



Spin and pseudospin symmetries of the Dirac equation for the generalised Morse potential and a class of Yukawa potential

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Abstract. We have studied the bound-state solutions of the spin and pseudospin limits of the Dirac equation with the generalised Morse potential and a class of Yukawa potential using the Nikiforov–Uvarov method and an appropriate approximation scheme. The energy eigenvalues and the corresponding normalised eigenfunction of the non-relativistic limits of the spin symmetry was obtained. By adjusting some potential parameters, six special potentials, namely, the generalised Morse, a class of Yukawa, Hellmann, inversely quadratic Yukawa, Hulthen and Coulomb potentials to which the generalised Morse potential plus a class of Yukawa potential (GMP + CYP) reduces to, were evaluated. The deduced corresponding energies of these special potentials were found to be in excellent agreement with those in the existing literature. We also studied and compared the energy spectra of the GMP + CYP with those of the special potentials with respect to internuclear distance. Moreover, we investigated and compared the behaviour of some selected diatomic molecules, when subjected to the (GMP + CYP) potential. Finally, the expectation values of some useful physical observables were deduced using the Hellmann–Feynman theorem.

Keywords. Dirac equation; Yukawa potential; generalised Morse potential; Coulomb-like; spin and pseudospin symmetries; Nikiforov–Uvarov method; Hellmann–Feynman potential.

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1. Introduction

The description of the dynamics of fermionic (i.e. spin 1/2) particles requires obtaining the exact or approximate solution of the Dirac equation for a given potential model, and this has led to empirical investigation of the relativistic spin and pseudospin symmetries of the equation in several hadronic and nuclear spectroscopies. A review of the empirical data supporting this empirical study, and some realistic relativistic mean-field calculations of nuclei and QCD sum rules to support approximate pseudospin symmetry can be found in [1] and references therein. The review not only provides the fundamental rationale and motivation for investigating pseudospin conservation in the nucleon–nucleon interaction, but also discusses the open questions regarding hadron spin symmetry and nuclear pseudospin symmetry.

Studies carried out by Page *et al* [2] using experimental data indicate the presence of a small spin–orbit splitting in hadrons, and identified a relativistic symmetry that suppresses these splittings in some mesons. The study further reveals that the relevance of the spin symmetry for mesons occurs when the difference between the repulsive vector potential $V(r)$ and the attractive Lorentz scalar potential $S(r)$ is constant in the nuclei, i.e., $\Delta(r) = V(r) - S(r) = c_{\text{spin}}$, while the pseudospin symmetry results is obtained when the sum of the vector and scalar potentials is constant, i.e., $\Sigma(r) = V(r) + S(r) = c_{\text{pseudospin}}$. Within the framework of the Dirac equation, in refs [3–6] the concept of pseudospin symmetry was used to investigate deformed nuclei and superdeformation. This enabled them to establish an effective nuclear shell model. The pseudospin symmetry usually refers to the quasidegeneracy of single nucleon doublets with non-relativistic

quantum numbers $n, l, j = l + \frac{1}{2}$ and $n - 1, l + 2, j = l + \frac{3}{2}$, where n, l and j are single-nucleon radial, orbital and total angular momentum quantum numbers respectively (see refs [7–9]). As shown in [10], the pseudospin symmetry in nuclei could arise from nucleons moving in a relativistic mean field which has an attractive scalar and repulsive core. Recently, the interests of many researchers have been focussed on exploring the nature of spin and pseudospin symmetries with different potential models. For instance, Ikot and Hassanabadi [11] have investigated the spin and pseudospin symmetries with Hellmann potential with three tensor interactions using Nikiforov–Uvarov (NU) method. They obtained the bound-state energy spectra and the radial wavefunctions within the framework of spin and pseudospin symmetry limits, and further reported some numerical results which revealed the effects of tensor interactions. In a related study, Ikot *et al* [12] solved the Dirac equation using the concept of spin and pseudospin symmetries with the shifted Hulthen potential (HP) in the framework of supersymmetry quantum mechanics (SUSYQM). Apart from obtaining approximate solutions to the equation, they also reported some numerical results to show the effects of tensors coupling to the Dirac equation. Hamzavi *et al* [13] on their part, investigated the pseudospin symmetry with Eckert potential including a Coulomb-like tensor potential using NU method, and obtained closed forms of eigenfunctions and energy eigenvalues. Onate *et al* [14] used the formula method to obtain the solutions of the Dirac equation with Coulomb–Hulthén-like tensor interaction within the framework of spin and pseudospin symmetries. They showed that in the presence of tensor interaction, the energy degeneracies in both symmetries break down leading to atomic stability. They also calculated Fisher information for both position and momentum spaces which can be used to determine the accuracy of predicting the localisation of a particle. Okorie *et al* [15] used modified factorisation method to explore the spin symmetry of the Dirac equation with shifted Tietz–Wei potential. They obtained both the relativistic and non-relativistic ro-vibrational energy spectra as well as numerical solutions for different diatomic molecules. The eigenfunction for this potential was also deduced in terms of hypergeometric function. Hassanabadi *et al* [16] used the NU method to obtain approximate analytical solution in the form of energy eigenvalues and the corresponding eigenfunctions of Dirac equation under the pseudospin and spin symmetry for Deng–Fan potential. They also considered the Yukawa potential as a tensor interaction and went on to investigate its effects. Bahar and Yasuk [17] used the asymptotic iteration method (AIM) to study fermionic

particles with position-dependent mass in the presence of inversely quadratic potential and arbitrary spin–orbit quantum state and obtained the energy eigenvalues and the corresponding normalised eigenfunctions and an approximation on the spin–orbit coupling term. Ikhdair and Hamzavi [18] used the generalised parametric NU method to obtain approximate analytical solutions of the Dirac equation with the Tietz–Hua potential for arbitrary spin–orbit quantum number using the Peskeris approximation scheme. Falaye and Ikhdair [19] investigated and solved the Dirac equation and obtained approximate bound-state solutions for fermions in the presence of trigonometric Poschl–Teller potential including a Coulomb-like tensor coupling with arbitrary spin and pseudospin quantum numbers using AIM. They presented numerical results in the presence and absence of tensor coupling and for various values of spin and pseudospin constants. Results for the non-relativistic limits were also obtained. Moshinsky and Szczepaniak [20] and later Ikhdair and Hamzavi [21] introduced the tensor interaction term into the Dirac equation and solved it by simply replacing the three-dimensional momentum operator \vec{p} with $\vec{p} - iM\omega\hat{\beta}\cdot\hat{r}U(r)$ and adding spin–orbit coupling to the Dirac Hamiltonian.

The aim of this paper is to obtain approximate analytical solutions of the Dirac equation with generalised Morse plus a class of Yukawa potential including a Coulomb-like tensor coupling for an arbitrary spin–orbit quantum number. Noting that the generalised Morse potential (GMP) is used to describe diatomic molecular spectra and electromagnetic transitions and that it is the true internuclear potential in diatomic molecules with the same behaviour as $r \rightarrow 0$, we shall use the results to study the spectra of some diatomic molecules namely for HCl, LiH, H₂, ScH and CH subjected to this potential.

The GMP is a modified version of the Morse potential as suggested by Deng–Fan [22,23], and is given as

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

where $r \in (0, \infty)$, D_e is the dissociation energy, $q = e^{\alpha r_e} - 1$ is the position corresponding to the minimum internuclear distance or equilibrium position r_e , r is the internuclear distance and α is the range of the potential. However, it has been shown in [24] that the Morse potential and the GMP are very close for large values of r_e , $\alpha = 1 \text{ \AA}^{-1}$ in the regions $r \rightarrow r_e$ and $r > r_e$ but are different for $r \rightarrow 0$. On the other hand, the class of Yukawa potential (CYP) is of the form [25,26]

$$V(r) = -\frac{b}{r} + \frac{ce^{-\alpha r}}{r} - \frac{ae^{-2\alpha r}}{r^2}, \quad (1b)$$

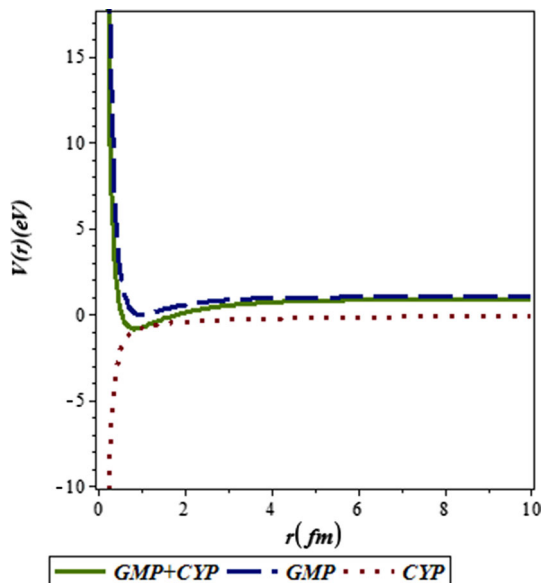


Figure 1. Plot of three potential energies vs. internuclear distance r , with $\alpha = 1 \text{ \AA}^{-1}$.

where a , b and c are potential strengths. Thus, eq. (1b) is a superposition of Hellmann and inversely quadratic Yukawa potentials which is applicable in describing the spectrum of diatomic molecules and electromagnetic transitions.

Recent studies in this field have been focussed on combining different potentials in both the relativistic and non-relativistic regimes so as to get a wider range of applications [27,28]. In this case, we propose a new potential $V(r)$, called the GMP + CYP, by expanding eq. (1a) and combining it with eq. (1b). Doing so, we get

$$V(r) = V - \frac{\eta e^{-\alpha r}}{1 - e^{-\alpha r}} + \frac{\Omega e^{-2\alpha r}}{(1 - e^{-\alpha r})^2} - \frac{b}{r} + \frac{ce^{-\alpha r}}{r} - \frac{ae^{-2\alpha r}}{r^2}, \tag{1c}$$

where $V = D_e$, $\eta = 2D_e q$, $\Omega = D_e q^2$ and r is the internuclear distance. A graphical illustration of the above potential $V(r)$, which is a combination of GMP and CYP and how it compares with its component potentials (GMP and CYP) is given in figure 1. From the figure it can be noticed that $V(r)$ behaves exactly like the generalised Morse potential (GMP) for large values of r_e and $\alpha = 1 \text{ \AA}^{-1}$ in the regions $r \rightarrow r_e$ and $r > r_e$; but behaves differently as $r \rightarrow 0$. In addition, the depth of the combined GMP + CYP potentials is lower and sharper than that of the GMP alone making it more suitable for use in molecular and particle physics spectroscopies.

