.670 751 754	10 726 160 798.4	53 778 143.2645	20 135 957.2952	93 865 980 863	1.028 581 75	12 036 627 749.4	7221 957.118 46	7021 276.741 94	6390 390 585
	10	2.707 930 317	10 717 218 863.8	53 733 310.7612	19 842 944.4155	92 219 375 660	1.029 514 25	12 037 387 342.8	7222 412.873 27	7015 359.790 57	6386 741 161
7	0	3.321 571 334	10 725 418 673.9	53 774 422.4479	16 189 452.8344	86 193 084 922	1.213 305 71	12 036 301 143.3	7221 761.155 33	5952 136.461 41	6220 935 758
	5	3.645 331 889	10 721 939 419.0	53 756 978.3808	14 746 799.4733	85 599 535 298	1.419 714 53	12 036 585 744.4	7221 931.915 53	5086 890.190 19	6219 565 251
	10	3.692 547 139	10 712 600 971.5	53 710 157.8663	14 545 557.8072	84 034 738 438	1.420 992 17	12 037 344 766.2	7222 387.327 38	5082 636.963 00	6215 909 951

$NO(X^2\Pi_r)$ Diatomic molecule / $Cl_2(X^1\Sigma_g^+)$ Diatomic molecule

n	ℓ	$\langle V\rangle_{n\ell}$	$\langle p^2\rangle_{n\ell}$	$\langle T\rangle_{n\ell}$	$\langle T/V\rangle_{n\ell}$	$\langle r^{-2}\rangle_{n\ell}$	$\langle V\rangle_{n\ell}$	$\langle p^2\rangle_{n\ell}$	$\langle T\rangle_{n\ell}$	$\langle T/V\rangle_{n\ell}$	$\langle r^{-2}\rangle_{n\ell}$
0	0	0.059 0176	26 580 624 128.6	17 071 992.8022	289 269 519.638	750 378 933	−0.017 349 478	1868 181 521.14	512 534.597 566	−29 541 787.8028	2541 386 767.17
	5	0.059 0366	26 581 001 395.9	17 072 235.1104	289 180 527.171	750 235 856	−0.017 350 980	1868 177 966.36	512 533.622 314	−29 539 174.2895	2541 272 947.27
	10	0.059 0936	26 582 007 513.8	17 072 881.3119	288 912 527.108	749 854 277	−0.017 354 794	1868 168 484.96	512 531.021 097	−29 532 532.6879	2540 969 404.79
5	0	1.239 0649	26 580 599 933.8	17 071 977.2625	13 778 113.8522	705 954 452	−0.364 630 615	1868 136 832.41	512 522.337 237	−1405 593.266 59	2626 168 878.47
	5	1.239 4521	26 580 976 932.6	17 072 219.3983	13 774 004.9803	705 810 846	−0.364 661 440	1868 133 492.16	512 521.420 841	−1405 471.938 14	2626 057 663.46
	10	1.240 4910	26 581 982 333.9	17 072 865.1395	13 762 989.9286	705 427 857	−0.364 743 463	1868 124 582.90	512 518.976 590	−1405 149.176 29	2625 761 068.01
7	0	1.457 1502	26 580 579 009.2	17 071 963.8232	11 715 994.5647	688 228 928	−0.433 577 209	1868 098 543.87	512 511.832 796	−1182 054.365 77	2659 649 378.39
	5	1.711 2425	26 580 955 900.5	17 072 205.8900	9976 497.130 01	688 085 112	−0.503 935 502	1868 095 287.81	512 510.939 498	−1017 016.934 64	2659 539 185.33
	10	1.712 6703	26 581 961 015.6	17 072 851.4474	9968 556.964 76	687 701 561	−0.504 047 245	1868 086 603.11	512 508.556 855	−101 678 674 358	2659 245 315.23

Table 6. Expectation values of $\langle V \rangle_{n\ell}(eV)$, $\langle p^2 \rangle_{n\ell}(eV)$, $\langle T \rangle_{n\ell}(eV\,\text{Å}^{-1})$, $\langle T/V \rangle_{n\ell}(eV\,\text{Å}^{-1})$, $\langle r^{-2} \rangle_{n\ell}(eV\,\text{Å}^{-1})$, $\langle V \rangle_{n\ell}(eV)$, $\langle p^2 \rangle_{n\ell}(eV)$, $\langle T \rangle_{n\ell}(eV\,\text{Å}^{-1})$, $\langle T/V \rangle_{n\ell}(eV\,\text{Å}^{-1})$, $\langle r^{-2} \rangle_{n\ell}(eV\,\text{Å}^{-1})$ corresponding to T-W potential with various n and ℓ quantum numbers for $H_2(X^1\Sigma_g^+)$, $CO(X^1\Sigma^+)$, $HF(X^1\Sigma^+)$, $O_2(X^3\Sigma_g^+)$, $NO(X^2\Pi_r)$ and $Cl_2(X^1\Sigma_g^+)$ diatomic molecules.

		$I_2(X(O_g^+))$ Diatomic molecule					$N_2(X^1\Sigma_g^+)$ Diatomic molecule				
n	ℓ	$\langle V \rangle_{n\ell}$	$\langle p^2 \rangle_{n\ell}$	$\langle T \rangle_{n\ell}$	$\langle T/V \rangle_{n\ell}$	$\langle r^{-2} \rangle_{n\ell}$	$\langle V \rangle_{n\ell}$	$\langle p^2 \rangle_{n\ell}$	$\langle T \rangle_{n\ell}$	$\langle T/V \rangle_{n\ell}$	$\langle r^{-2} \rangle_{n\ell}$
0	0	−0.006 648 8341	558 513 328.245	42 219.956 6751	−63 49 978.964 75	1409 346 961.10	−0.073 107 27	13 906 362 690.4	9526 604.594 97	−130 309 948.586	8348 868 372
	5	−0.006 648 9510	558 513 226.961	42 219.949 0187	−63 49 866.169 67	1409 336 874.82	−0.073 124 01	13 906 169 383.6	9526 472.169 44	−130 278 306.256	8347 453 937
	10	−0.006 649 2578	558 512 956.830	42 219.928 5986	−63 49 570.112 71	1409 309 977.40	−0.073 162 54	13 905 653 924.6	9526 119.052 37	−130 204 870.585	8343 682 339
5	0	−0.139 681 5777	558 503 274.986	42 219.196 7145	−302 253.148 981	1433 074 557.92	−1.535 802 25	13 906 316 966.1	9526 573.271 37	−6202 994.735 40	8738 662 788
	5	−0.139 683 9663	558 503 189.934	42 219.190 2851	−302 247.934 415	1433 064 691.37	−1.536 161 58	13 906 124 198.4	9526 441.215 15	−6201 457.801 82	8737 250 549
	10	−0.139 690 3321	558 502 963.077	42 219.173 1362	−302 234.037 972	1433 038 379.92	−1.537 113 65	13 905 610 176.6	9526 089.082 64	−6197 387.605 43	8733 484 812
7	0	−0.166 220 5103	558 494 650.466	42 218.544 7571	−253 991.187 254	1442 464 239.81	−1.835 087 55	13 906 277 500.7	9526 546.235 46	−5191 330.645 48	8893 782 600
	5	−0.192 965 5280	558 494 571.802	42 218.538 8107	−218 787.983 783	1442 454 459.66	−2.122 047 01	13 906 084 947.8	9526 414.326 39	−4489 256.968 15	8892 371 246
	10	−0.192 974 2157	558 494 361.947	42 218.522 9470	−218 778.051 741	1442 428 378.52	−2.123 357 04	13 905 571 499.1	9526 062.586 48	−4486 321.615 74	8888 607 862

