

Bound state solutions of the Deng–Fan molecular potential with the Pekeris-type approximation using the Nikiforov–Uvarov (N–U) method

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Abstract By employing the Pekeris-type approximation to deal with the centrifugal term, we solve the Schrödinger equation with the Deng–Fan molecular potential for all values of l (orbital angular momentum quantum number). Using the Nikiforov–Uvarov (N–U) method, the approximate analytical bound state energy eigenvalues and the corresponding wave functions are obtained. The results obtained are in good agreement with those ones found in the literature. The bound state energy eigenvalues for a set of diatomic molecules (HCl, LiH, H₂, ScH, TiH, VH, CrH, CuLi, TiC, NiC, ScN and ScF) corresponding to the Deng–Fan molecular potential for arbitrary values of n and l quantum numbers are reported.

Keywords Schrödinger equation · Diatomic molecules · Deng–Fan molecular potential · Pekeris-type approximation scheme · Nikiforov–Uvarov (N–U) method

1 Introduction

It is well known in non-relativistic quantum mechanics that the motions of the particles are completely described by the Schrödinger equation [1–10, 13–40, 50, 51]. The

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analytical solutions of this equation with physical potentials play an important role in the understanding of physical background of such a system [1–10, 13–40, 50, 51]. This is attributed to the fact that the wave functions associated with these problems contain all the necessary information regarding the quantum systems under consideration.

Thus, in recent years, considerable efforts have been directed towards obtaining the non-relativistic energy eigenvalues and the corresponding wave functions by solving the Schrödinger equation [1–5]. However, one of the major challenging tasks of theoretical physics is to obtain the analytical solutions of some quantum mechanical problems in the presence of the centrifugal term ($l \neq 0$).

Molecular potentials in quantum mechanics are forms of potential energy functions within which molecules can interact. They vary in nature and mostly depend on their internuclear distance between their atoms. Any physical potential $V(r)$ in such a quantum molecular system has to behave properly at the limits of the coordinate. i.e. $V_{r \rightarrow 0}(r) = \infty$ and $V_{r \rightarrow \infty}(r)$ approaches a constant. For a stable molecule, the potential has minimum at bond length r_e , i.e. $V_{r \rightarrow r_e}(r) = 0$ [6–12]. Thus, seeking for the approximate analytical solutions of the Schrödinger equation associated with these forms of potentials is essential.

Some quantum molecular systems have been solved analytically by adopting different methods, these include: pseudoharmonic potential [13–15], Kratzer potential [16–20]. Some of these quantum molecular potentials exist in the form of the two-, three-, four-, and five-parameter potential functions [21].

However, it is not possible to obtain analytical solutions of some of these problems due to the presence of the centrifugal barrier term. For such problems to be solvable, we resort to the use of one of the approximation schemes to deal with this centrifugal term [22]. One of such schemes is the Pekeris-type approximation introduced by Pekeris [22], also, for a short-range potential, Greene and Aldrich in 1976 proposed a similar approximation [23]. The proposed approximation was used to study arbitrary l -states pseudo-Hulthén wave functions by using variational trial functions [23].

Moreover, some quantum molecular systems have been solved by applying an improved approximation scheme to the centrifugal term, the approximate analytical solutions to some of these potential models have been obtained by using different methods. These methods include: Nikiforov–Uvarov (N–U) method [19, 24–27], Hypergeometric function [3]. Other methods are: asymptotic iteration method [28], Factorization method [15, 20], Pseudo-perturbative shifted l -expansion techniques [29].

Other examples that have been investigated so far are: the two-point quasi-rational approximation technique [30], the tridiagonal J-matrix representation [31], exact quantization rule [32, 33], supersymmetry [7, 21, 34, 35], variational method and supersymmetric quantum mechanics [36].

In the list of these molecular potentials, the Morse potential is one of the most useful models in many different fields of physics such as molecular physics, solid state physics and chemical physics [5]. However, irrespective of the fact that the Morse Potential is a typical anharmonic potential and it has been the subject of interest since it was proposed by Morse [37]. It is also worth noting that as bond length approaches zero, the Morse potential goes to a large value, whereas an ideal potential should approach infinity. This shortcoming of the Morse Potential is attributed to the small

but non-zero wave functions for bound vibrational states as the bond length approaches zero [6].

In an attempt to overcome this shortcoming, the Morse potential is modified in several ways. These modified Morse potentials have more parameters than the usual Morse potential itself and lead to better agreement with experiment, but do not have correct behaviour at $r = 0$ [6]. With this modification, a modified form was introduced by Deng and Fan [8]. The Deng–Fan exponential–type potential is a simple modified Morse potential, sometimes, called generalized Morse potential [8]. This has been proposed in an attempt of finding a more suitable diatomic potential to describe the vibrational spectrum [3]. It is qualitatively similar to the Morse potential but has the correct asymptotic behaviour as the internuclear distance approaches zero [6].