This paper is divided into six sections. The introduction is given in §1, while in §2, we give a review of the Nikiforov–Uvarov method. In §3, we present the solutions of the spin and pseudospin symmetries of the Dirac equation and the non-relativistic limit of the equation. The results and discussions for some special cases of which the potential reduces to by varying the values of the potential parameters are presented in §4. Then, in §5, the Hellmann–Feynman theorem is used to obtain the expectation values for some physical quantities. And finally, in §6, we summarize and give our concluding remarks.

2. Review of Nikiforov–Uvarov method

The Nikiforov–Uvarov (NU) method [29–31] (summarised in the Appendix) is an analytical technique developed to solve hypergeometric-type second-order differential equations by means of the special orthogonal functions. For instance, for any given potential, an equation such as the Schrödinger or a Schrödinger-like equation in special coordinates can be reduced to a generalised hypergeometric-type equation with an appropriate coordinate transformation $s = s(r)$, and then solved to obtain its solution. One such hypergeometric-type second-order differential equation that can be solved using the NU method is of the form

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)} \psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)} \psi(s) = 0, \tag{2}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials of at most second-degree, $\tilde{\tau}(s)$ is a polynomial of at most first-degree and $\psi(s)$ is a hypergeometric-type function, and the prime denotes differentiation with respect to s . In order to find an exact solution to eq. (2), a common ansatz for the wave function ψ is chosen as

$$\psi(s) = \phi(s) \chi(s). \tag{3}$$

Substituting the above expression into eq. (2) gives

$$\sigma(s) \chi''(s) + \tau(s) \chi'(s) + \lambda \chi(s) = 0. \tag{4}$$

The parameter λ is defined as

$$\lambda = k + \pi'(s), \tag{5}$$

where k is a constant, and the function $\pi(s)$ is given by

$$\pi(s) = \frac{\sigma'(s) - \tilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)}. \tag{6}$$

The parameter k is determined by setting the discriminant in the quadratic expression in the square root of

eq. (6) equal to zero. Thus, the new eigenvalue equation for λ takes the form

$$\lambda = \lambda_n = -n\tau(s) - \frac{n(n-1)}{2}\sigma''(s), \quad n=0, 1, 2, \dots, \quad (7)$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s). \quad (8)$$

Equation (7) gives the energy eigenvalues of the equation under study.

The eigenfunctions $\chi(s)$ are polynomials of degree n written in the form of Rodrigue’s relation as

$$\chi_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n \rho(s)], \quad (9)$$

where B_n is the normalisation constant and $\rho(s)$ is the weight function which satisfies the condition

$$\frac{d}{ds} [(\sigma(s)\rho(s))] = \tau(s)\rho(s). \quad (10)$$

Since $\rho(s) > 0$ and $\sigma(s) > 0$, the derivative of $\tau(s)$ should be negative, i.e. $\tau'(s) < 0$ as this is a condition for a bound-state solution [32]. The other part of the wave function $\phi(s)$ is defined as the logarithmic derivative

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}, \quad (11)$$

where $\pi(s)$ is given by eq. (6).

3. Dirac equation including tensor coupling potential

The Dirac equation for a spin- $\frac{1}{2}$ particle of mass M subjected to an external attractive scalar potential $S(r)$, repulsive vector potential $V(r)$ and tensor coupling $U(r)$ in relativistic unit $\hbar = c = 1$ is given by

$$[\vec{\alpha} \cdot \vec{p} + \beta(M + S(r)) - i\beta\vec{\alpha} \cdot \hat{r}U(r)]\psi(r) = [E - V(r)]\psi(r), \quad (12)$$

where E is the relativistic energy of the system, $\vec{p} = -i\vec{\nabla}$ is the three-dimensional momentum operator [7, 13,16], $\vec{\alpha}$ and β are 4×4 Dirac matrices given as

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma}_i \\ \vec{\sigma}_i & 0 \end{pmatrix}, \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad (13)$$

where I is a 2×2 unitary matrix given by

$$I = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (14)$$

and σ_i are the Pauli spin matrices given by

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

(15)

For a spherically symmetric nuclei, the total nuclear angular momentum \vec{J} and spin matrix operator $\hat{K} = -\vec{\beta} \cdot (\vec{\sigma} \cdot \vec{L} + 1)$, where \vec{L} the orbital angular momentum of the spherical nucleus, commutes with the Dirac Hamiltonian

$$H = \alpha \cdot \vec{p} + \beta(M + S(r)) + V(r). \quad (16)$$

The eigenvalues of \hat{K} are $\kappa = \pm(j + \frac{1}{2})$ where $\kappa = +(j + \frac{1}{2}) > 0$ is for unaligned spin $j = l - \frac{1}{2}$ and $\kappa = -(j + \frac{1}{2}) < 0$ is for the aligned spin $j = l + \frac{1}{2}$. Thus, the conjugate set of conserved quantities can be written as (H^2, K, J^2, J_z) . The spin wave functions can be classified according to the radial quantum number n and spin-orbit quantum number κ and can be written using the Pauli-Dirac representation as [16,32]

$$\psi_{n\kappa}(r) = \begin{pmatrix} \frac{F_{n\kappa}(r)}{r} Y_{jm}^l(\theta, \varphi) \\ i \frac{G_{n\kappa}(r)}{r} Y_{jm}^{\tilde{l}}(\theta, \varphi) \end{pmatrix}, \quad (17)$$

where $F_{n\kappa}(\vec{r})$ is the upper component and $G_{n\kappa}(\vec{r})$ is the lower component of the Dirac spinors. $Y_{jm}^l(\theta, \varphi)$ and $Y_{jm}^{\tilde{l}}(\theta, \varphi)$ are the spin and pseudospin spherical harmonics respectively and m is the projection of the angular momentum on the z -axis. Substituting eq. (17) into eq. (12) [1,2,16] and using the following identities

$$(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) = \vec{A} \cdot \vec{B} + i\vec{\sigma} \cdot (\vec{A} \times \vec{B}), \quad (18a)$$

$$(\vec{\sigma} \cdot \vec{P}) = \vec{\sigma} \cdot \hat{r} \left(\hat{r} \cdot \vec{P} + i \frac{\vec{\sigma} \cdot \vec{L}}{r} \right) \quad (18b)$$

as well as the following relations:

$$\begin{aligned} (\vec{\sigma} \cdot \vec{L}) Y_{jm}^{\tilde{l}}(\theta, \varphi) &= (\kappa - 1) Y_{jm}^{\tilde{l}}(\theta, \varphi) \\ (\vec{\sigma} \cdot \vec{L}) Y_{jm}^l(\theta, \varphi) &= -(\kappa - 1) Y_{jm}^l(\theta, \varphi) \\ (\vec{\sigma} \cdot \hat{r}) Y_{jm}^{\tilde{l}}(\theta, \varphi) &= -Y_{jm}^l(\theta, \varphi) \\ (\vec{\sigma} \cdot \hat{r}) Y_{jm}^l(\theta, \varphi) &= Y_{jm}^{\tilde{l}}(\theta, \varphi) \end{aligned} \quad (19)$$

we obtain two coupled first-order differential (Dirac) equations for the upper and lower radial wave functions $F_{n\kappa}(r)$ and $G_{n\kappa}(r)$ given as

$$\begin{aligned} \left(\frac{d}{dr} + \frac{\kappa}{r} - U(r) \right) F_{n\kappa}(r) \\ = (M + E_{n\kappa} - \Delta(r)) G_{n\kappa}(r) \end{aligned} \quad (20a)$$

and

$$\begin{aligned} \left(\frac{d}{dr} - \frac{\kappa}{r} + U(r) \right) G_{n\kappa}(r) \\ = (M - E_{n\kappa} + \Sigma(r)) F_{n\kappa}(r), \end{aligned} \quad (20b)$$

where

$$\Delta(r) = V(r) - S(r) \tag{21a}$$

and

$$\Sigma(r) = V(r) + S(r) \tag{21b}$$

are the difference and sum of potentials respectively. Eliminating $F_{n\kappa}(r)$ and $G_{n\kappa}(r)$ from eqs (20a) and (20b), we obtain two second-order Schrödinger-like differential equations for the upper and lower spinor components respectively as

$$\left\{ \begin{aligned} & \frac{d^2}{dr^2} - \frac{\kappa(\kappa+1)}{r^2} + \frac{2\kappa}{r}U(r) - \frac{dU(r)}{dr} - U^2(r) \\ & - (M + E_{n\kappa} - \Delta(r))(M - E_{n\kappa} + \Sigma(r)) \\ & + \frac{\frac{d\Delta(r)}{dr}}{M + E_{n\kappa} - \Delta(r)} \left(\frac{d}{dr} + \frac{\kappa}{r} - U(r) \right) \end{aligned} \right\} F_{n\kappa}(r) = 0, \tag{22a}$$

$$\left\{ \begin{aligned} & \frac{d^2}{dr^2} - \frac{\kappa(\kappa+1)}{r^2} + \frac{2\kappa}{r}U(r) - \frac{dU(r)}{dr} - U^2(r) \\ & - (M + E_{n\kappa} - \Delta(r))(M - E_{n\kappa} + \Sigma(r)) \\ & + \frac{\frac{d\Sigma(r)}{dr}}{M + E_{n\kappa} - \Sigma(r)} \left(\frac{d}{dr} + \frac{\kappa}{r} - U(r) \right) \end{aligned} \right\} G_{n\kappa}(r) = 0, \tag{22b}$$

where

$$\kappa(\kappa - 1) = \tilde{l}(\tilde{l} + 1) \text{ and } \kappa(\kappa + 1) = l(l + 1).$$

The quantum number κ is related to the quantum numbers for spin and pseudospin symmetries l and \tilde{l} respectively as [2,7,13]

$$\begin{aligned} -l + 1 &= -(j + \frac{1}{2}), (s_{1/2}, p_{3/2}, \text{ etc.}), \\ j &= l + \frac{1}{2}, \text{ aligned spin } (\kappa < 0), \\ +l &= +(j + \frac{1}{2}), (p_{1/2}, d_{3/2}, \text{ etc.}), \\ j &= l - 1, \text{ unaligned spin } (\kappa > 0), \end{aligned} \tag{23}$$

and the quasidegenerate doublet structure can be expressed in terms of the pseudospin angular momentum $\tilde{s} = \frac{1}{2}$ and pseudo-orbital angular momentum \tilde{l} , which is defined as

$$\begin{aligned} +(\tilde{l} + 1) &= +(j + \frac{1}{2}), (d_{3/2}, f_{5/2}, \text{ etc.}), \\ j &= \tilde{l} + 1, \text{ unaligned spin } (\kappa > 0), \end{aligned} \tag{24}$$

where $\kappa = \pm 1, \pm 2, \dots$. Thus, as an example, $(1s_{1/2}, 0d_{3/2})$ and $(0p_{3/2}, 0f_{5/2})$ can be considered as pseudospin doublets [13].