|		$O_2^+(X^2\Pi_g)$ Diatomic molecule					$NO^+(X^1\Sigma^+)$ Diatomic molecule				
0	0	−0.059 0531	17 376 639 579.0	10 425 955.5513	−176 552 214.046	8073 402 239.2	−0.073 7188	16 182 723 972.9	10 477 599.7280	−142 129 276.765	8888 672 445
	5	−0.059 0698	17 376 605 854.2	10 425 935.3165	−176 501 957.286	8071 902 694.6	−0.073 7345	16 182 434 514.2	10 477 412.3163	−142 096 472.022	8887 171 024
	10	−0.059 1083	17 376 515 914.2	10 425 881.3526	−176 386 080.341	8067 903 742.1	−0.073 7702	16 181 662 688.7	10 476 912.5933	−142 020 932.481	8883 167 721
5	0	−1.240 5016	17 376 610 367.6	10 425 938.0245	−8404 614.733 67	8514 294 721.8	−1.548 5101	16 182 688 492.1	10 477 576.7558	−6766 230.814 90	9276 047 969
	5	−1.240 8588	17 376 576 977.4	10 425 917.9904	−8402 179.192 67	8512 803 533.9	−1.548 8481	16 182 399 470.1	10 477 389.6268	−6764 633.424 54	9274 543 700
	10	−1.241 8058	17 376 487 929.6	10 425 864.5619	−8395 728.673 44	8508 826 861.9	−1.549 7435	16 181 628 808.8	10 476 890.6576	−6760 403.032 89	9270 532 816
7	0	−1.472 1570	17 376 585 124.8	10 425 922.8788	−7082 072.685 73	8690 035 133.6	−1.858 9035	16 182 657 844.7	10 477 556.9129	−5636 417.873 71	9430 334 769
	5	−1.714 0431	17 376 551 867.4	10 425 902.9245	−6082 637.551 24	8688 547 269.4	−2.139 3993	16 182 368 997.2	10 477 369.8969	−4897 341.930 00	9428 829 391
	10	−1.715 3485	17 376 463 175.1	10 425 849.7092	−6077 977.570 86	8684 579 467.2	−2.140 6326	16 181 598 801.1	10 476 871.2289	−4894 287.431 15	9424 815 522
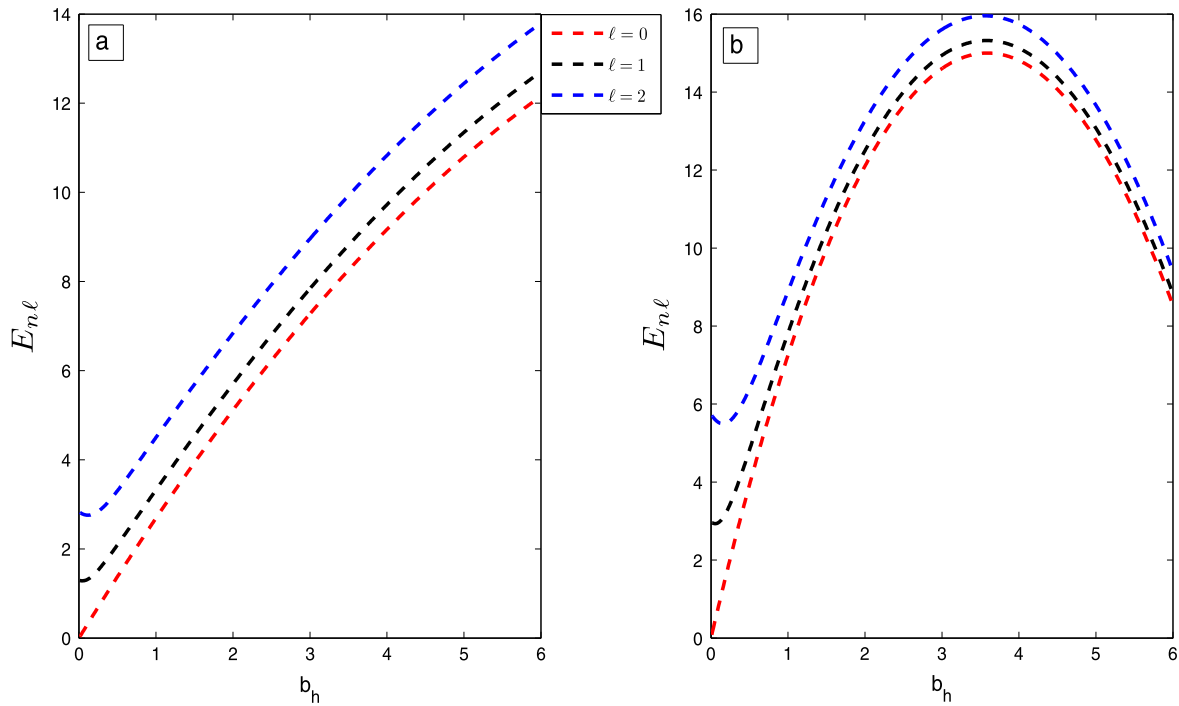
Figure 2. (a) The variation of the ground state energy spectrum for various values of ℓ as a function of the parameter b_h. We choose $c_h = 0.03$, $\mu = 1$, $r_e = 1.207$ and $D = 15$. (b) The variation of the first excited energy state for various ℓ as a function of the parameter b_h.
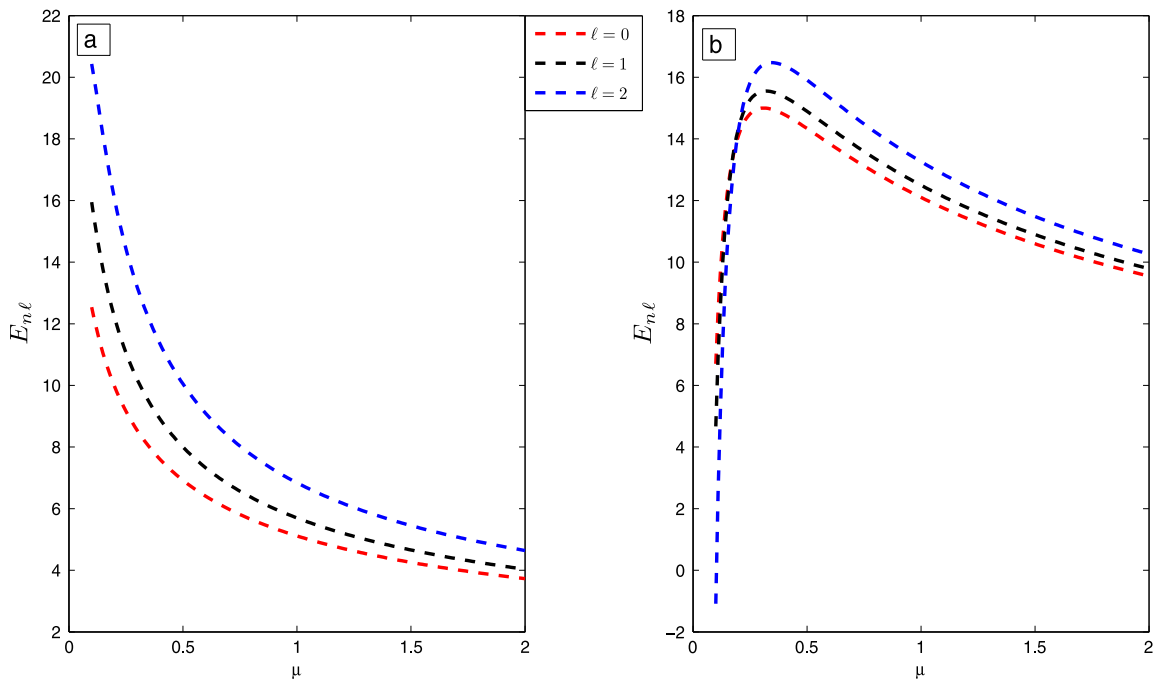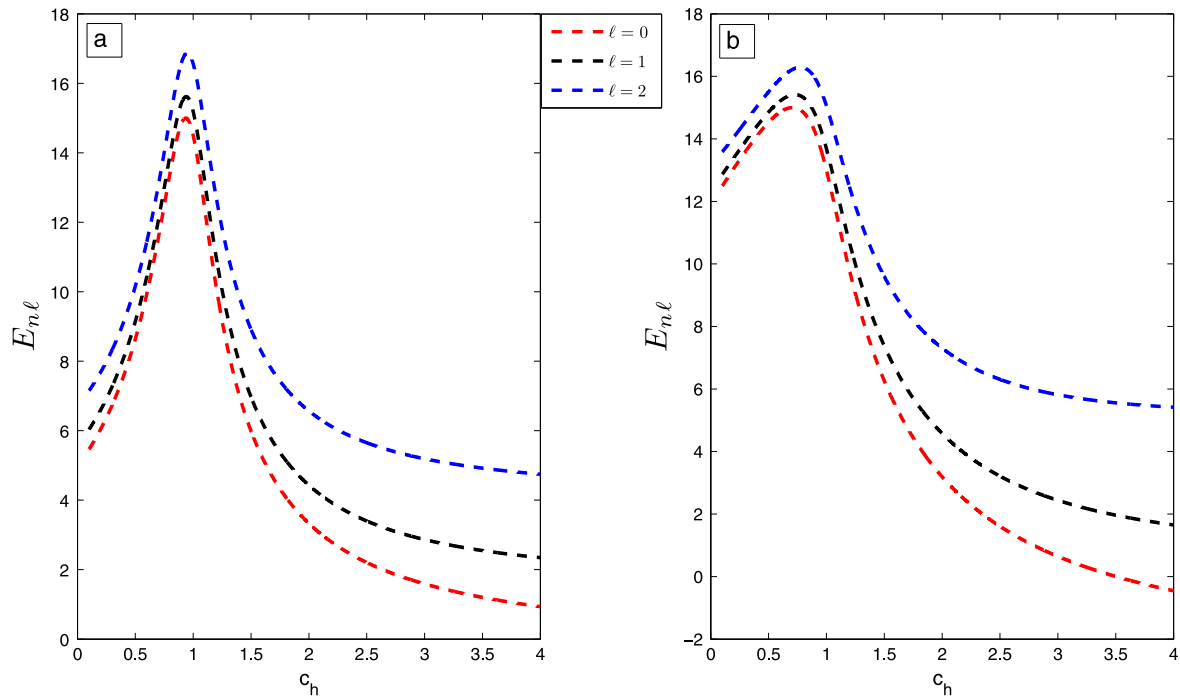