The Deng–Fan molecular potential for a diatomic molecule was proposed by Deng and Fan [8] as

$$V(r) = D_e \left[1 - \frac{b}{e^{ar} - 1} \right]^2, \quad b = e^{ar_e} - 1, \quad r \in [0, \infty) \quad (1)$$

where D_e is the dissociation energy, r_e is the equilibrium inter-nuclear distance, a is the range of the potential well and b is the position of minimum r_e . It is worth noting that this molecular potential has correct physical boundary conditions at the origin and at infinity [3, 6–12, 38, 39].

The analytical expressions for the energy eigenvalues and the wave functions for $l = 0$ state have been obtained by Deng and Fan [8]. In an attempt of solving this molecular potential, some of the following methods have been used: functional analysis method [3, 6, 9]. In 2011, Ikhdair obtained the approximate analytical solutions with this potential for the Dirac equation with spin and pseudospin symmetry conditions by using a new improved approximation scheme (Pekeris-type) with the Nikiforov–Uvarov method [26].

The approximate bound state solutions of the pseudospin and spin symmetric Dirac equation with the generalized Morse potential has been obtained by using an improved approximation scheme to deal with the centrifugal (pseudo-centrifugal) term, this has been done by employing the basic concept of the supersymmetric shape invariance formalism [40]. In the same way, Zhang et al. [7] used the basic concept of the supersymmetric shape invariance formalism and functional analysis method to obtain the approximate solutions of the generalized Morse potential model including the centrifugal term.

Recently, the bound state solutions of the Klein–Gordon and Dirac equations of the Deng–Fan potential have been obtained by using the functional analysis method for $l \neq 0$ [38], the Nikiforov–Uvarov method for $l \neq 0$ [11] and for $l = 0$ [12]. By using a proper approximation scheme to the centrifugal term, Wei and Chen [39] obtained the l -wave continuum states of the Schrödinger equation for the modified Morse potential. In their work, they obtained the normalized analytical wave functions and the corresponding phase shifts. Also, it has been shown that the energy levels of the continuum states reduce to those of the bound states at the poles of the scattering amplitude [39].

This potential has been used to describe diatomic molecular energy spectra and electromagnetic transitions and it is an ideal internuclear potential in diatomic molecules with the same behaviour for $r \rightarrow 0$ [10]. The comparison between the Deng–Fan and Morse molecular potentials have been studied by various authors [6,9].

Furthermore, the interest in the Deng–Fan molecular potential is due to its significant applications in the study of the diatomic molecules in the field of molecular physics [3,6,7].

In this work, our focus is to obtain the approximate analytical solutions of the Schrödinger equations for the Deng–Fan molecular potential with the Pekeris-type approximation using the Nikiforov–Uvarov (N–U) method. The successful applications of the results obtained are used to find the bound state energy eigenvalues for a set of diatomic molecules (HCl, LiH, H₂, ScH, TiH, VH, CrH, CuLi, TiC, NiC, ScN and ScF) for arbitrary values of n and l quantum numbers.

The work is organized as follows, in Sect. 2, we review the Nikiforov–Uvarov method. In Sect. 3, the Schrödinger equation is solved by using the Nikiforov–Uvarov method with the non-zero angular momentum quantum numbers for the Deng–Fan molecular potential. Section 4 contains the applications of the results. In Sect. 5, the conclusion is given.

2 Overview of the Nikiforov–Uvarov (N–U) method

This method has been successfully applied to mathematical, nuclear and chemical physics as well [11,12,19,24–27,41–47,51]. The Nikiforov–Uvarov (N–U) method reduces the second order linear differential equation to generalized equation of hypergeometric type [43]. With an appropriate coordinate transformation $s = s(r)$, the equation take the form

$$\Psi''(s) + \frac{\bar{\tau}(s)}{\sigma(s)}\Psi'(s) + \frac{\bar{\sigma}(s)}{\sigma^2(s)}\Psi(s) = 0, \quad (2)$$

where $\sigma(s)$ and $\bar{\sigma}(s)$ are polynomials, at most second degree and $\bar{\tau}(s)$ is a first degree polynomials.

By taking the following factorization

$$\Psi(s) = \phi(s)y(s), \quad (3)$$

Equation (1) reduces to the hypergeometric type equation of the form [43]

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0, \quad (4)$$

where

$$\tau(s) = \bar{\tau}(s) + 2\pi(s), \quad (5)$$

satisfies the condition $\tau'(s) < 0$, which will have a negative derivative is related to the function $\phi(s)$ by

$$\pi(s) = \sigma(s) \frac{d}{ds} [\ln \phi(s)] \quad (6)$$

The parameter λ is defined by

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

the energy eigenvalues can be calculated from Eq. (7). In order to calculate the energy eigenvalues, we need first, to determine λ by using the first derivative of $\pi(s)$ and defining

$$K = \lambda - \pi'(s). \quad (8)$$

By solving the resulting quadratic equation for $\pi(s)$, we obtain the following expression

$$\pi(s) = \left(\frac{\sigma' - \bar{\tau}}{2} \right) \pm \sqrt{\left(\frac{\sigma' - \bar{\tau}}{2} \right)^2 - \bar{\sigma} + k\sigma}. \quad (9)$$