3.1 Spin symmetry limit

The exact spin symmetry of the Dirac equation as shown by [4,10,33–36] occurs when $\frac{d\Delta(r)}{dr=0}$ or $\Delta(r) = c_{\text{spin}} =$

constant. For the spin symmetry case, we take $\Sigma(r)$ as the generalised Morse potential plus a class of Yukawa potential (GMP + CYP) given by eq. (1c) as

$$\begin{aligned} V(r) &= V - \frac{\eta e^{-\alpha r}}{1 - e^{-\alpha r}} + \frac{\Omega e^{-2\alpha r}}{(1 - e^{-\alpha r})^2} - \frac{b}{r} \\ &+ \frac{ce^{-\alpha r}}{r} - \frac{ae^{-2\alpha r}}{r^2}, \end{aligned} \tag{25}$$

with the Coulomb-like tensor potential given as [7]

$$U(r) = -\frac{H}{r}, \tag{26}$$

where $H = Z_p Z_t e^2 / 4\pi\epsilon_0$, with $r \geq R_c$. $R_c = 7.78$ fm is the Coulomb radius, Z_p and Z_t are the charges of the projectile p and the target t respectively. Inserting eqs (25) and (26) into eq. (22a) gives

$$\begin{aligned} & \left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa+1) + 2\kappa H + H(H+1)}{r^2} \right] F_{n\kappa}(r) \\ & = \left[(M + E_{n\kappa} - c_s) \left(\begin{aligned} & M - E_{n\kappa} + V - \frac{\eta e^{-\alpha r}}{1 - e^{-\alpha r}} + \frac{\Omega e^{-2\alpha r}}{(1 - e^{-\alpha r})^2} \\ & - \frac{b}{r} + \frac{ce^{-\alpha r}}{r} - \frac{ae^{-2\alpha r}}{r^2} \end{aligned} \right) \right] F_{n\kappa}(r) \end{aligned} \tag{27}$$

$$\begin{aligned} -\tilde{l} &= -(j + \frac{1}{2}), (s_{1/2}, p_{3/2}, \text{ etc.}), \\ j &= l - \frac{1}{2}, \text{ aligned pseudospin } (\kappa < 0), \end{aligned}$$

$$\begin{aligned} \text{where } \kappa(\kappa + 1) &= l(l + 1), \kappa = l \text{ for } \kappa < 0 \text{ and } \kappa = \\ &-(l + 1) \text{ for } \kappa > 0. \end{aligned}$$

Since eq. (27) can be solved exactly only for s -wave case where $\kappa = -1$ and $H = 0$ due to the centrifugal term, we resort to the approximation scheme given by [37]

$$\frac{1}{r^2} \approx \frac{\alpha^2}{(1 - e^{-\alpha r})^2} \tag{28}$$

to circumvent the centrifugal barrier.

Substituting eq. (28) into eq. (27) and introducing a new variable $z \rightarrow e^{-\alpha r}$, we obtain

$$\begin{aligned} \frac{d^2 F_{n\kappa}(z)}{dz^2} + \frac{(1-z)}{z(1-z)} \frac{dF_{n\kappa}(z)}{dz} \\ + \frac{1}{z^2(1-z)^2} [-(\tilde{\epsilon} + \delta - \tilde{\gamma})z^2 + (2\tilde{\epsilon} + \delta - \omega - \tilde{\beta})z \\ - (\tilde{\epsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1))] F_{n\kappa}(z) = 0, \end{aligned} \tag{29}$$

where

$$\left\{ \begin{aligned} \tilde{\epsilon} &= \frac{1}{\alpha^2} [(M + E_{n\kappa} - c_{\text{spin}})(M - E_{n\kappa} + V)] \\ \delta &= (M + E_{n\kappa} - c_{\text{spin}}) \frac{\eta}{\alpha^2} \\ \tilde{\gamma} &= (M + E_{n\kappa} - c_{\text{spin}}) \left(a - \frac{\Omega}{\alpha^2} \right) \\ \omega &= (M + E_{n\kappa} - c_{\text{spin}}) \frac{b}{\alpha} \\ \tilde{\beta} &= (M + E_{n\kappa} - c_{\text{spin}}) \frac{c}{\alpha} \\ \lambda_\kappa &= \kappa + H + 1 \end{aligned} \right. \tag{30}$$

Comparing eqs (30) and (2), we obtain the following equation:

$$\left\{ \begin{aligned} \tilde{\tau}(s) &= 1 - s \\ \sigma(s) &= s(1 - s) \\ \tilde{\sigma}(s) &= -(\tilde{\epsilon} + \delta - \tilde{\gamma})s^2 + (2\tilde{\epsilon} + \delta - \omega - \tilde{\beta})s \\ &\quad - (\tilde{\epsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)) \end{aligned} \right. \tag{31}$$

Substituting eq. (31) into (6), we get the quadratic root of $\pi(s)$ as

$$\pi(s) = -\frac{s}{2} \pm \sqrt{\left(\frac{1}{4} + \tilde{\epsilon} + \delta - \tilde{\gamma} - k\right)s^2 + (-2\tilde{\epsilon} - \delta + \omega + \tilde{\beta} + k)s + (\tilde{\epsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1))}. \tag{32}$$

To find the value of k , we set the discriminant under the square root to zero. Doing so gives

$$k_{\pm} = \delta + \omega - \tilde{\beta} - 2\lambda_\kappa(\lambda_\kappa - 1) \pm 2\sqrt{\tilde{\epsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)}$$

$$\times \sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)}. \tag{33}$$

Substituting the negative value of eq. (33) into eq. (32) yields

$$\begin{aligned} \pi(s) = -\frac{s}{2} \pm \left[\left(\sqrt{\tilde{\epsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)} \right. \right. \\ \left. \left. + \sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)} \right) s \right. \\ \left. - \sqrt{\tilde{\epsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)} \right]. \end{aligned} \tag{34}$$

Using eq. (8) to confirm the validity of the solution, we obtain

$$\begin{aligned} \tau'(s) = -2 + 2\sqrt{\tilde{\epsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)} \\ - 2\sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)} < 0. \end{aligned} \tag{35}$$

We now define the constant λ in eq. (5) as

$$\begin{aligned} \lambda &= \delta + \omega - \tilde{\beta} - 2\lambda_\kappa(\lambda_\kappa - 1) \\ &\quad - 2\sqrt{\tilde{\epsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)} \\ &\quad \times \sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)} - \frac{1}{2} \\ &\quad - \sqrt{\tilde{\epsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)} \\ &\quad - \sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)} \end{aligned} \tag{36}$$

and from eq. (7) we now get

$$\lambda_n = 2n + 2n\sqrt{\tilde{\epsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)}$$

$$+ 2n\sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)} - n(n - 1). \tag{37}$$

The energy eigenvalue is obtained by equating eqs (36) and (37) as follows:

$$\tilde{\varepsilon} = \omega - \lambda_\kappa(\lambda_\kappa - 1) + \frac{1}{4} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)} \right)^2 + \lambda_\kappa(\lambda_\kappa - 1) + \tilde{\gamma} - \omega - \delta}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)} \right)} \right]^2, \tag{38}$$

$$\begin{aligned} & (M + E_{n\kappa} - c_{\text{spin}})(M - E_{n\kappa} + V) \\ &= (M + E_{n\kappa} - c_{\text{spin}})b\alpha - \lambda_\kappa(\lambda_\kappa - 1)\alpha^2 \\ &+ \frac{\alpha^2}{4} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - (M + E_{n\kappa} - c_{\text{spin}})\left(a - \frac{\Omega}{\alpha^2}\right) + (M + E_{n\kappa} - c_{\text{spin}})\frac{c}{\alpha} + \lambda_\kappa(\lambda_\kappa - 1)} \right)^2 - (M + E_{n\kappa} - C_s)\frac{\eta}{\alpha^2} - (M + E_{n\kappa} - C_s)\frac{b}{\alpha} + (M + E_{n\kappa} - c_{\text{spin}})\left(a - \frac{\Omega}{\alpha^2}\right) + \lambda_\kappa(\lambda_\kappa - 1)}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - (M + E_{n\kappa} - C_s)\left(a - \frac{\Omega}{\alpha^2}\right) + (M + E_{n\kappa} - c_{\text{spin}})\frac{c}{\alpha} + \lambda_\kappa(\lambda_\kappa - 1)} \right)} \right]^2. \end{aligned} \tag{39}$$

Now evaluating eqs (8)–(11) and substituting into eq. (3), we obtain the corresponding upper spinor component of the wave function as

$$\begin{aligned} F_{n\kappa}(s) &= N_{n\kappa} s \sqrt{\tilde{\varepsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)} \\ &\times (1 - s)^{\frac{1}{2} + \sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)}} \\ &\times P_n^{(2\sqrt{\tilde{\varepsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)}, 2\sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)})}(1 - 2s). \end{aligned} \tag{40}$$

From the definition of Jacobi polynomials we can deduce that

$$\begin{aligned} & P_n^{(2A, 2B)}(1 - 2e^{-\alpha r}) \\ &= \frac{(2A + 1)n}{n!} {}_2F_1(-n, 2A + 2B + n + 1, 2A + 1; e^{-\alpha r}) \end{aligned} \tag{41}$$

or

$$\begin{aligned} F_{n\kappa}(r) &= N_{n\kappa} \frac{(2A + 1)n}{n!} e^{-A\alpha r} (1 - e^{-\alpha r})^{\frac{1}{2} + B} \\ &\times {}_2F_1(-n, 2A + 2B + n + 1, 2A + 1; e^{-\alpha r}), \end{aligned} \tag{42}$$

where

$$A = \sqrt{\tilde{\varepsilon} - \omega + \lambda_\kappa(\lambda_\kappa - 1)}$$

and

$$B = \sqrt{\frac{1}{4} - \tilde{\gamma} + \tilde{\beta} + \lambda_\kappa(\lambda_\kappa - 1)}. \tag{43}$$