Figure 3. (a) The variation of the ground state energy spectrum for various values of ℓ as a function of the particle mass μ. We choose $c_h = 0.03$, $b_h = 2$, $r_e = 1.207$ and $D = 15$. (b) The variation of the first excited energy state for various ℓ as a function of the particle mass μ.

Schrödinger, Klein–Gordon and Dirac equations for TW diatomic molecular potential. For each type of wave equation, and by applying an approximation to the centrifugal term, we have obtained the energy eigenvalues and the corresponding wave functions for any quantum state. As a further guide to interested readers, we have provided some numerical data and figures that discuss the energy spectrum in each case. The probability distributions of TW diatomic molecular

Figure 4. (a) The variation of the ground state energy spectrum for various values of ℓ as a function of the potential constant c_h. We choose $\mu = 1$, $b_h = 2$, $r_e = 1.207$ and $D = 15$. (b) The variation of the first excited energy state for various ℓ as a function of the potential constant c_h.
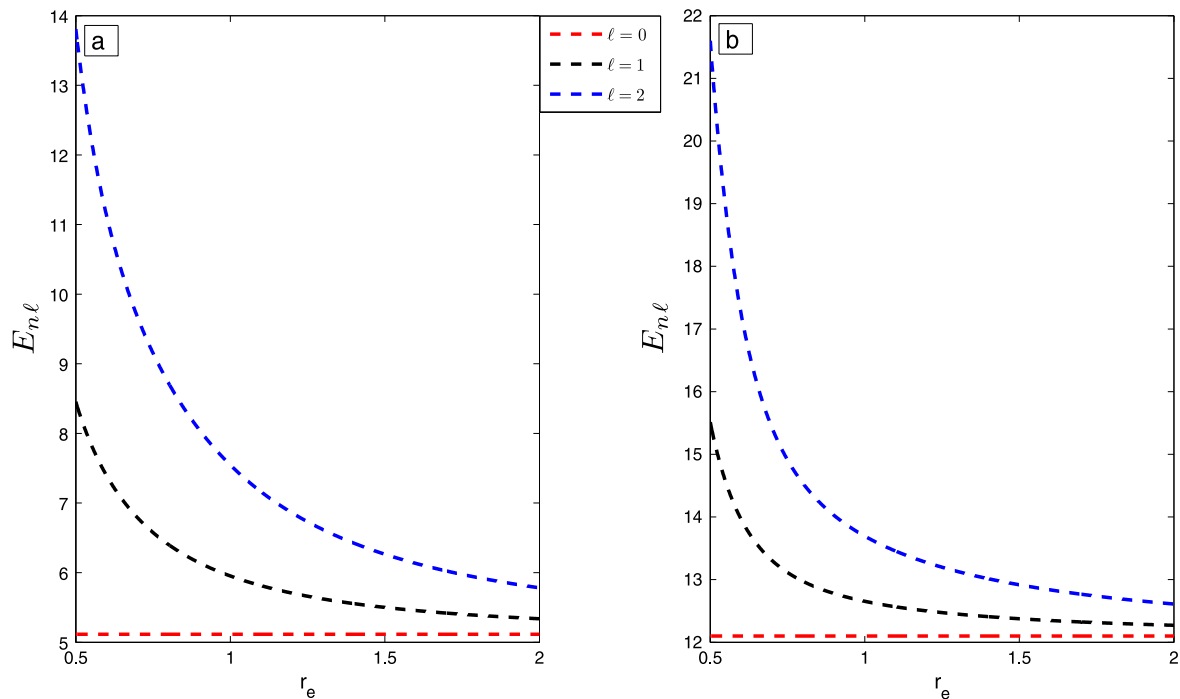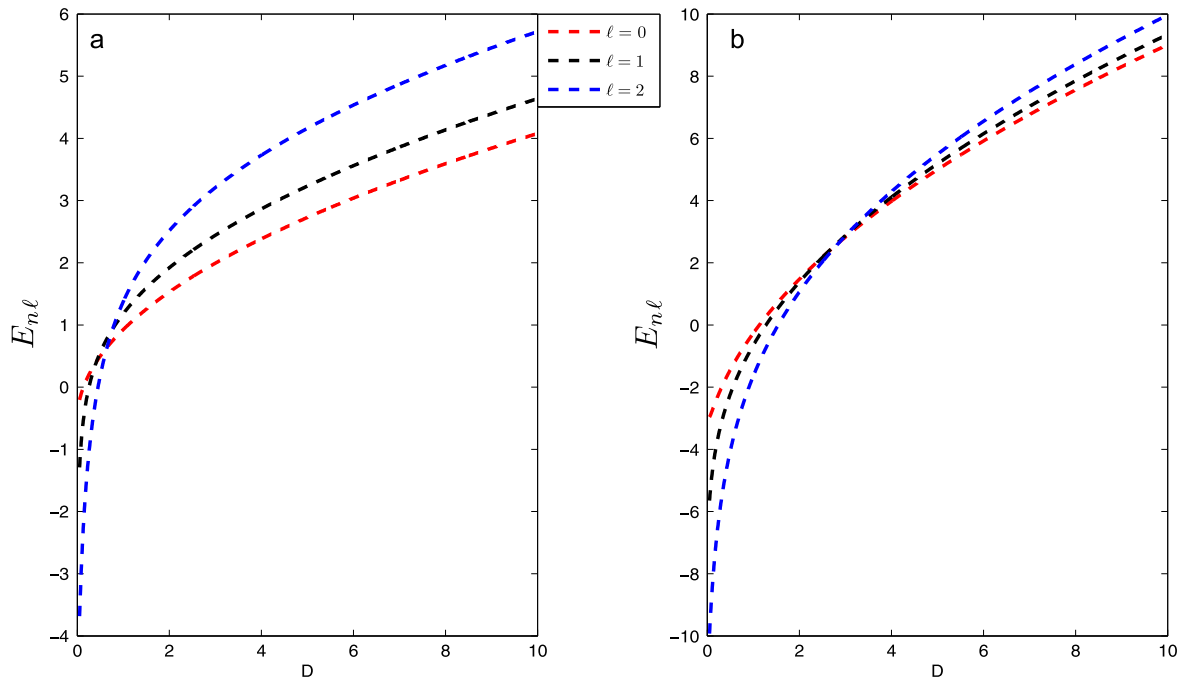

Figure 5. (a) The variation of the ground state energy spectrum for various values of ℓ as a function of the molecular bond length r_e. We choose $\mu = 1$, $b_h = 2$, $c_h = 0.03$ and $D = 15$. (b) The variation of the first excited energy state for various ℓ as a function of the molecular bond length r_e.

potential were also analyzed. Our obtained solutions could find application in various branches of physics and chemistry where non-relativistic and relativistic systems are investigated.