Here, $\pi(s)$ is a polynomial with the parameter s and the prime denote the first derivative of the functions $\sigma(s)$ and $\tau(s)$, respectively. The determination of k is the essential point in the calculation of $\pi(s)$. It is simply defined by setting the discriminant of the square root to zero [43], therefore, a general quadratic expression for k can be obtained. The wave function $\phi(s)$ in relation in Eq. (3) satisfies the condition

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)}, \quad (10)$$

can now be determined and using the Rodrigues' relation. The polynomial solutions $y_n(s)$ are given by

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s) \rho(s)], \quad (11)$$

where B_n is a normalization constant and the weight function $\rho(s)$ satisfies the following relation

$$\frac{d}{ds} [\sigma(s) \rho(s)] = \tau(s) \rho(s). \quad (12)$$

3 Any l -State solutions of the Schrödinger equation

3.1 Separation of variables for the Schrödinger equation with the Deng–Fan molecular potential

The Schrödinger equation for motion of a particle with the reduced mass μ in the spherical symmetric potential described by the spherical coordinates is given by:

$$-\frac{\hbar^2}{2\mu} \left[\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right) + V(r) \right] \Psi_{nlm}(r, \theta, \phi) = E_{nl} \Psi_{nlm}(r, \theta, \phi). \quad (13)$$

By considering the solution of the form

$$\psi_{nlm}(r, \theta, \phi) = U_{nl}(r) Y_{lm}(\theta, \phi), \quad (14)$$

we obtain the radial part of Schrodinger equation as:

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) U_{nl}(r) - \frac{2\mu}{\hbar^2} \left[V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2} \right] U_{nl}(r) + \frac{2\mu E_{nl}}{\hbar^2} U_{nl}(r) = 0, \quad (15)$$

where the relationship between the effective potential $V_{eff}(r)$ and the centrifugal term \tilde{V}_l is defined as

$$V_{eff}(r) = V(r) + \tilde{V}_l = V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2}. \quad (16)$$

By substituting of $U_{nl}(r) = \frac{R_{nl}(r)}{r}$, we have,

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) \frac{R_{nl}(r)}{r} = \frac{1}{r} \frac{d^2}{dr^2} R_{nl}(r) \quad (17)$$

and accordingly, the radial Schrödinger equation given by Eq. (15) can now be written in the form

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2} [E_{nl} - V_{eff}] R_{nl}(r) = 0. \quad (18)$$

3.2 Approximate analytical solutions of the Deng–Fan molecular potential

In order to obtain the bound state solutions of $l \neq 0$, we insert the potential in Eq. (1) into Eq. (16), then the effective potential becomes:

$$V_{eff}(r) = D_e \left[1 - \frac{be^{-ar}}{1 - e^{-ar}} \right]^2 + \frac{l(l+1)\hbar^2}{2\mu r^2}. \quad (19)$$

Using the following new improved approximation scheme to deal with the centrifugal term (Pekeris-type approximation scheme), near the minimum point $r = r_e$ [7, 11, 26, 40]:

$$\begin{aligned} \frac{1}{r^2} &= a^2 \left[d_0 + \frac{e^{-ar}}{(1 - e^{-ar})^2} \right] \\ &= a^2 \left[d_0 + \frac{1}{(ar)^2} - \frac{1}{12} + \frac{(ar)^2}{240} - \frac{(ar)^4}{6048} + \frac{(ar)^6}{172800} + 0((ar)^8) \right] \end{aligned} \quad (20)$$

where $ar \ll 1$ and the dimensionless parameter $d_0 = \frac{1}{12}$ by the above series expansion. It has been shown that this approximation scheme is better than the Greene and Aldrich [23] approximation scheme used by Dong and Gu [3], as pointed out by Zhang et al. [7].

Substituting Eq. (20) into Eq. (18), we obtain the radial Schrödinger equation with the Deng–Fan potential and the centrifugal barrier term as:

$$\begin{aligned} \frac{d^2 R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[E_{nl} - D_e \left(1 - \frac{be^{-ar}}{1 - e^{-ar}} \right)^2 \right. \\ \left. - \frac{l(l+1)\hbar^2 a^2}{2\mu} \left(d_0 + \frac{e^{-ar}}{(1 - e^{-ar})^2} \right) \right] R_{nl} = 0. \end{aligned} \quad (21)$$

Taking a transformation equation of the form $s = e^{-ar}$, Eq. (21) reduces to

$$\begin{aligned} \frac{d^2 R_{nl}(s)}{ds^2} + \frac{1-s}{s(1-s)} \frac{dR_{nl}(s)}{ds} + \frac{1}{s^2(1-s)^2} \left[-(\varepsilon_{nl}^2 + (2+b)\beta^2 b) s^2 \right. \\ \left. + (2(\beta^2 b + \varepsilon_{nl}^2) - \gamma) s - \varepsilon_{nl}^2 \right] R_{nl}(s) = 0 \end{aligned} \quad (22)$$

where we have used the following dimensional parameters:

$$\varepsilon^2 = \frac{2\mu E_{nl}}{\hbar^2 a^2}, \quad \beta^2 = \frac{2\mu D_e}{\hbar^2 a^2}, \quad \gamma = l(l+1) \text{ and } -\varepsilon_{nl}^2 = \varepsilon^2 - \beta^2 - \gamma d_0. \quad (23)$$