The normalisation constant N_n is explicitly obtained from the normalisation condition as

$$N_{n\kappa} = \sqrt{\frac{n! \alpha (2A - 1) \Gamma(2A + 2B + n + 1)}{\Gamma(2A + n) \Gamma(2B + n + 2)}}. \tag{44}$$

From eq. (20a), we obtain the lower spinor component of the wave function as

$$G_{n\kappa}(r) = \frac{1}{M + E_{n\kappa} - c_{\text{spin}}} \left(\frac{d}{dr} + \frac{\kappa}{r} - U(r) \right) F_{n\kappa}(r), \tag{45}$$

where

$$E_{n\kappa} \neq -M + c_{\text{spin}}. \tag{46}$$

3.2 Pseudospin symmetry limit

The exact pseudospin symmetry of the Dirac equation [38,39] occurs when

$$\frac{d\Sigma(r)}{dr} = 0$$

or when

$$\Sigma(r) = c_{\text{pseudospin}} = \text{constant}.$$

So, for equal vector and scalar potentials, we take $\Delta(r)$ as the generalised Morse potential plus class of Yukawa potential, eq. (1c) with a Coulomb-like tensor potential [7]. Substituting these limits into eq. (22b), we obtain

$$\left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa + 1) + 2\kappa H + H(H - 1)}{r^2} \right] G_{n\kappa}(r) = \left[(M - E_{n\kappa} + C_{ps}) \left(\begin{matrix} M + E_{n\kappa} - V + \frac{\eta e^{-\alpha r}}{1 - e^{-\alpha r}} - \frac{\Omega e^{-2\alpha r}}{(1 - e^{-\alpha r})^2} \\ +\frac{b}{r} - \frac{ce^{-\alpha r}}{r} + \frac{ae^{-2\alpha r}}{r^2} \end{matrix} \right) \right] G_{n\kappa}(r). \tag{47}$$

To avoid repetition, let us map the following into eq. (39) as follows:

$$F_{n\kappa} \Leftrightarrow G_{n\kappa}, \quad \kappa \rightarrow \kappa - 1, \quad \lambda_\kappa \rightarrow \eta_\kappa, \quad V(r) \rightarrow -V(r), \\ E_{n\kappa} \rightarrow -E_{n\kappa}, \quad c_{spin} \rightarrow -c_{pseudospin}. \tag{48}$$

We then obtain

$$\varepsilon = -\omega - \eta_\kappa(\eta_\kappa - 1) + \frac{1}{4} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \tilde{\gamma} - \tilde{\beta} + \eta_\kappa(\eta_\kappa - 1)} \right)^2 + \eta_\kappa(\eta_\kappa - 1) - \tilde{\gamma} + \omega + \delta}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \tilde{\gamma} - \tilde{\beta} + \eta_\kappa(\eta_\kappa - 1)} \right)} \right]^2, \tag{49}$$

where

$$\frac{1}{\alpha^2} (M - E_{n\kappa} + c_{pseudospin}) (M + E_{n\kappa} - V). \tag{50}$$

$$(M - E_{n\kappa} + C_{ps}) (M + E_{n\kappa} - V) = -(M - E_{n\kappa} + C_{ps}) b\alpha - \eta_\kappa (\eta_\kappa - 1) \alpha^2 + \frac{\alpha^2}{4} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - (M - E_{n\kappa} + C_{ps}) \left(\frac{\Omega}{\alpha^2} - a \right) - (M - E_{n\kappa} + C_{ps}) \frac{c}{\alpha} + \eta_\kappa (\eta_\kappa - 1)} \right)^2 + (M - E_{n\kappa} + C_{ps}) \frac{\eta}{\alpha^2} + (M - E_{n\kappa} + C_{ps}) \frac{b}{\alpha} + (M + E_{n\kappa} - C_s) \left(\frac{\Omega}{\alpha^2} - a \right) + \eta_\kappa (\eta_\kappa - 1)}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - (M - E_{n\kappa} + C_{ps}) \left(\frac{\Omega}{\alpha^2} - a \right) - (M - E_{n\kappa} + C_{ps}) \frac{c}{\alpha} + \eta_\kappa (\eta_\kappa - 1)} \right)} \right]^2. \tag{51}$$

The lower spinor is obtained as

$$G_{n\kappa}(s) = N_{n\kappa} s^{\sqrt{\varepsilon + \omega + \eta_\kappa(\eta_\kappa - 1)}} \times (1 - s)^{\frac{1}{2} + \sqrt{\frac{1}{4} + \tilde{\gamma} - \tilde{\beta} + \eta_\kappa(\eta_\kappa - 1)}} \times P_n \left(2\sqrt{\varepsilon + \omega + \eta_\kappa(\eta_\kappa - 1)}, 2\sqrt{\frac{1}{4} + \tilde{\gamma} - \tilde{\beta} + \eta_\kappa(\eta_\kappa - 1)} \right) (1 - 2s). \tag{52}$$

Similarly, the upper spinor is given according to eq. (20b) as

$$F_{n\kappa}(r) = \frac{1}{M - E_{n\kappa} + C_{ps}} \left(\frac{d}{dr} - \frac{\kappa}{r} + U(r) \right) G_{n\kappa}(r), \tag{53}$$

where

$$E_{n\kappa} \neq M + c_{\text{pseudospin}}. \tag{54}$$

3.3 Non-relativistic limit

Noting that the Schrödinger equation is non-relativistic, we now deduce the non-relativistic limit of the spin symmetry limit of the Dirac equation. This is because it has been reported in literature that at this limit, there exists some relationship between their solutions [40–42]. We achieved this by setting the constant, $c_{\text{spin}} = H = 0$ and using the following transformations:

$$M + E_{n\kappa} \rightarrow \frac{2\mu}{\hbar^2}, \quad M - E_{n\kappa} \rightarrow -E_{nl} \quad \text{and} \quad \kappa \rightarrow l$$

$$E_{nl} = \frac{\hbar^2 \alpha^2}{2\mu} l(l+1) + V - \frac{\hbar^2 \alpha^2}{8\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu\Omega}{\hbar^2 \alpha^2} + l(l+1)} \right)^2 - \frac{2\mu\Omega}{\hbar^2 \alpha^2} - \frac{2\mu\eta}{\hbar^2 \alpha^2} + l(l+1)}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu\Omega}{\hbar^2 \alpha^2} + l(l+1)} \right)} \right]^2. \tag{59}$$

on eq. (37). Doing so, we obtain the non-relativistic energy equation E_{nl} as

$$E_{nl} = \frac{\hbar^2 \alpha^2}{2\mu} l(l+1) + V - b\alpha - \frac{\hbar^2 \alpha^2}{8\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \xi + \frac{2\mu c}{\hbar^2 \alpha^2} + l(l+1)} \right)^2 + \xi - \frac{2\mu\eta}{\hbar^2 \alpha^2} - \frac{2\mu b}{\hbar^2 \alpha^2} + l(l+1)}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \xi + \frac{2\mu c}{\hbar^2 \alpha^2} + l(l+1)} \right)} \right]^2, \tag{55}$$

where

$$\xi = \frac{2\mu}{\hbar^2} \left(a - \frac{\Omega}{\alpha^2} \right). \tag{56}$$

Also, the upper spinor component of the wave function reduces to the radial wave function

$$R_{nl}(s) = N_{nl} s \sqrt{-\frac{2\mu}{\hbar^2 \alpha^2} (E_{nl} - V) - \frac{2\mu b}{\hbar^2 \alpha^2} + l(l+1)} \times (1-s)^{\frac{1}{2} + \sqrt{\frac{1}{4} - \xi + \frac{2\mu c}{\hbar^2 \alpha^2} + l(l+1)}} \times P_n \left(2\sqrt{-\frac{2\mu}{\hbar^2 \alpha^2} (E_{nl} - V) - \frac{2\mu b}{\hbar^2 \alpha^2} + l(l+1)}, 2\frac{1}{2} + \sqrt{\frac{1}{4} - \xi + \frac{2\mu c}{\hbar^2 \alpha^2} + l(l+1)} \right) \times (1-2s) \tag{57}$$

4. Results and discussion

Below, we deduce the results obtained, as limiting cases, when some parameters in eq. (1c) are adjusted. We further present and discuss the numerical results of the energy eigenvalues for the generalised Morse potential (GMP) for different quantum states and those obtained when this potential is combined individually, with the Hellmann, inversely quadratic Yukawa, Yukawa and a class of Yukawa potentials.

4.1 Generalised Morse potential

If we set $a = b = c = 0$ in eq. (1c), we realise the GMP

$$V(r) = V - \frac{\eta e^{-\alpha r}}{1 - e^{-\alpha r}} + \frac{\Omega e^{-2\alpha r}}{(1 - e^{-\alpha r})^2} \tag{58}$$

and the energy eigenvalue eq. (55) becomes

Equation (59) is the energy eigenvalue for the the GMP which is consistent with the results obtained in [43].