Acknowledgements

Figure 6. (a) The variation of the ground state energy spectrum for various values of ℓ as a function of the potential well depth D. We choose $\mu = 1$, $b_h = 2$, $c_h = 0.03$ and $r_e = 1.207$. (b) The variation of the first excited energy state for various ℓ as a function of the potential well depth D.
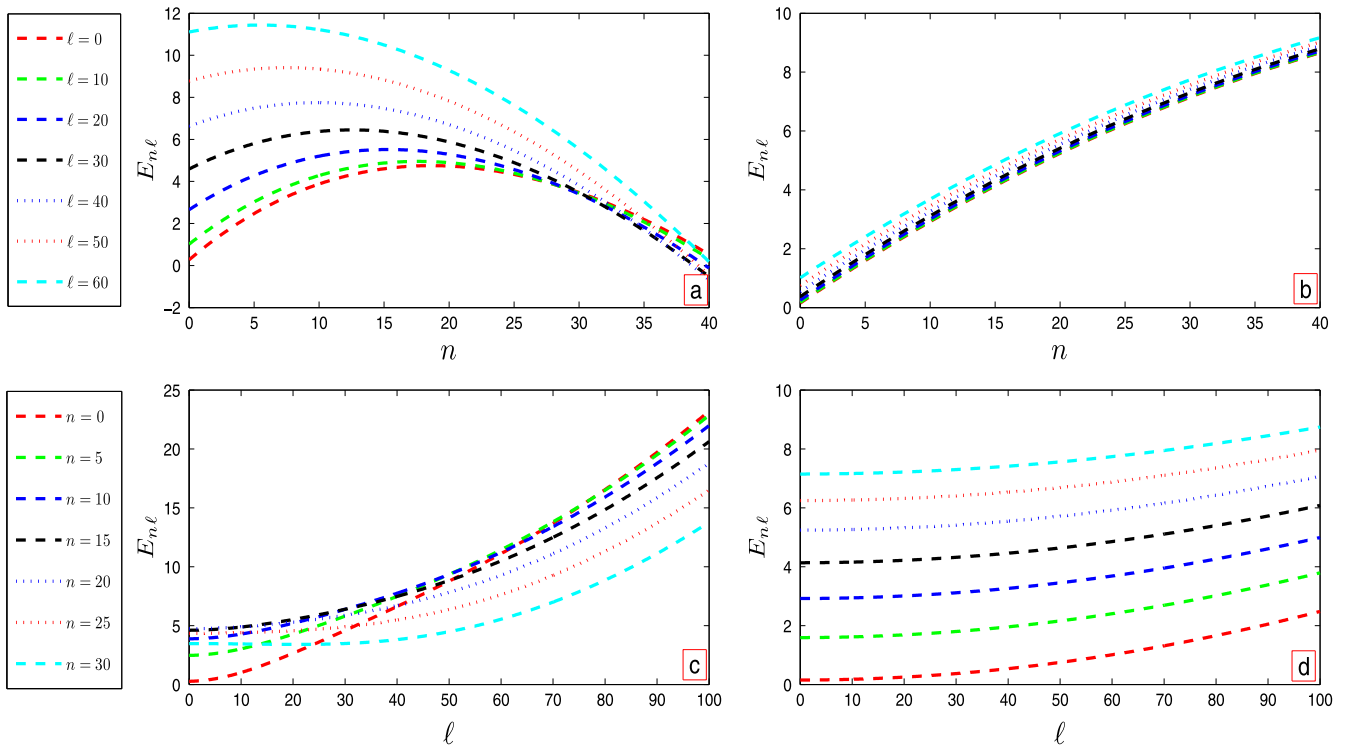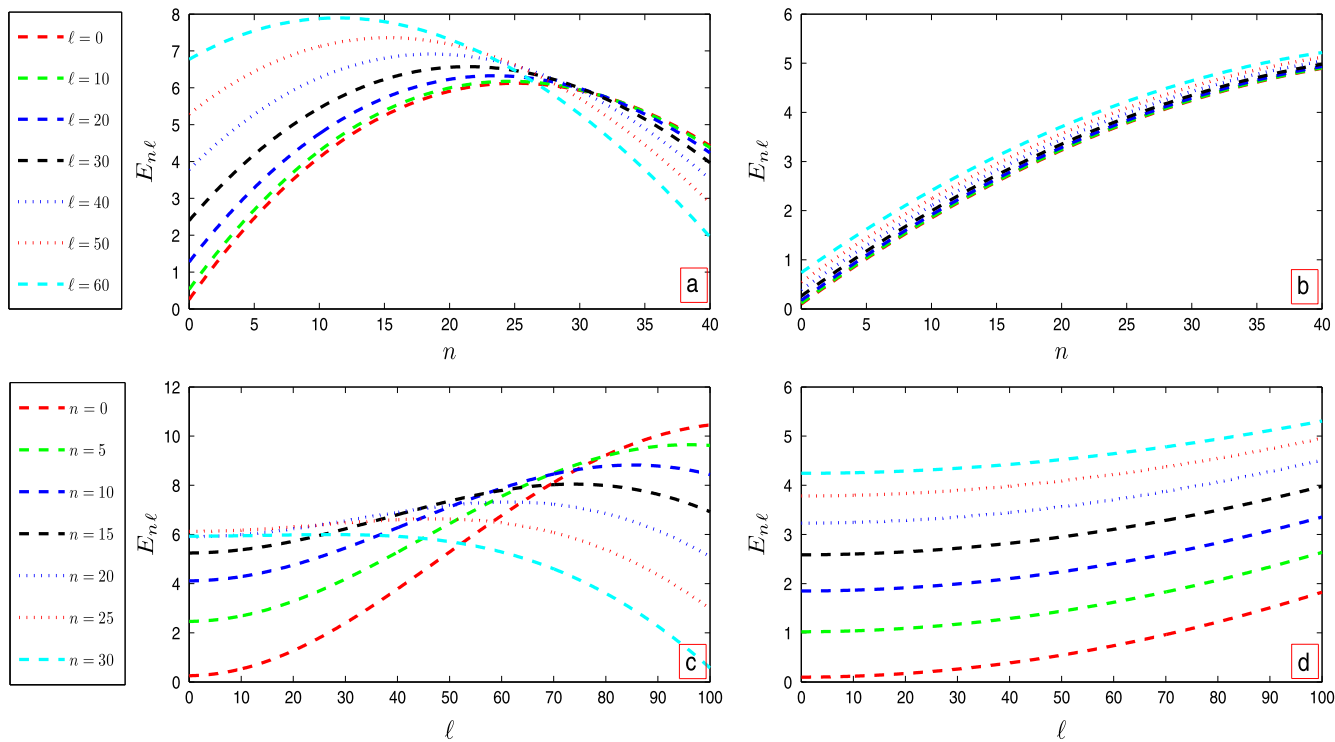

Figure 7. (a) The variations of energy (in eV) in TW diatomic molecular potential, with respect to vibrational (n) for $H_2\left(X^1\Sigma_g^+\right)$ molecules. (b) Same as (a) but for $CO\left(X^1\Sigma^+\right)$ (c) The variations