In order to solve Eq. (22) by using the Nikiforov–Uvarov (N–U) method, we compare it with Eq. (2) and obtain the following polynomials:

$$\begin{aligned} \bar{\tau}(s) &= 1 - s, \quad \sigma(s) = s(1 - s), \quad \sigma^2(s) = s^2(1 - s)^2, \\ \bar{\sigma}(s) &= -(\varepsilon_{nl}^2 + (2+b)\beta^2 b) s^2 + (2(\beta^2 b + \varepsilon_{nl}^2) - \gamma) s - \varepsilon_{nl}^2 \\ &= -As^2 + Bs - C, \end{aligned} \quad (24)$$

where

$$A = \varepsilon_{nl}^2 + (2 + b) \beta^2 b, \quad B = 2 \left(\beta^2 b + \varepsilon_{nl}^2 \right) - \gamma, \quad C = \varepsilon_{nl}^2. \tag{25}$$

Substituting these polynomials into Eq. (9), we obtain the following four possible solutions for $\pi(s)$ as

$$\pi(s) = -\frac{s}{2} \pm \frac{1}{2} \left[\left(\sqrt{(1 + 2l)^2 + 4\beta^2 b^2 + 2\varepsilon_{nl}} \right) s - 2\varepsilon_{nl} \right] \tag{26}$$

$$k_{\pm} = 2\beta^2 b - l(l + 1) \pm \varepsilon_{nl} \sqrt{(1 + 2l)^2 + 4\beta^2 b^2}. \tag{27}$$

In an attempt of making the first derivative of $\tau(s) = \bar{\tau}(s) + 2\pi(s)$ negative, we need to select the most suitable form of $\pi(s)$ as

$$\begin{aligned} \pi(s) &= -\frac{s}{2} - \frac{1}{2} \left[\left(\sqrt{(1 + 2l)^2 + 4\beta^2 b^2 + 2\varepsilon_{nl}} \right) s - 2\varepsilon_{nl} \right]; \\ k_- &= 2\beta^2 b - l(l + 1) - \varepsilon_{nl} \sqrt{(1 + 2l)^2 + 4\beta^2 b^2}. \end{aligned} \tag{28}$$

According to Eqs. (7) and (8), $\lambda = \lambda_n$ gives energy equation as

$$\begin{aligned} E_{nl} &= D_e + \frac{l(l + 1) \hbar^2 a^2 d_0}{2\mu} - \frac{\hbar^2 a^2}{2\mu} \left[\frac{(2+b)\mu D_e b}{\hbar^2 a^2} - \frac{n + \eta}{2} \right]^2; \\ \beta^2 &= \frac{2\mu D_e}{\hbar^2 a^2}, \quad \eta = \frac{1}{2} \left[1 + \sqrt{(1 + 2l)^2 + \frac{8\mu D_e b^2}{\hbar^2 a^2}} \right], \end{aligned} \tag{29}$$

where n and l are the principal and orbital quantum numbers, respectively.

Since the polynomial solutions of the hypergeometric function $y(s)$ depend on the determination of the weight function $\rho(s)$ which satisfies the differential equation in Eq. (12). Thus, $\rho(s)$ is obtained as:

$$\rho(s) = s^{2\varepsilon_{nl}} (1 - s)^{2\eta - 1}, \tag{30}$$

where we have used

$$2\eta - 1 = \sqrt{(1 + 2l)^2 + \frac{8\mu D_e b^2}{\hbar^2 a^2}} \tag{31}$$

Substituting Eq. (30) into the Rodrigue’s relation given in Eq. (11), we obtain

$$y_{nl}(s) = B_n s^{-2\varepsilon_{nl}} (1 - s)^{-(2\eta - 1)} \frac{d^n}{ds^n} \left[s^{n + 2\varepsilon_{nl}} (1 - s)^{n + 2\eta - 1} \right], \tag{32}$$

where

$$\varepsilon_{nl} = \frac{(2 + b) \beta^2 b}{2n + 1 + \sqrt{(1 + 2l)^2 + 4\beta^2 b^2}} - \frac{2n + 1 + \sqrt{(1 + 2l)^2 + 4\beta^2 b^2}}{4} \tag{33}$$

and B_n is the normalization constant.