4.2 Class of Yukawa potential

Setting $V = \eta = \Omega = 0$ in eq. (1c), we obtain the class of Yukawa potential as

$$V(r) = -\frac{b}{r} + \frac{ce^{-\alpha r}}{r} - \frac{ae^{-2\alpha r}}{r^2} \tag{60}$$

and the energy eigenvalue eq. (55) reduces to

$$E_{nl} = \frac{\hbar^2 \alpha^2}{2\mu} l(l+1) - b\alpha - \frac{\hbar^2 \alpha^2}{8\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \frac{2\mu a}{\hbar^2} + \frac{2\mu c}{\hbar^2 \alpha} + l(l+1)} \right)^2 + \frac{2\mu a}{\hbar^2} - \frac{2\mu b}{\hbar^2 \alpha} + l(l+1)}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \frac{2\mu a}{\hbar^2} + \frac{2\mu c}{\hbar^2 \alpha} + l(l+1)} \right)} \right]^2 \tag{61}$$

which is in agreement with the results obtained in [25]. and the corresponding energy eigenvalues from eq. (55) becomes

$$E_{nl} = \frac{\hbar^2 \alpha^2}{2\mu} l(l+1) - \frac{\hbar^2 \alpha^2}{8\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \frac{2\mu a}{\hbar^2} + l(l+1)} \right)^2 + \frac{2\mu a}{\hbar^2} + l(l+1)}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} - \frac{2\mu a}{\hbar^2} + l(l+1)} \right)} \right]^2 \tag{65}$$

4.3 Hellmann potential

Setting $V = \eta = \Omega = a = 0$ in eq. (1c), we obtain the Hellmann potential

$$V(r) = -\frac{b}{r} + \frac{ce^{-\alpha r}}{r} \tag{62}$$

and the corresponding energy eigenvalues eq. (55) becomes

which is the energy eigenvalue expression for the the inversely quadratic Yukawa potential.

$$E_{nl} = \frac{\hbar^2 \alpha^2}{2\mu} l(l+1) - b\alpha - \frac{\hbar^2 \alpha^2}{8\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu c}{\hbar^2 \alpha} + l(l+1)} \right)^2 - \frac{2\mu b}{\hbar^2 \alpha} + l(l+1)}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu c}{\hbar^2 \alpha} + l(l+1)} \right)} \right]^2 \tag{63}$$

which is in good agreement with the results obtained in [44].

4.4 Inversely quadratic Yukawa potential (IQYP)

Setting $V = \eta = \Omega = c = b = 0$ in eq. (1c), we obtain the inversely quadratic Yukawa potential

$$V(r) = -\frac{ae^{-2\alpha r}}{r^2} \tag{64}$$

4.5 Hulthen potential (HP)

Setting $V = \Omega = c = b = a = 0$ in eq. (1c), we realise the Hulthen potential given as

$$V(r) = -\frac{\eta e^{-\alpha r}}{1 - e^{-\alpha r}} \tag{66}$$

and the corresponding energy eigenvalues from eq. (55) reduces to

$$E_{nl} = \frac{\hbar^2 \alpha^2}{2\mu} l(l+1) - \frac{\hbar^2 \alpha^2}{8\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + l(l+1)} \right)^2 - \frac{2\mu \eta}{\hbar^2 \alpha^2} + l(l+1)}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + l(l+1)} \right)} \right]^2 \tag{67}$$

Table 1. Energy eigenvalues (in units of fm⁻¹) for the generalised Morse potential (GMP), GMP + YP, GMP + IQYP, GMP + HP and GMP + CYP with $\alpha = \text{\AA}^{-1}$ in different quantum states.

<i>n</i>	<i>l</i>	GMP	GMP + YP	GMP + IQYP	GMP + HP	GMP + CYP
0	0	0.5166	0.9852	-0.7102	-3.1571	-3.2062
1	0	0.8094	0.9783	0.5692	-2.4807	-2.5195
2	0	0.9116	0.9705	0.8281	-1.9354	-1.9664
	1	0.9322	0.9710	0.8945	-1.9111	-1.9417
3	0	0.9574	0.9618	0.9203	-1.4898	-1.5150
	1	0.9684	0.9622	0.9506	-1.4695	-1.4944
	2	0.9766	0.9627	0.9655	-1.4493	-1.4739
4	0	0.9804	0.9522	0.9620	-1.1219	-1.1425
	1	0.9868	0.9527	0.9778	-1.1046	-1.1250
	2	0.9917	0.9531	0.9861	-1.0876	-1.1077
	3	0.9957	0.9535	0.9919	-1.0707	-1.0905
5	0	0.9924	0.9419	0.9830	-0.8150	-0.8321
	1	0.9962	0.9423	0.9917	-0.8003	-0.8172
	2	0.9992	0.9427	0.9966	-0.7857	-0.8024
	3	1.0017	0.9430	1.0000	-0.7712	-0.7877
	4	1.0038	0.9434	1.0027	-0.7569	-0.7732

Equation (67) is the energy eigenvalue for the Hulthen potential which is in good agreement with the results obtained in [45,46].

4.6 Coulomb potential

Setting $V = \Omega = \eta = c = a = 0$ in eq. (1c), we obtain the Coulomb potential

$$V(r) = -\frac{b}{r} \tag{68}$$

and the corresponding energy eigenvalues with $\alpha \rightarrow 0$ in eq. (55) becomes

$$E_{nl} = -\frac{\mu b^2}{2\hbar^2(n+l+1)}. \tag{69}$$

Equation (69) is the energy eigenvalue for the Coulomb potential which is in good agreement with results stated in [47,48].

To test the accuracy of our work and elucidate the relationship between the pure GMP and when it is combined with other potentials, we present in table 1, the numerical results of the energy eigenvalue for five molecular potentials, namely: GMP ($a = b = c = 0$), GMP plus Hellmann potential ($a = 0, b = 2, c = 4$), GMP plus inversely quadratic Yukawa ($a = 1, b = c = 0$), GMP plus Yukawa potential ($a = 0, b = 2, c = 0$) and GMP plus class of Yukawa potential ($a = 1, b = 2, c = 4$) for $\hbar = \mu = D_e = r_e = 1, \alpha = 0.05 \text{\AA}^{-1}$. From the results, it can readily be observed that adding the Yukawa potential to the GMP slightly increases the energy spectrum, while the spectrum is slightly decreased when combined with the IQYP. But the GMP

with either Hellmann or class of Yukawa potentials rapidly decreases the energy approximately in the same order. Tables 2 and 3 give the ro-vibrational energies of the five selected diatomic molecules for the excited and ground states respectively for different potential ranges, α , in the order of $0.025 (\text{\AA})^{-1}$. It can be observed that the energy of the diatomic molecules increases sharply as the potential range α increases, but increases slowly for increasing ro-vibrational states. In table 4, we present the dissociation energies D_e (in eV), equilibrium separation distance r_e (in \AA) and the reduced masses μ (in a.m.u.) using the GMP + CYP potential, and these have been found to be close to those obtained experimentally.

To show the characteristics of the various potentials under study, we present in figure 2, a plot of the variation of the five potentials (in eV) with the internuclear distance in \AA . Notice the similarity between the curve for GMP + HP and that for GMP + CYP. This indicates that to a large extent, both potentials can be used interchangeably to describe diatomic molecules. Figure 3 is a plot showing the variation of GMP + CYP for some selected diatomic molecules with internuclear distance. The difference in potential depth for different molecules reveals that different molecules have different equilibrium bond lengths r_e . Figures 4–8 give the variations of non-relativistic energy eigenvalues with the following potential parameters: D_e, r_e and α for different ro-vibrational quantum numbers (n, l). Specifically, figure 4 gives the variation of the energy eigenvalues with rotational quantum number $l = 1$ for the selected diatomic molecules. Here, we notice that as the principal quantum number n increases, the non-relativistic

Table 2. Energy eigenvalues (in eV) for various vibrational quantum number for HCl, LiH, H₂, ScH and CH diatomic molecules with $\hbar c = 1973.29 \text{ eV} \cdot \text{\AA}$ for excited quantum states.

States	α	HCl	LiH	H ₂	ScH	CH
2p	0.025	-38.1846	-37.6505	-37.6001	-37.3381	-38.4113
	0.050	-18.6140	-18.1430	-18.2096	-17.8464	-18.8434
	0.075	-12.1471	-11.7179	-11.8372	-11.4430	-12.3748
	0.100	-8.9419	-8.5458	-8.6979	-8.2922	-9.1665
	0.150	-5.7823	-5.4397	-5.6310	-5.2237	-5.9987
3p	0.025	-37.6074	-37.0729	-36.7679	-36.8035	-37.8087
	0.050	-18.1950	-17.7424	-17.5808	-17.4824	-18.4003
	0.075	-11.7944	-11.3937	-11.2881	-11.1530	-11.9981
	0.100	-8.6265	-8.2659	-8.1907	-8.0450	-8.8272
	0.150	-5.5076	-5.2096	-5.1646	-5.0245	-5.7004
3d	0.025	-37.6054	-37.0707	-36.7636	-36.8017	-37.8065
	0.050	-18.1931	-17.7404	-17.5763	-17.4807	-18.3981
	0.075	-11.7925	-11.3918	-11.2834	-11.1514	-11.9959
	0.100	-8.6246	-8.2640	-8.1856	-8.04349	-8.8249
4p	0.025	-37.0414	-36.5073	-35.9593	-36.2794	-37.2186
	0.050	-17.7868	-17.3527	-16.9764	-17.1277	-17.9695
	0.075	-11.4519	-11.0796	-10.7644	-10.8715	-11.6335
4d	0.025	-37.0395	-36.5052	-35.9553	-36.2776	-37.2164
	0.500	-17.7849	-17.3507	-16.9721	-17.1260	-17.9673
	0.750	-11.4501	-11.0778	-10.7598	-10.8700	-11.6314
4f	0.025	-37.0375	-36.5032	-35.9512	-36.2758	-37.2143
	0.050	-17.7830	-17.3488	-16.9678	-17.1244	-17.9652
	0.075	-11.4482	-11.0759	-10.7553	-10.8684	-11.6292
5p	0.025	-36.4865	-35.9535	-35.1737	-35.7655	-36.6405
	0.050	-17.3889	-16.9736	-16.3952	-16.7820	-17.5504
	0.075	-11.1194	-10.7754	-10.2643	-10.5981	-11.2805
5d	0.025	-36.4846	-35.9515	-35.1697	-35.7637	-36.6384
	0.050	-17.3870	-16.9717	-16.3911	-16.7804	-17.5483
	0.075	-11.1176	-10.7736	-10.2600	-10.5966	-11.2784
5f	0.025	-36.4827	-35.9494	-35.1657	-35.7620	-36.6363
	0.050	-17.3852	-16.9698	-16.3869	-16.7788	-17.5462
	0.075	-11.1157	-10.7718	-10.2556	-10.5951	-11.2763
5g	0.025	-36.4808	-35.9474	-35.1618	-35.7602	-36.6343
	0.050	-17.3834	-16.9679	-16.3828	-16.7772	-17.5441
	0.075	-11.1139	-10.7700	-10.2513	-10.5936	-11.2742
6p	0.025	-35.9423	-35.4111	-34.4100	-35.2615	-36.0743
	0.050	-17.0010	-16.6047	-15.8360	-16.4450	-17.1427
6d	0.025	-35.9405	-35.4091	-34.4061	-35.2598	-36.0723
	0.050	-16.9992	-16.6029	-15.8320	-16.4435	-17.1407
6f	0.025	-35.9386	-35.4071	-34.4023	-35.2581	-36.0702
	0.050	-16.9974	-16.6010	-15.8280	-16.4419	-17.1387
6g	0.025	-35.9367	-35.4051	-34.3984	-35.2563	-36.0682
	0.050	-16.9956	-16.5992	-15.8240	-16.4403	-17.1366