of energy (in eV) in TW diatomic molecular potential, with respect to rotational ℓ for $H_2\left(X^1\Sigma_g^+\right)$ molecules. (d) Same as (c) but for $CO\left(X^1\Sigma^+\right)$.
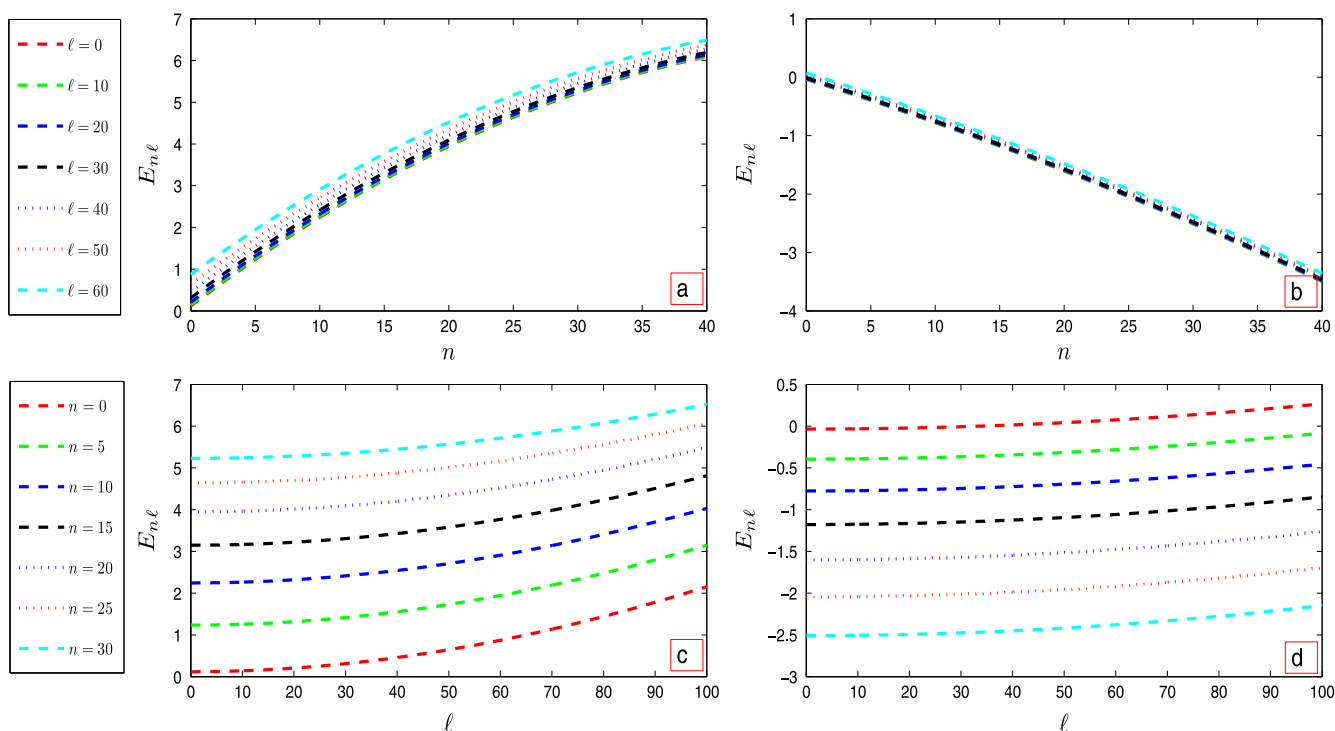
Figure 8. (a) The variations of energy (in eV) in TW diatomic molecular potential, with respect to vibrational (n) for $HF\left(X^1\Sigma^+\right)$ molecules. (b) Same as (a) but for $O_2\left(X^3\Sigma_g^+\right)$ (c) The variations of energy (in eV) in TW diatomic molecular potential, with respect to rotational ℓ for $HF\left(X^1\Sigma^+\right)$ molecules. (d) Same as (c) but for $O_2\left(X^3\Sigma_g^+\right)$.