Equation (33) may be expressed in terms of Jacobi polynomials as Gradshteyn and Ryzhik [48]:

$$y_{nl}(s) \equiv P_n^{(2\varepsilon_{nl}, 2\eta-1)}(s), \tag{34}$$

the Jacobi polynomial $P_n^{(\alpha, \beta)}$ is related to the hypergeometric functions by the relation

$$P_n^{(\alpha, \beta)}(s) = \frac{\Gamma(n + 1 + \alpha)}{n! \Gamma(1 + \alpha)} {}_2F_1 \left(-n, n + \alpha + \beta + 1; \alpha + 1; \frac{1}{2}(1 - s) \right), \tag{35}$$

solving for $\phi(s)$ by using $\pi(s)$ and $\sigma(s)$ in the expression given in Eq. (10), we have

$$\phi(s) = s^{\varepsilon_{nl}} (1 - s)^\eta. \tag{36}$$

Hence, using Eqs. (35) and (36) in relation in Eq. (3), we obtain the un-normalized radial wave functions as:

$$R_{nl}(s) = N_{nl} \frac{\Gamma(n + 2\varepsilon_{nl} + 1)}{n! \Gamma(1 + 2\varepsilon_{nl})} e^{-\varepsilon_{nl} ar} (1 - e^{-ar})^\eta {}_2F_1 \left(-n, n + 2(\varepsilon_{nl} + \eta); 2\varepsilon_{nl} + 1; \frac{1 - e^{-ar}}{2} \right) \tag{37}$$

where N_{nl} is the normalization constant which is obtained as:

$$N_{nl} = \frac{1}{\Gamma(2\varepsilon_{nl} + 1)} \left[\frac{a\varepsilon_{nl}(n + \varepsilon_{nl} + \eta) \Gamma(n + 2\varepsilon_{nl} + 1) \Gamma(n + 2\varepsilon_{nl} + 2\eta)}{2(n + \eta) n! \Gamma(n + 2\eta)} \right]^{1/2}. \tag{38}$$

4 Applications

In order to know the contribution of the improved Pekeris-type approximation scheme with the N–U method used and the accuracy of our results obtained in Sect. 3, we compare our results with the results of Dong and Gu (functional method) [3], numerical integration method obtained by using the MATHEMATICA program of Lucha and Schöberl [53] (as reported by Dong and Gu (functional method) [3]) and Zhang et al. (SUSY method) [7]. From Tables 1 and 2, our results (N–U method) and the results of Zhang et al. (SUSY method) [7] are better than the results obtained by numerical integration method (as reported by Dong and Gu [3]) for large values of l . In addition,

Table 1 Energy eigenvalues E_{nl} (eV) for the Deng–Fan potential as a function of the parameter l for some spectroscopic states for $r_c = 0.40$ and $D_c = 15$ ($\hbar = \mu = 1$)

State	l	N–U method	SUSY method [7]	Numerical method [3]	Functional method [3]
2p	0.05	7.860804493	7.86080	7.8628	7.8606
	0.10	7.953304454	7.95330	7.95537	7.95247
	0.15	8.045099870	8.04510	8.04724	8.04322
	0.20	8.136203772	8.13620	8.13842	8.13287
	0.25	8.226629167	8.22663	8.22892	8.22142
	0.30	8.316389030	8.31639	8.31874	8.30889
3p	0.05	10.99776305	10.9978	10.9998	10.9976
	0.10	11.16256046	11.1626	11.1647	11.1617
	0.15	11.32424872	11.3242	11.32647	11.3224
	0.20	11.48283762	11.4828	11.48513	11.4795
	0.25	11.63833667	11.6383	11.64068	11.6331
	0.30	11.79075502	11.7908	9.67565	11.7833
3d	0.05	10.21598027	10.21598	10.21651	10.2154
	0.10	10.35353947	10.35354	10.35409	10.351
	0.15	10.48935439	10.48935	10.48992	10.4837
	0.20	10.62346374	10.62346	10.62403	10.6135
	0.25	10.75590641	10.75591	10.75645	10.7403
	0.30	10.88672151	10.88672	10.88719	10.8642
4p	0.05	12.49760242	12.4976	12.4992	12.4974
	0.10	12.69679604	12.69680	12.69851	12.696
	0.15	12.88834813	12.88835	12.8901	12.8865
	0.20	13.07224462	13.07224	13.07400	13.0689
	0.25	13.24847044	13.24847	13.2501	13.2433
4d	0.05	12.09829027	12.09829	12.0989	12.0977
	0.10	12.28500942	12.28501	12.2857	12.2825
	0.15	12.46641937	12.46642	12.46715	12.4608
	0.20	12.64256756	12.64257	12.64324	12.6326
4f	0.05	11.82078623	11.82079	11.8209	11.8195
	0.10	11.99796121	11.99796	11.9981	11.993
	0.15	12.17169661	12.17170	12.1718	12.1604
	0.20	12.34207217	12.34207	12.3421	12.3221
5p	0.10	13.54214250	13.54214	13.5434	13.5413
	0.20	13.92898633	13.92899	13.9301	13.9257
5d	0.10	13.30679690	13.30680	13.3075	13.3043
	0.20	13.69266395	13.69266	13.6931	13.6827
5f	0.10	13.14759771	13.14760	13.1478	13.1426
	0.20	13.53344225	13.53344	13.5333	13.5134
5g	0.10	13.03797622	13.03798	13.0379	13.0296
	0.20	13.42711266	13.42711	13.42667	13.3938