energy eigenvalues (in eV) of GMP + CYP decreases, and this decreasing trend is more pronounced in the HCl molecule than in others. Figure 5 gives the energy eigenvalues for GMP + CYP for increasing l when the molecules are in the ground state ($n = 1$). Here, it can be seen that there is an exponential increase in the non-relativistic energy eigenvalues for increasing orbital quantum number l . Figure 6 gives the variation of the non-relativistic energy eigenvalues with dissociation

energy D_e for GMP + CYP when $l = 0$. We notice here that there is an initial rapid increase of energy eigenvalues with D_e up to the point $D_e = 0.5 \text{ eV}$, after which the rate of increase reduces asymptotically to constant values specific to each quantum number n . Figure 7 gives variation of the eigenvalues with equilibrium bond length r_e for GMP + CYP for different principal quantum numbers n , and $l = 0$. Here, we see that the spectra converges, irrespective of the value of n , when

Table 3. Energy eigenvalues (in eV) for various vibrational quantum numbers for HCl, LiH, H₂, ScH and CH diatomic molecules with $\hbar c = 1973.29 \text{ eV \AA}$ for the ground state.

States	α	HCl	LiH	H ₂	ScH	CH
1s	0.025	-39.0290	-38.2427	-38.4614	-37.8854	-39.0290
	0.050	-18.7154	-18.5572	-18.8690	-18.2218	-19.3014
	0.075	-12.7665	-12.0548	-12.4183	-11.7434	-12.7665
	0.100	-9.5209	-8.8379	-9.23875	-8.5490	-9.5208
	0.150	-6.3119	-5.6808	-6.1340	-5.4316	-6.3119
2s	0.025	-38.4135	-37.6526	-37.6044	-37.3400	-38.4135
	0.050	-18.8456	-18.1451	-18.2142	-17.8481	-18.8456
	0.075	-12.3771	-11.7199	-11.8421	-11.4446	-12.3771
	0.100	-9.1689	-8.5478	-8.7032	-8.2937	-9.1689
	0.150	-6.0012	-5.4416	-5.6370	-5.2252	-6.0012
3s	0.025	-37.8109	-37.0750	-36.7720	-36.8054	-37.8109
	0.050	-18.4025	-17.7443	-17.5853	-17.4841	-18.4025
	0.075	-12.0004	-11.3956	-11.2929	-11.1546	-12.0004
4s	0.025	-37.2207	-36.5094	-35.9634	-36.2812	-37.2207
	0.050	-17.9716	-17.3546	-16.9807	-17.1293	-17.9716
	0.075	-11.6357	-11.0815	-10.7689	-10.8731	-11.6357
5s	0.025	-36.6426	-35.9555	-35.1776	-35.7673	-36.6426
	0.050	-17.5525	-16.9755	-16.3993	-16.7836	-17.5525

Table 4. Some analytically deduced parameters for the selected diatomic molecules.

Parameter	HCl	LiH	H ₂	ScH	CH
D_e (in eV)	4.6190	2.5153	4.7446	2.2500	3.9479
r_e (in \AA)	1.2746	1.5956	0.7416	1.7760	1.1198
μ (in a.m.u.)	0.9801	0.8801	0.5039	0.9860	0.9299

the equilibrium bond length $r_e \geq 1 \text{ \AA}$. Finally, figure 8 gives the variation of non-relativistic energy eigenvalues with screening parameter α , for selected diatomic molecules. Here, we notice that the spectra for H₂ depart remarkably from the trends of other molecules.

5. Hellmann–Feynmann theorem (HFT)

We now calculate the expectation values of some physical variables for GMP+CYP using the Hellmann–Feynmann theorem (HFT). According to the theorem, suppose the Hamiltonian H of a given quantum system is a function of some generalised parameter q , i.e. $H(q)$, then the energy eigenvalue $E_{nl}(q)$ and the normalised eigenfunction $\psi_{nl}(q)$ satisfy the expression [49–51]

$$\frac{\partial E_{nl}(q)}{\partial q} = \left\langle \psi_{nl}(q) \left| \frac{\partial \hat{H}(q)}{\partial q} \right| \psi_{nl}(q) \right\rangle. \tag{70}$$

Here we use the effective non-relativistic Hamiltonian \hat{H} corresponding to the non-relativistic energy spectrum eq. (55) and radial wave function eq. (57) given as

$$\hat{H} = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu r^2} l(l+1) + V - \frac{\eta e^{-\alpha r}}{1 - e^{-\alpha r}} + \frac{\Omega e^{-2\alpha r}}{(1 - e^{-\alpha r})^2} - \frac{b}{r} + \frac{ce^{-\alpha r}}{r} - \frac{ae^{-2\alpha r}}{r^2}. \tag{71}$$

5.1 Expectation value of r^{-2}

In order to calculate $\langle r^{-2} \rangle$, we set $q = l$ in eq. (70) to get

$$\frac{\partial E_{nl}(l)}{\partial l} = \left\langle \psi_{nl}(l) \left| \frac{\partial \hat{H}(l)}{\partial l} \right| \psi_{nl}(l) \right\rangle. \tag{72}$$

Taking the partial derivative of the left-hand side of eq. (55) with respect to l gives

$$\frac{\partial E_{nl}(l)}{\partial l} = \frac{\hbar^2 \alpha^2}{2\mu} (2l+1) - \frac{\hbar^2 \alpha^2}{8\mu \chi_2^2} \left[2\chi_1 (2l+1) + 2\chi_1 \frac{(2l+1)}{\sqrt{\chi_3}} - \frac{\chi_1 (2l+1)}{\chi_2 \sqrt{\chi_3}} \right], \tag{73}$$

where

$$\begin{aligned}\chi_1 &= \chi_2^2 + \xi - \frac{2\mu\eta}{\hbar^2\alpha^2} - \frac{2\mu b}{\hbar^2\alpha} + l(l+1) \\ \chi_2 &= n + \frac{1}{2} + \sqrt{\chi_3} \\ \chi_3 &= \frac{1}{4} - \xi + \frac{2\mu c}{\hbar^2\alpha} + l(l+1).\end{aligned}\quad (74)$$

Evaluating the right-hand side of eq. (72) using eq. (71) gives

$$\left\langle \psi_{nl}(l) \left| \frac{\partial \hat{H}(l)}{\partial l} \right| \psi_{nl}(l) \right\rangle = \frac{\hbar^2}{2\mu} (2l+1) \langle r^{-2} \rangle. \quad (75)$$

Equating eqs (73) and (75) yields

$$\begin{aligned}\langle r^{-2} \rangle &= \alpha^2 - \frac{\alpha^2(2l+1)}{4\chi_2^2} \left[2\chi_1(2l+1) \right. \\ &\quad \left. + 2\chi_1 \frac{(2l+1)}{\sqrt{\chi_3}} - \chi_1 \frac{(2l+1)}{2\sqrt{\chi_3}} \right].\end{aligned}\quad (76)$$

5.2 Expectation value of r^{-1}

Here, we set $q = b$, in eq. (70), and then evaluate its partial derivative with respect to b . Doing so we have

$$\frac{\partial E_{nl}(b)}{\partial b} = -\alpha - \frac{\hbar^2\alpha^2}{8\mu\chi_2^2} \left[-\frac{4\mu}{\hbar^2\alpha} \chi_1 \right] \quad (77)$$

and

$$\left\langle \psi_{nl}(b) \left| \frac{\partial \hat{H}(b)}{\partial b} \right| \psi_{nl}(b) \right\rangle = -\langle r^{-1} \rangle. \quad (78)$$

Equating eqs (77) and (78) gives

$$\langle r^{-1} \rangle = \alpha - \frac{\alpha\chi_1}{2\chi_2^2}. \quad (79)$$

5.3 Expectation value of $(e^{\alpha r} - 1)^{-1}$

Here, independently equating the partial derivatives of eqs (55) and (70) with respect to η gives

$$\langle (e^{\alpha r} - 1)^{-1} \rangle = -\frac{\chi_1}{2\chi_2^2}. \quad (80)$$

5.4 Expectation value of $(1 - e^{-\alpha r})^{-2}$

Here, we evaluate the partial derivative of eq. (55) with respect to Ω to get

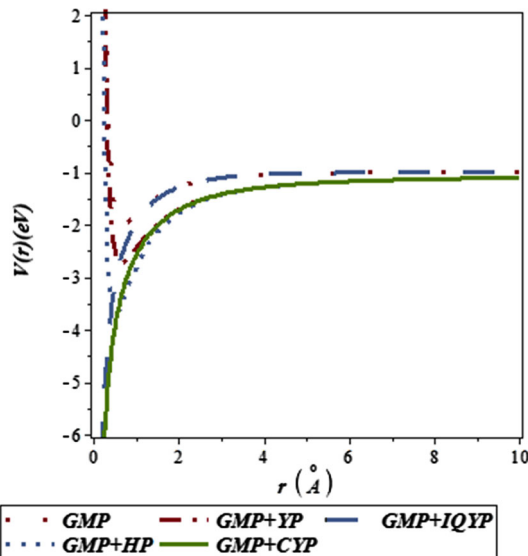


Figure 2. Plot of five potential energies vs. internuclear distance.