Figure 9. (a) The variations of energy (in eV) in TW diatomic molecular potential, with respect to vibrational (n) for $NO\left(X^2\Pi_r\right)$ molecules. (b) Same as (a) but for $Cl_2\left(X^1\Sigma_g^+\right)$ (c) The variations of energy (in eV) in TW diatomic molecular potential, with respect to rotational ℓ for $NO\left(X^2\Pi_r\right)$ molecules. (d) Same as (c) but for $Cl_2\left(X^1\Sigma_g^+\right)$.

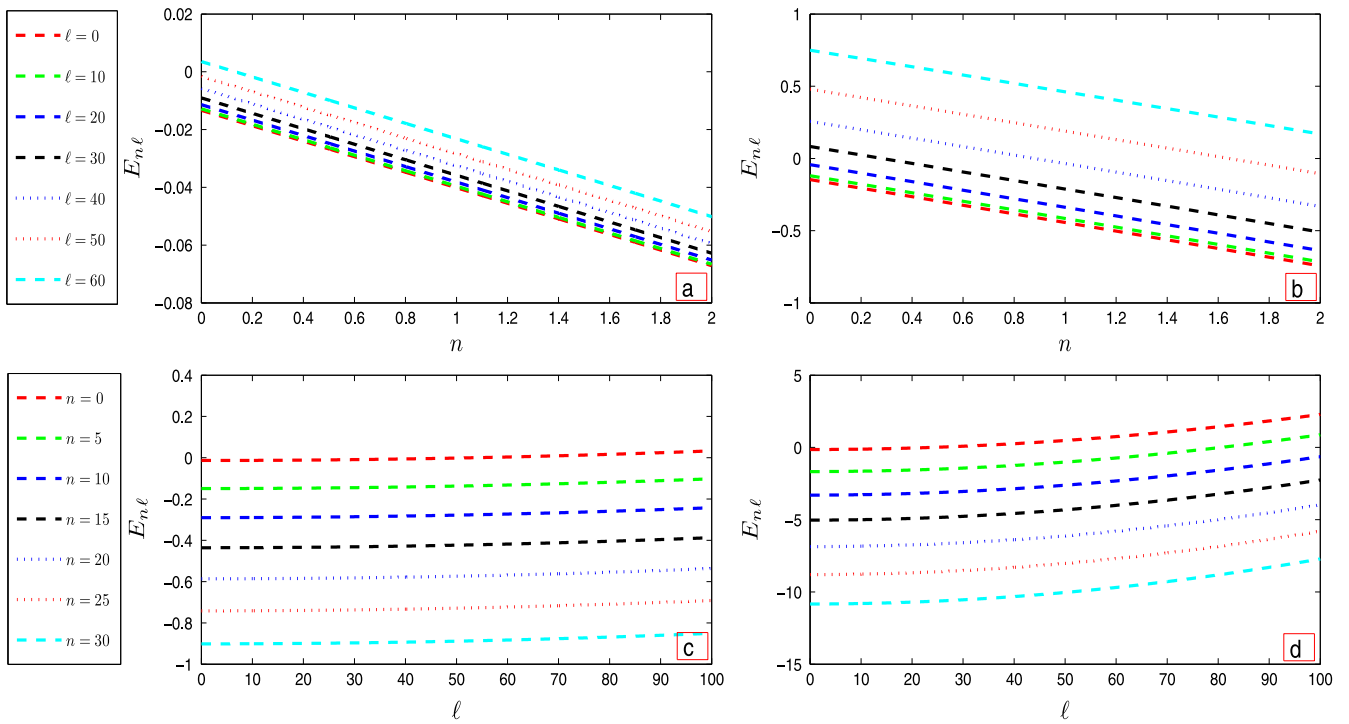**Figure 10.** (a) The variations of energy (in eV) in TW diatomic molecular potential, with respect to vibrational (*n*) for $I_2\left(X\left(O_g^+\right)\right)$ molecules. (b) Same as (a) but for $N_2\left(X^1\Sigma_g^+\right)$ (c) The variations of energy (in eV) in TW diatomic molecular potential, with respect to rotational ℓ for $I_2\left(X\left(O_g^+\right)\right)$ molecules. (d) Same as (c) but for $N_2\left(X^1\Sigma_g^+\right)$.
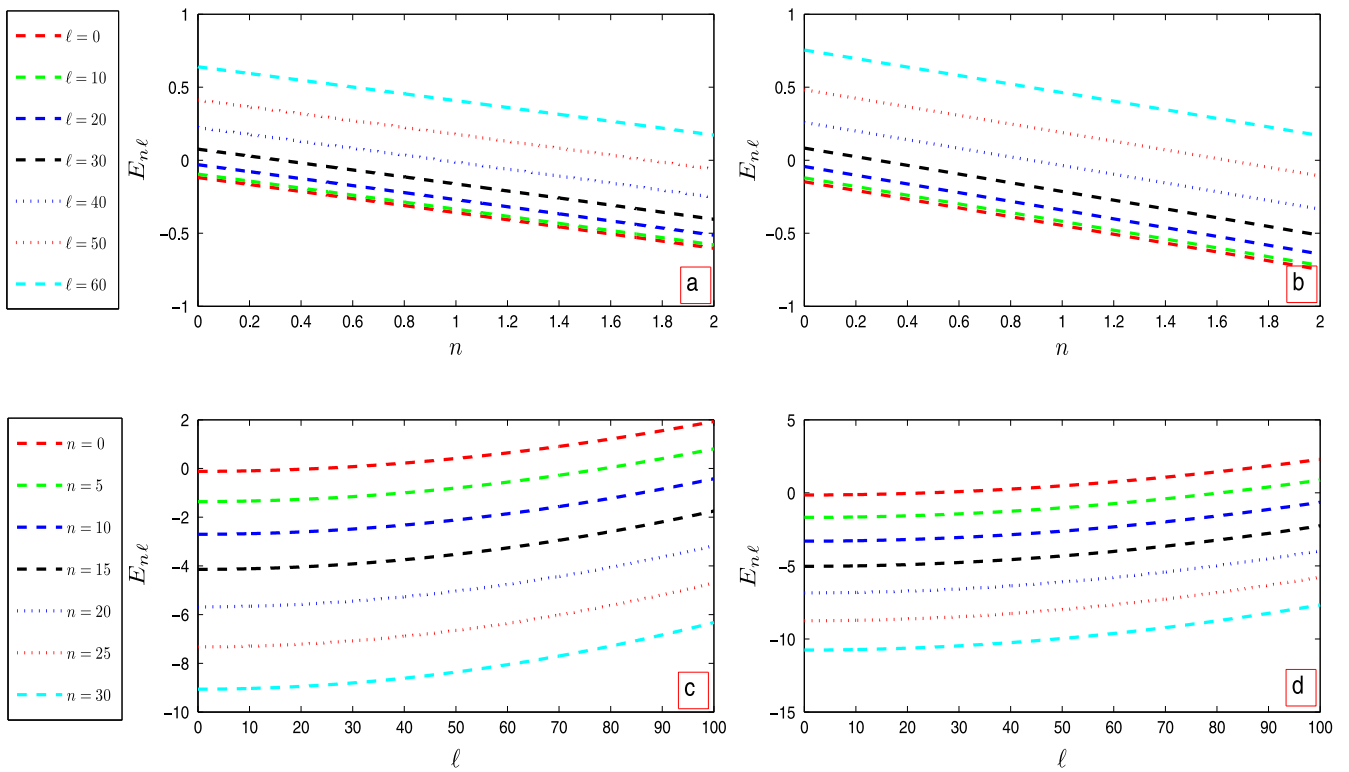