Table 1 continued

State	l	N–U method	SUSY method [7]	Numerical method [3]	Functional method [3]
6p	0.10	14.05208861	14.05209	14.0530	14.0513
6d	0.10	13.90704846	13.90705	13.9075	13.9045
6f	0.10	13.81118995	13.81119	13.8113	13.8062
6g	0.10	13.74661283	13.74661	13.7466	13.7383

Table 2 Energy eigenvalues E_{nl} (eV) for the Deng–Fan potential as a function of the parameter l for some spectroscopic states for $r_e = 0.80$ and $D_e = 15$ ($\hbar = \mu = 1$)

State	l	N–U method	SUSY method [7]	Numerical method [3]	Functional method [3]
2p	0.05	4.140887263	4.140887	4.14208	4.14068
	0.10	4.219180128	4.219180	4.2204	4.21835
	0.15	4.297393199	4.297393	4.2987	4.29552
	0.20	4.375546508	4.375547	4.3769	4.37221
	0.25	4.453659654	4.453660	4.4551	4.44845
	0.30	4.531751791	4.531752	4.5332	4.52425
3p	0.05	7.532791561	7.532792	7.5350	7.53258
	0.10	7.724764274	7.724764	7.7271	7.72393
	0.15	7.915178655	7.915179	7.9177	7.9133
	0.20	8.104040627	8.104041	8.1066	8.10071
	0.25	8.291354169	8.291354	8.2841	8.28615
	0.30	8.477121312	8.477121	8.4799	8.46962
3d	0.05	5.739751228	5.739751	5.7404	5.73913
	0.10	5.845770281	5.845770	5.8465	5.84327
	0.15	5.950678133	5.950678	5.9515	5.94505
	0.20	6.054533598	6.054534	6.0553	6.04453
	0.25	6.157395321	6.157395	6.1582	6.14177
	0.30	6.259321745	6.259322	6.2601	6.23682
4p	0.05	9.613013087	9.613013	9.6156	9.6128
	0.10	9.883523698	9.883524	9.8862	9.88269
	0.15	10.14855572	10.14856	10.1514	10.1467
	0.20	10.40805775	10.40806	10.4111	10.4047
	0.25	10.66197388	10.66197	10.665	10.6568
	0.30	10.91589001	10.91589	10.919	10.9101
4d	0.05	8.493343486	8.493344	8.4948	8.49272
	0.10	8.707110984	8.707111	8.7087	8.70461
	0.15	8.917807599	8.917808	8.9194	8.91218
	0.20	9.125505093	9.125505	9.1272	9.11551
4f	0.05	7.434705812	7.434706	7.4351	7.43346
	0.10	7.586418806	7.586419	7.5868	7.58142

Table 2 continued

State	l	N–U method	SUSY method [7]	Numerical method [3]	Functional method [3]
	0.15	7.735732273	7.735732	7.7361	7.72448
	0.20	7.882757512	7.882758	7.8831	7.86276
5p	0.10	11.30207244	11.30207	11.3047	11.3012
	0.20	11.91322375	11.91322	11.9161	11.9099
5d	0.10	10.52008608	10.52009	10.5219	10.5176
	0.20	11.06937161	11.06937	11.0713	11.0594
5f	0.10	9.796658033	9.796658	9.7975	9.79166
	0.20	10.27303707	10.27304	10.2738	10.253
5g	0.10	9.152223355	9.152223	9.1524	9.14389
	0.20	9.552869479	9.552869	9.5528	9.51954
6p	0.10	12.27979921	12.27980	12.2822	12.279
6d	0.10	11.73643864	11.73644	11.7383	11.7339
6f	0.10	11.24481492	11.24481	11.2459	11.2398
6g	0.10	10.81533228	10.81533	10.8158	10.807

our results (N–U method) and the results of Zhang et al. (SUSY method) [7] are better than the results of Dong and Gu [3], since their results are obtained by using conventional approximation scheme to deal with the centrifugal term. Hence, the new improved approximation scheme to deal with the centrifugal term in Eq. (20) is better than the one proposed by Dong and Gu [3].

Furthermore, the approximate analytical solutions for some selected diatomic molecules are obtained. In this work, some diatomic molecules have been selected for the purposes which they serve in various aspect of chemical synthesis, nature of bonding, temperature stability and electronic transport properties in chemical physics [15, 32, 41, 49, 50]. Some of these selected diatomic molecules composed of the homogeneous diatomic molecules (H_2); the heterogeneous diatomic molecules (HCl, LiH); the neutral transition metal hydrides (ScH, TiH, VH, CrH); the transition-metal lithide (CuLi); the transition-metal carbides (TiC, NiC); the transition-metal nitrite (ScN) and the transition-metal fluoride (ScF).

The spectroscopic data in Table 3 are used to obtain approximate ro-vibrational energy states for some of these selected diatomic molecules for the Deng–Fan potential, the results are tabulated in Tables 4, 5, 6.