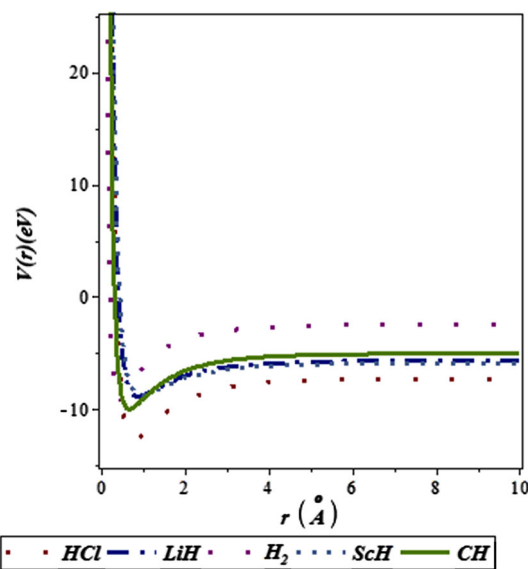


Figure 3. Plot of potential energy vs. internuclear distance for some diatomic molecules.

$$\frac{\partial E_{nl}(\Omega)}{\partial \Omega} = -\frac{1}{4\chi_2^3} \left[2\chi_1\chi_2 \left(\frac{\chi_1}{\sqrt{\chi_3}} - 1 \right) - \frac{\chi_1^2}{\sqrt{\chi_3}} \right] \quad (81)$$

and also evaluate the right-hand side of eq. (70) with respect to Ω to get

$$\left\langle \psi_{nl}(\Omega) \left| \frac{\partial \hat{H}(\Omega)}{\partial \Omega} \right| \psi_{nl}(\Omega) \right\rangle = -\langle (1 - e^{-\alpha r})^{-2} \rangle. \quad (82)$$

Equating eqs (81) and (82) gives

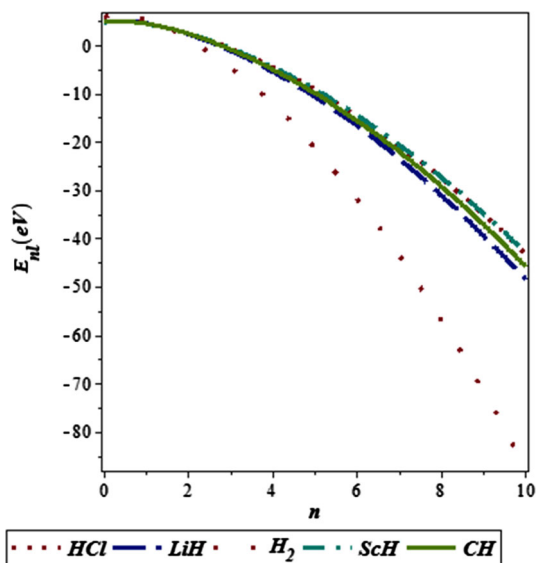


Figure 4. Energy eigenvalues vs. principal quantum numbers for some diatomic molecules when $l = 1$.

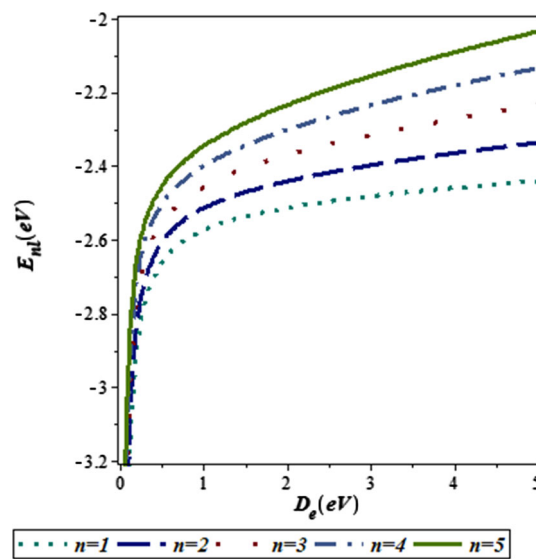


Figure 6. Variation of energy eigenvalues with dissociation energy D_e for GMP + CYP for different principal quantum numbers n , when $l = 0$.

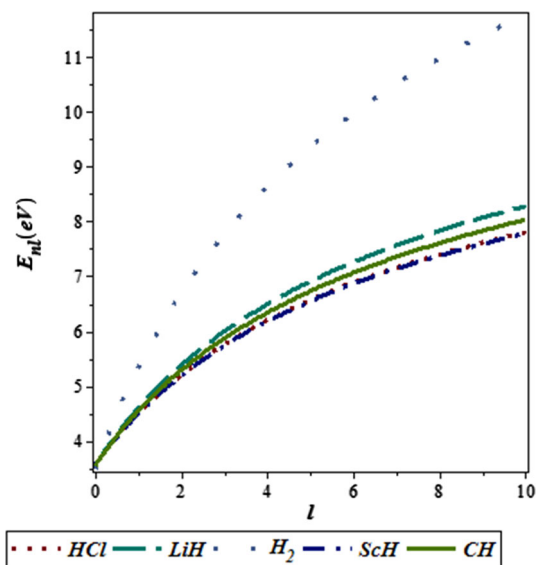


Figure 5. Energy eigenvalue vs. vibrational quantum number for some diatomic molecules when $n = 1$.

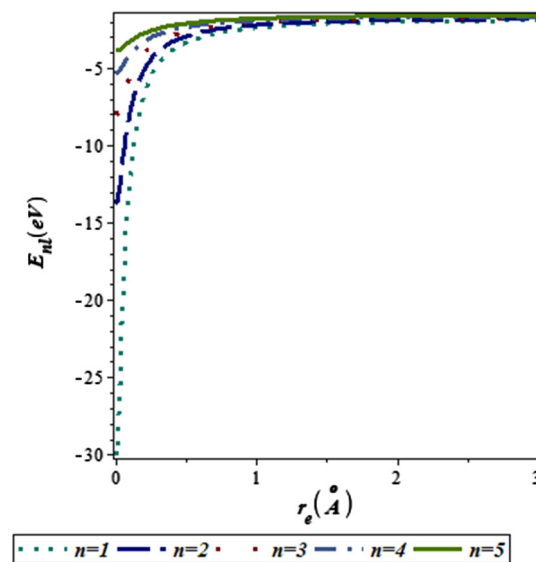


Figure 7. Variation in energy eigenvalues with equilibrium bond length r_e for GMP + CYP for different principal quantum numbers n , when $l = 0$.

$$\begin{aligned} & \langle (1 - e^{-\alpha r})^{-2} \rangle \\ &= \frac{1}{4\chi_2^3} \left[2\chi_1\chi_2 \left(\frac{\chi_1}{\sqrt{\chi_3}} - 1 \right) - \frac{\chi_1^2}{\sqrt{\chi_3}} \right]. \end{aligned} \quad (83)$$

5.5 Expectation value of p^2 and T

Here, we take the partial derivative of eq. (55) with respect to μ to obtain

$$\begin{aligned} \frac{\partial E_{nl}(\mu)}{\partial \mu} &= \frac{\hbar^2 \alpha^2}{2\mu^2} l(l+1) \\ &- \frac{\hbar^2 \alpha^2 \chi_1}{4\mu \chi_2^3} \left[\frac{2\chi_2^2}{\sqrt{\chi_3}} \left(\frac{2c}{\hbar^2 \alpha} - \frac{\xi}{\mu} \right) + \frac{\xi}{\mu} - \frac{2\eta}{\hbar^2 \alpha^2} - \frac{2b}{\hbar^2 \alpha} \right. \\ &\quad \left. - \frac{\chi_1}{2\sqrt{\chi_3}} \left(\frac{2c}{\hbar^2 \alpha} - \frac{\xi}{\mu} \right) \right] - \frac{\hbar^2 \alpha^2}{8\mu^2} \left(\frac{\chi_1}{\chi_2} \right)^2 \end{aligned} \quad (84)$$

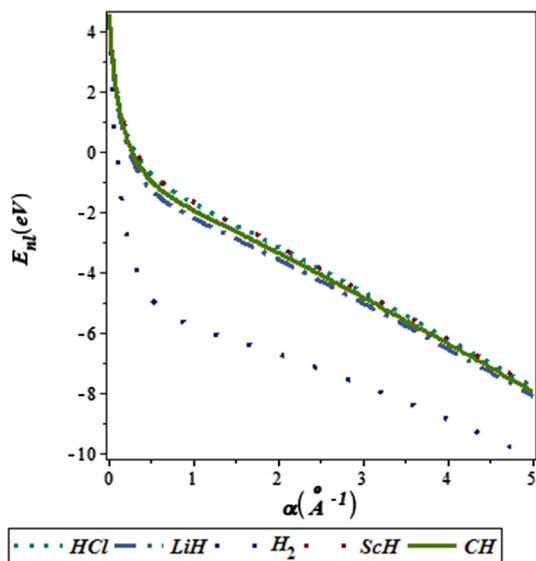


Figure 8. Variation in energy eigenvalues with screening parameter α for some diatomic molecules.

and evaluating the right-hand side of eq. (70) using μ as the dependent variable gives

$$\begin{aligned} & \langle \psi_{nl}(\mu) \left| \frac{\partial \hat{H}(\mu)}{\partial \mu} \right| \psi_{nl}(\mu) \rangle \\ &= -\frac{1}{\mu} \left(\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu r^2} l(l+1) \right) \\ &= -\frac{1}{\mu} [\hat{H} - V] = -\frac{1}{\mu} \langle T \rangle. \end{aligned} \tag{85}$$

Equating eqs (84) and (85) gives

$$\begin{aligned} \langle T \rangle &= \frac{\hbar^2 \alpha^2}{2\mu l(l+1)} + \frac{\hbar^2 \alpha^2 \chi_1}{4\chi_2^3} \left[\frac{2\chi_2^2}{\sqrt{\chi_3}} \left(\frac{2c}{\hbar^2 \alpha} - \frac{\xi}{\mu} \right) \right. \\ &+ \left. \frac{\xi}{\mu} - \frac{2\eta}{\hbar^2 \alpha^2} - \frac{2b}{\hbar^2 \alpha} - \frac{\chi_1}{2\sqrt{\chi_3}} \left(\frac{2c}{\hbar^2 \alpha} - \frac{\xi}{\mu} \right) \right] \\ &+ \frac{\hbar^2 \alpha^2}{8\mu} \left(\frac{\chi_1}{\chi_2} \right)^2. \end{aligned} \tag{86}$$