Figure 11. (a) The variations of energy (in eV) in TW diatomic molecular potential, with respect to vibrational (*n*) for $O_2^+\left(X^2\Pi_g\right)$ molecules. (b) Same as (a) but for $NO^+\left(X^1\Sigma^+\right)$ (c) The variations of energy (in eV) in TW diatomic molecular potential, with respect to rotational ℓ for $O_2^+\left(X^2\Pi_g\right)$ molecules. (d) Same as (c) but for $NO^+\left(X^1\Sigma^+\right)$.

Table 7. The positive-energy degenerate states in units of fm^{-1} of the spin-symmetry TW diatomic molecular potential for various values of n and b_h. We use the following parameters: $ch = 0.027262$, $M = 5$ fm^{-1}, $r_e = 0.8$, $D = 15$ fm^{-1}.

ℓ	$n, \kappa<0, \kappa>0$	b_h	Degenerate states	$E_{n\kappa}(C_s = 5$ fm$^{-1})$	$E_{n\kappa}(C_s = 0)$	ℓ	$n, \kappa<0, \kappa>0$	b_h	Degenerate states	$E_{n\kappa}(C_s = 5$ fm$^{-1})$	$E_{n\kappa}(C_s = 0)$
1	0, −2, 1	0.005	$(0p_{1/2},\ 0p_{3/2})$	5.985 911 24	−5.558 871 52	1	1, −2, 1	0.005	$(1p_{1/2},\ 1p_{3/2})$	−1.948 501 26	6.208 186 81
				−0.985 831 05	5.558 951 66					6.948 685 19	−6.208 002 86
		0.010		−0.984 421 17	5.558 317 92			0.010		6.946 199 96	−6.205 858 92
				5.984 742 42	−5.557 996 75					−1.945 462 81	6.206 595 93
		0.015		5.983 708 35	−5.557 111 37			0.015		6.943 985 91	−6.203 665 97
				−0.982 984 07	5.557 835 19					−1.942 324 05	6.205 327 08
		0.020		−0.981 519 69	5.557 503 91			0.020		−1.939 084 61	−6.201 423 91
				5.982 809 72	−5.556 215 33					6.942 044 59	6.204 381 52
2	0, −3, 2	0.005	$(0d_{3/2},\ 0d_{5/2})$	−1.871 566 70	6.153 157 90	2	1, −3, 2	0.005	$(1d_{3/2},\ 1d_{5/2})$	−3.186 871 40	7.147 889 10
				6.871 624 80	−6.153 099 70					8.186 989 60	−7.147 771 00
		0.010		6.869 650 28	6.151 816 20			0.010		8.183 140 07	−7.144 451 73
				−1.869 416 85	−6.151 582 81					−3.182 666 53	7.144 925 26
		0.015		6.867 762 53	6.150 577 42			0.015		8.179 443 70	7.142 150 24
				−1.867 236 13	−6.150 051 14					−3.178 375 88	−7.141 082 60
		0.020		6.865 962 28	−6.148 504 68			0.020		8.175 901 52	−7.137 663 36
				−1.865 024 32	6.149 442 23					−3.173 999 07	7.139 565 23
3	0, −4, 3	0.005	$(0f_{5/2},\ 0f_{7/2})$	−2.800 587 70	−6.844 433 90	3	1, −4, 3	0.005	$(1f_{5/2},\ 1f_{5/2})$	−4.34151230	−8.096 690 90
				7.800 637 10	6.844 483 50					9.341 604 20	8.096 782 90
		0.010		7.798 039 49	6.842 515 94			0.010		9.336 783 07	−8.092 405 55
				−2.797 841 21	−6.842 317 64					−4.336 415 00	8.092 773 62
		0.015		−2.795 061 25	−6.840 182 80			0.015		−4.331 239 46	−8.088 069 26
				7.795 508 42	6.840 629 92					9.332 069 49	8.088 899 24
		0.020		−2.792 247 58	−6.838 029 32			0.020		9.327 464 31	−8.083 681 96
				7.793 044 49	6.838 826 05					−4.325 985 40	8.085 160 68
4	0, −5, 4	0.005	$(0g_{7/2},\ 0g_{9/2})$	8.756 718 40	−7.608 943 20	4	1, −5, 4	0.005	$(1g_{7/2},\ 1g_{9/2})$	10.456 2481	9.058 264 90
				−3.756 673 70	7.608 988 00					−5.456 170 40	−9.058 187 20
		0.010		8.753 586 68	−7.606 267 90			0.010		10.450 6344	9.053 380 94
				−3.753 407 55	7.606 447 08					−5.450 323 68	−9.053 070 26
		0.015		8.750 509 95	−7.603 974 70			0.015		10.445 1040	9.048 602 17
				−3.750 105 91	−7.603 570 68					−5.444 403 34	−9.047 901 58
		0.020		−3.746 768 52	−7.600 851 45			0.020		10.439 6574	−9.042 681 01
				8.747 488 66	7.601 571 43					−5.438 408 94	9.043 929 31

Table 8. The energy degenerate states in units of fm⁻¹ of the pseudospin-symmetry TW diatomic molecular potential for various values of n and b_h. We use the following parameters: $ch = 0.027\,262$, $M = 5$ fm⁻¹, $r_e = 0.8$, $D = 15$ fm⁻¹.