5 Conclusion

In the present study, we have obtained the approximate analytical solutions of the Schrödinger equation for the Deng–Fan molecular potential by using the Nikiforov–Uvarov (N–U) method. This is done by introducing a Pekeris-type approximation to deal with the centrifugal term of the Schrödinger equation for the Deng–Fan molecular potential. The approximate analytical energy eigenvalues and the corresponding

Table 3 Spectroscopic data for some selected diatomic molecules

Molecules	$D_e(eV)$	$r_e(\text{\AA})$	$a(\text{\AA}^{-1})$	μ (a.m.u)
HCl	4.619061175	1.2746	1.8677	0.9801045
LiH	2.515283695	1.5956	1.1280	0.8801221
H ₂	4.7446	0.7416	1.9426	0.50391
ScH	2.25	1.776	1.41113	0.986040
ScN	4.56	1.768	1.50680	10.682771
TiH	2.05	1.781	1.32408	0.987371
VH	2.33	1.719	1.44370	0.988005
CrH	2.13	1.694	1.52179	0.988976
NiC	2.76	1.621	2.25297	9.974265
CuLi	1.74	2.310	1.00818	6.259494
TiC	2.66	1.790	1.52550	9.606079
ScF	5.85	1.794	1.46102	13.358942

where $\hbar c = 1973.29 eV \text{\AA}$ [15, 19, 20, 32, 41, 49–52]

Table 4 The bound state energies E_{nl} (eV) for HCl, LiH and H₂ molecules for different values of the vibrational n and rotational l quantum numbers of the Deng–Fan potential

n	l	HCl	LiH	H ₂
0	0	0.201984174	0.103334650	0.349980221
0	1	0.204854248	0.105236729	0.364688765
1	0	0.590747827	0.302005955	0.996777053
1	1	0.593537612	0.303838653	1.010323238
2	0	0.960011044	0.490685861	1.580248366
2	1	0.962721591	0.492450759	1.592700793
2	2	0.968141645	0.495978997	1.617539648
3	0	1.310027865	0.669601019	2.104086156
3	1	1.312660203	0.671299648	2.115507769
3	2	1.317923855	0.674695388	2.138289195
3	3	1.325816775	0.679785205	2.172307398
4	0	1.641047243	0.838970564	2.571680443
4	1	1.643602379	0.840604402	2.582129083
4	2	1.648711644	0.843870601	2.602968445
4	3	1.656373023	0.848766203	2.634083222
4	4	1.666583499	0.855286782	2.675301759
5	0	1.953313156	0.999006401	2.986148433
5	1	1.955792078	1.00057688	2.995677323
5	2	1.960748932	1.003716397	3.014680784
5	3	1.968181734	1.008422072	3.043050669
5	4	1.978087513	1.014689589	3.080625975
5	5	1.990462308	1.022513206	3.127194276

Table 5 The bound state energies E_{nl} (eV) for ScH, TiH, VH and CrH molecules for different values of the vibrational n and rotational l quantum numbers of the Deng–Fan potential

n	l	ScH	TiH	VH	CrH
0	0	0.104850694	0.095195135	0.109283701	0.109051761
0	1	0.106349671	0.096647888	0.110873673	0.110713465
1	0	0.306246538	0.277949104	0.319115401	0.317715462
1	1	0.307704129	0.279358078	0.320660504	0.319328938
2	0	0.496950687	0.450924416	0.517711754	0.514210716
2	1	0.498367397	0.452290234	0.519212554	0.515776561
2	2	0.501200316	0.455021255	0.522213593	0.518907656
3	0	0.677093198	0.614259487	0.705213873	0.698688309
3	1	0.678469522	0.615582758	0.706670923	0.700207111
3	2	0.681221677	0.618228694	0.709584473	0.703244131
3	3	0.685348677	0.622196086	0.713953418	0.707798199
4	0	0.846801673	0.768089723	0.881760121	0.871296119
4	1	0.848138097	0.769371041	0.883173966	0.872768456
4	2	0.850810460	0.771933083	0.886001113	0.875712554
4	3	0.854817791	0.775774658	0.890240476	0.880127261
4	4	0.860158632	0.780893985	0.895890425	0.886010849
5	0	1.006201313	0.912547598	1.047486184	1.032179179
5	1	1.007498315	0.913787546	1.048857357	1.033605616
5	2	1.010091841	0.916266858	1.051599167	1.036457924
5	3	1.013980933	0.919984364	1.055710546	1.040734966
5	4	1.019164157	0.924938312	1.061189889	1.046435042
5	5	1.025639693	0.931126367	1.068035065	1.053555885