Note that

$$\begin{aligned} -\frac{1}{\mu} \langle T \rangle &= -\frac{1}{2\mu^2} \langle p^2 \rangle \\ \langle p^2 \rangle &= \hbar^2 \alpha^2 l(l+1) \\ &+ \frac{\hbar^2 \alpha^2 \mu \chi_1}{2\chi_2^3} \left[\frac{2\chi_2^2}{\sqrt{\chi_3}} \left(\frac{2c}{\hbar^2 \alpha} - \frac{\xi}{\mu} \right) \right. \\ &+ \left. \frac{\xi}{\mu} - \frac{2\eta}{\hbar^2 \alpha^2} - \frac{2b}{\hbar^2 \alpha} - \frac{\chi_1}{2\sqrt{\chi_3}} \left(\frac{2c}{\hbar^2 \alpha} - \frac{\xi}{\mu} \right) \right] \\ &+ \frac{\hbar^2 \alpha^2}{4} \left(\frac{\chi_1}{\chi_2} \right)^2. \end{aligned} \tag{87}$$

6. Conclusion

We have studied the bound-state solutions of the spin and pseudospin limits of the Dirac equation with the generalised Morse and a class of Yukawa potential using the NU method and an appropriate approximation scheme. The energy eigenvalues and the corresponding normalised eigenfunction of the non-relativistic limits of the spin symmetry were obtained. We also studied and compared the energy spectra with respect to internuclear distance, of five classes of potentials namely, GMP, GMP+HP, GMP+IQYP, GMP+YP and GMP+CYP. In addition, we investigated and compared the behaviour of some selected diatomic molecules, i.e., HCl, LiH, H₂, ScH and CH when subjected to this potential. This was achieved by generating plots of the variation of their potential energies with internuclear distance r , energy spectra vs. rovibrational quantum numbers, energy spectra vs. dissociation energy, energy spectra vs. bond length r_e and energy spectra vs. screening parameter (potential range) α .

Moreover, by adjusting some potential parameters, six potentials (GMP, CYP, Hellmann potential, IQYP, Hulthen potential and Coulomb potential) of which GMP+CYP potential reduces to were evaluated. Also, the corresponding energies of these special potentials deduced using eq. (55) were found to be in excellent agreement with those in the existing literature. Finally, we reported the expectation values of some useful physical observables deduced by using the Hellmann–Feynman theorem.

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Appendix: Parameterised formulation of the NU method

The Nikiforov–Uvarov (NU) method [29] is an analytical technique developed to solve hypergeometric-type second-order differential equations by means of special orthogonal functions. For instance, for any given potential, an equation such as the Schrödinger or a Schrödinger-like equation in special coordinates can be reduced to a generalised hypergeometric-type equation with an appropriate coordinate transformation $s = s(r)$, and then solved to obtain its solution. One such hypergeometric-type second-order differential equation

that can be solved using the NU method is of the form (eq. (2)):

$$\psi_n''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi_n'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s) = 0, \tag{A.1}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials of at most second degree, $\tilde{\tau}(s)$ is a first-degree polynomial and $\psi(s)$ is a hypergeometric-type function, and the prime denotes differentiation with respect to s .

In order to find an exact solution to eq. (A.1), a common ansatz for the wave function ψ is chosen as

$$\psi(s) = \phi(s)\chi(s). \tag{A.2}$$

Substituting eq. (A.2) into eq. (A.1) and dividing by $\phi(s)$ gives

$$\begin{aligned} \chi''(s) + \left(2\frac{\phi'(s)}{\phi(s)} + \frac{\tilde{\tau}(s)}{\sigma(s)}\right)\chi'(s) \\ + \left(\frac{\phi''(s)}{\phi(s)} + \frac{\phi'(s)\tilde{\tau}(s)}{\phi(s)\sigma(s)} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\right)\chi(s) = 0. \end{aligned} \tag{A.3}$$

Let the coefficient of $\chi'(s)$ in eq. (A.3) takes the form $\tau(s)/\sigma(s)$, where $\tau(s)$ is a polynomial of degree at most one, i.e.,

$$2\frac{\phi'(s)}{\phi(s)} + \frac{\tilde{\tau}(s)}{\sigma(s)} = \frac{\tau(s)}{\sigma(s)}. \tag{A.4}$$

Re-arranging eq. (A.4) and deducing its logarithmic derivative, we obtain

$$\frac{\phi'(s)}{\phi(s)} = \frac{1}{2} \left[\frac{\tau(s)}{\sigma(s)} - \frac{\tilde{\tau}(s)}{\sigma(s)} \right] = \frac{\pi(s)}{\sigma(s)}, \tag{A.5}$$

where

$$\pi(s) = \frac{1}{2} [\tau(s) - \tilde{\tau}(s)], \tag{A.6}$$

and therefore

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s). \tag{A.7}$$

The parameter $\pi(s)$ is also a first-degree polynomial. The term $\phi_n''(s)/\phi_n(s)$ appearing in the coefficient of $\chi(s)$ in eq. (A.3) is obtained by finding the second logarithmic derivative of eq. (A.5) using the Leibnitz's formula. Doing so we get

$$\begin{aligned} \frac{\phi''(s)}{\phi(s)} &= \left(\frac{\phi'(s)}{\phi(s)}\right)' + \left(\frac{\phi'(s)}{\phi(s)}\right)^2 \\ &= \left(\frac{\pi(s)}{\sigma(s)}\right)' + \left(\frac{\pi(s)}{\sigma(s)}\right)^2. \end{aligned} \tag{A.8}$$

Taking the equality given by eq. (A.5), the coefficient of $\chi(s)$ in eq. (A.3) can then be re-written in a more suitable form as

$$\frac{\phi_n''(s)}{\phi_n(s)} + \frac{\phi'(s)\tilde{\tau}(s)}{\phi(s)\sigma(s)} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)} = \frac{\tilde{\sigma}(s)}{\sigma^2(s)}, \tag{A.9}$$

where

$$\begin{aligned} \tilde{\sigma}(s) &= \tilde{\sigma}(s) + \pi^2(s) + \pi(s) [\tilde{\tau}(s) - \sigma'(s)] \\ &\quad + \pi'(s)\sigma(s). \end{aligned} \tag{A.10}$$

Substituting the right-hand sides of eqs (A.4) and (A.9) into eq. (A.3) yields the following hypogeometric-type equation:

$$\chi''(s) + \frac{\tau(s)}{\sigma(s)}\chi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\chi(s) = 0. \tag{A.11}$$

Assuming that $\tilde{\sigma}(s)$ in the above expression is divisible by $\sigma(s)$ so that we can write $\tilde{\sigma}(s)$ as

$$\tilde{\sigma}(s) = \lambda\sigma(s), \tag{A.12}$$

where λ is a constant, eq. (A.11) reduces to the hypergeometric-type equation

$$\sigma(s)\chi''(s) + \tau(s)\chi'(s) + \lambda\chi(s) = 0, \tag{A.13}$$

and its solution is given as a hypogeometric-type function. To determine the polynomial $\pi(s)$, eq. (10) is compared with eq. (12) and then a quadratic equation for $\pi(s)$ is obtained as follows:

$$\pi^2(s) + \pi(s) [\tilde{\tau}(s) - \sigma'(s)] + \tilde{\sigma}(s) - k\sigma(s) = 0, \tag{A.14}$$

where

$$k = \lambda - \pi'(s). \tag{A.15}$$

Solving eq. (A.14) for $\pi(s)$ yields the following inequality:

$$\begin{aligned} \pi(s) &= \frac{\sigma'(s) - \tilde{\tau}(s)}{2} \\ &\quad \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)}. \end{aligned} \tag{A.16}$$

The constant k is determined by setting the discriminant of this quadratic equal to zero. After determining k , the polynomial $\pi(s)$ is obtained from eq. (A.16), and $\tau(s)$ and λ are also obtained by using eqs (A.7) and (A.15), respectively.

To generalise the solutions of eq. (A.13) is to show that all the derivatives of hypergeometric-type functions are also of the hypergeometric-type [52]. Following this procedure, we differentiate eq. (A.13) by using the representation $\eta_1(s) = \chi'(s)$ to obtain

$$\sigma(s)\eta_1''(s) + \tau_1(s)\eta_1'(s) + \mu_1\eta_1(s) = 0, \tag{A.17}$$

where $\tau_1(s) = \tau(s) + \sigma'(s)$ is a first-degree polynomial and $\mu_1 = \lambda + \tau'(s)$ is a parameter that is independent of the variable s . We can see that eq. (A.17) is a hypogeometric-type equation. Taking a new representation given by $\eta_2(s) = \psi''(s)$, the second derivative of eq. (A.13) becomes

$$\sigma(s)\eta_2''(s) + \tau_2(s)\eta_2'(s) + \mu_2\eta_2(s) = 0, \quad (\text{A.18})$$

where

$$\tau_2(s) = \tau_1(s) + \sigma'(s) = \tau(s) + 2\sigma'(s), \quad (\text{A.19})$$

$$\mu_2 = \mu_1 + \tau_1'(s) = \lambda + 2\tau'(s) + \sigma''(s). \quad (\text{A.20})$$

In a similar way, several hypergeometric-type equations can be constructed as a family of particular solutions of eq. (A.13) by taking $\eta_n(s) = \chi^{(n)}(s)$, i.e.

$$\sigma(s)\eta_n''(s) + \tau_n(s)\eta_n'(s) + \mu_n\eta_n(s) = 0. \quad (\text{A.21})$$

From the foregoing discussion, the general recurrence relations for $\tau_n(s)$ and $\mu_n(s)$ are given respectively as

$$\tau_n(s) = \tau(s) + n\sigma'(s), \quad (\text{A.22})$$

$$\mu_n = \lambda + n\tau'(s) + \frac{n(n-1)}{2}\sigma''(s). \quad (\text{A.23})$$

When $\mu_n = 0$, eq. (A.23) reduces to

$$\lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s); \quad (n=0, 1, 2, \dots), \quad (\text{A.24})$$

and so eq. (A.21) has a particular solution of the form $\chi(s) = \chi_n(s)$ which is a polynomial of degree n . Furthermore, to obtain an eigenvalue solution through the NU method, the relationship between λ and λ_n must be established by means of eqs (A.15) and (A.24).

The function χ_n is the hypergeometric-type function whose polynomial solutions are given by the Rodrigues relation

$$\chi_n^{(n)}(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n \rho(s)], \quad (\text{A.25})$$

where B_n is the normalisation constant and $\rho(s)$ is the weight function which must satisfy the condition

$$(\sigma(s)\rho(s))' = \tau(s)\rho(s). \quad (\text{A.26})$$

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