ℓ	$n,\ \kappa<0,\ \kappa>0$	b_h	Degenerate states	$E_{n\kappa}(C_{ps}=-5\ \mathrm{fm}^{-1})$	$E_{n\kappa}(C_{ps}=0)$	ℓ	$n,\ \kappa<0,\ \kappa>0$	b_h	Degenerate states	$E_{n\kappa}(C_{ps}=5\ \mathrm{fm}^{-1})$	$E_{n\kappa}(C_{ps}=0)$
1	1, −1, 2	0.005	$(1s_{1/2},\ 0d_{3/2})$	−6.948 397 50	−6.207 854 54	1	2, −1, 2	0.005	$(2s_{1/2},\ 1d_{3/2})$	−7.736 951 90	−6.795 181 87
				1.948 582 00	6.208 039 01					2.737 239 90	6.795 469 88
		0.010		1.945 785 52	−6.205 264 56			0.010		2.733 409 61	−6.791 304 68
				−6.945 048 01	6.20 600 224					−7.732 256 09	6.792 458 42
		0.015		−6.941 387 71	6.203 988 59			0.015		2.729 690 57	−6.786 890 75
				1.943 051 07	−6.202 324 49					−7.727 089 05	6.789 493 32
		0.020		1.940 378 87	6.201 997 93			0.020		−7.721 446 73	6.786 574 69
				−6.937 414 15	−6.199 030 82					2.726 083 25	−6.781 934 85
2	1, −2, 3	0.005	$(1p_{3/2},\ 0f_{5/2})$	3.186 938 00	7.147 807 07	2	2, −2, 3	0.005	$(2p_{3/2},\ 1f_{5/2})$	4.250 686 00	8.020 072 00
				−8.186 819 00	−7.147 688 04					−9.250 507 00	−8.019 893 11
		0.010		3.182 931 90	−7.144 119 91			0.010		4.245 293 80	8.015 491 71
				−8.182 457 90	7.144 593 95					−9.244 579 50	−8.014 777 62
		0.015		−8.177 905 50	−7.140 334 41			0.015		4.239 977 40	8.010 949 81
				3.178 973 70	7.141 402 81					−9.238 367 60	−8.009 339 81
		0.020		−8.173 160 02	7.138 233 401			0.020		4.234 738 23	8.006 446 03
				3.175 063 73	−7.136 329 09					−9.231 869 68	−8.003 576 71
3	1, −3, 4	0.005	$(1d_{5/2},\ 0g_{7/2})$	4.341 572 000	−8.096 633 11	3	2, −3, 4	0.005	$(2d_{5/2},\ 1g_{7/2})$	5.594 302 01	−9.179 599 00
				−9.341 478 00	8.096 727 13					−10.594 1661	9.179 735 13
		0.010		−9.336 280 12	−8.092 177 82			0.010		−10.587 1961	−9.173 375 21
				4.336 648 81	8.092 546 61					5.587 734 22	9.173 913 30
		0.015		4.331 765 73	8.088 386 33			0.015		5.581 226 03	−9.166 910 81
				−9.330 935 51	−8.087 555 90					−10.580 0132	9.168 124 09
		0.020		4.326 922 91	−8.082 766 41			0.020		−10.572 6151	−9.160 204 93
				−9.325 443 20	8.084 246 50					5.574 776 90	9.162 367 11
4	1, −4, 5	0.005	$(0f_{7/2},\ 0h_{9/2})$	−10.456 1441	9.058 223 02	4	2, −4, 5	0.005	$(2f_{7/2},\ 1h_{9/2})$	−10.456 144	9.058 223 08
				5.456 225 03	−9.058 143 01					5.456 225 01	−9.058 143 03
		0.010		5.450 537 20	9.053 209 61			0.010		5.450 537 21	9.053 209 61
				−10.450 2258	−9.052 898 50					−10.450 2258	−9.052 898 50
		0.015		5.444 883 40	9.048 215 88			0.015		5.444 883 45	9.048 215 11
				−10.444 1828	−9.047 514 46					−10.444 1828	−9.047 514 42
		0.020		−10.438 0157	9.043 239 29			0.020		5.439 264 42	9.043 239 23
				5.439 264 42	−9.041 990 06					−10.438 0157	−9.041 990 15

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Appendix A. Some useful standard integrals

$$\int_{-1}^{1}\left(\frac{1-s}{2}\right)^{a}\left(\frac{1+x}{2}\right)^{b}\left[P_{n}^{(a+1,\,b+1)}(x)\right]^{2}\mathrm{d}x$$

$$= \frac{2^{2n+1}n!\,\Gamma(n+a+2)}{[\Gamma(2n+a+b+3)]^{2}}\Gamma(n+b+2)\Gamma(n+a+b+2)$$

$$\times\left(\frac{n+a+1}{b+1}+2+\frac{n+b+1}{a+1}\right). \tag{A.1}$$

$$\int_{-1}^{1}\left(\frac{1-x}{2}\right)^{a-1}\left(\frac{1+x}{2}\right)^{b}\left[P_{n}^{(a,\,b)}(x)\right]^{2}\mathrm{d}x$$

$$= \frac{2\Gamma(a+n+1)\Gamma(b+n+1)}{n!\,a\Gamma(a+b+n+1)}. \tag{A.2}$$

$$\int_{-1}^{1}\left(\frac{1-x}{2}\right)^{a}\left(\frac{1+x}{2}\right)^{b}\left[P_{n}^{(a,\,b)}(x)\right]^{2}\mathrm{d}x$$

$$= \frac{2\Gamma(a+n+1)\Gamma(b+n+1)}{n!\,a\Gamma(a+b+2n+1)\Gamma(a+b+n+1)}. \tag{A.3}$$

$$\int_{0}^{1}x^{\rho-1}(1-x)^{b-\rho-1}\,_{2}F_{1}(a,b;c;x)\mathrm{d}x$$

$$= \frac{\Gamma(\rho)\Gamma(\sigma)}{\Gamma(\rho+\sigma)}\,_{3}F_{2}(a,b,\rho;\gamma,\rho+\sigma;1). \tag{A.4}$$

$$\int_{0}^{1}x^{\rho-1}(1-x)^{\sigma-1}\,_{2}F_{1}(a,b;c;x)\mathrm{d}x$$

$$= \frac{\Gamma(\rho)\Gamma(\gamma)\Gamma(b-\rho)\Gamma(\gamma-a-\rho)}{\Gamma(b)\Gamma(\gamma-a)\Gamma(\gamma-\rho)}. \tag{A.5}$$

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