Table 6 The bound state energies E_{nl} (eV) for CuLi, TiC, NiC, ScN and ScF molecules for different values of the vibrational n and rotational l quantum numbers of the Deng–Fan potential

n	l	CuLi	TiC	NiC	ScN	ScF
0	0	0.026818307	0.039113293	0.055344362	0.048241243	0.047570217
1	0	0.026955324	0.039272617	0.055579192	0.048386343	0.047682126
1	1	0.079745219	0.116393424	0.164294062	0.143880175	0.142069247
2	0	0.079880854	0.116551564	0.164527691	0.144024459	0.142180660
2	1	0.131756662	0.192439939	0.270947523	0.238420357	0.235733223
2	2	0.131890919	0.192596892	0.271179952	0.238563831	0.235844142
3	0	0.132159429	0.192910789	0.271644807	0.238850775	0.236065981
3	1	0.182857099	0.267256594	0.375308427	0.331864375	0.328563726
3	2	0.182989988	0.267412364	0.375539658	0.332007039	0.328674152
3	3	0.183255759	0.267723901	0.376002118	0.332292365	0.328895002
4	0	0.183654398	0.268191197	0.376695804	0.332720351	0.329226276
4	1	0.233050973	0.340847133	0.477380444	0.424214801	0.420562331

Table 6 continued

n	<i>l</i>	CuLi	TiC	NiC	ScN	ScF
4	2	0.233182495	0.341001723	0.477610482	0.424356658	0.420672264
4	3	0.233445541	0.341310904	0.478070549	0.424640373	0.420892131
4	4	0.233840092	0.341774668	0.478760649	0.425065934	0.421221926
5	0	0.234366131	0.342393002	0.479680772	0.425633343	0.421661649
5	1	0.282342675	0.413215272	0.577167239	0.515474202	0.511730608
5	2	0.282472844	0.413368688	0.577396081	0.515615254	0.511840049
5	3	0.282733177	0.413675522	0.577853763	0.515897355	0.512058932
5	4	0.283123662	0.414135763	0.578540282	0.516320503	0.512387253
5	5	0.283644273	0.414749401	0.579455631	0.516884691	0.512825013

normalized wave functions for arbitrary *l* state are obtained. For comparison sake, the energy eigenvalues of this potential as a function of the parameter *l* for different spectroscopic states are obtained as shown in Tables 1 and 2.

Also, we have obtained ro-vibrational energy states for some selected diatomic molecules (HCl, LiH, H₂, ScH, TiH, VH, CrH, CuLi, TiC, NiC, ScN and ScF) for this molecular potential. For these selected diatomic molecules, the energy eigenvalues increases as *n* and *l* increases as it can be seen in Tables 4, 5, 6. As we have observed, the N–U method allows no constraint on the potential parameter, see Tables 1 and 2 values involved and it is easy to implement. The results obtained are sufficiently accurate. Therefore, we have applied the present solutions to obtain the ro-vibrational energies for some selected diatomic molecules for the Deng–Fan molecular potential for various arbitrary values of rotational and vibrational quantum numbers.

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References

1. O. Bayrak, G. Kocak, I. Boztosun, J. Phys. A Math. Gen **39**, 6955 (2006)
2. O. Bayrak, I. Boztosun, H. Ciftci, Int. J. Quant. Chem. **107**, 540 (2007)
3. S.H. Dong, X.Y. Gu, J. Phys. Conf. Ser. **96**, 012109 (2008)
4. S. Flügge, *Practical Quantum Mechanics* (Springer, Berlin, 1994)
5. T. Barakat, O.M. Al-Dossary, Int. J. Mod. Phys. A. **22**(1), 203 (references therein, 2007)
6. Z. Rong, H.G. Kjaergaard, M.L. Sage, Mol. Phys. **101**(14), 2285 (2003)
7. L.H. Zhang, X.P. Li, C.S. Jia, Int. J. Quant. Chem **111**, 1870 (2011)
8. Z.H. Deng, Y.P. Fan, Shandong Univ. J. **7**, 162 (1957)
9. Z. Rong, M.L. Sage, Interdiscip. Sci. Comput. Life Sci. **1**, 163 (2009)
10. A.D.S. Mesa, C. Quesne, Y.F. Smirnov, J. Phys. A. Math. Gen **31**, 321 (1998)
11. O.J. Oluwadare, K.J. Oyewumi, C.O. Akoshile, O.A. Babalola, Phys. Scr. **86**, 035002 (2012)
12. O.J. Oluwadare, K.J. Oyewumi, O.A. Babalola, Afr. Rev. Phys. **7**(0016), 165 (2012b)
13. S.M. Ikhdair, R. Sever, J. Mol. Struct. THEOCHEM **806**, 155 (2007)

14. K.J. Oyewumi, F.O. Akinpelu, A.D. Agboola, *Int. J. Theor. Phys* **47**, 1039 (2008)
15. K.J. Oyewumi, K.D. Sen, *J. Math. Chem.* **50**, 1039 (references therein, 2012)
16. A. Kratzer, *Z. Phys.* **3**, 289 (1920)
17. K.J. Oyewumi, *Found. Phys. Lett.* **18**(1), 75 (2005)
18. P.G. Hajiogeorgiou, *J. Mol. Spec.* **235**, 111 (2006)
19. C. Berkdemir, A. Berkdemir, J. Han, *Chem. Phys. Lett.* **417**, 326 (2006)
20. K.J. Oyewumi, *Int. J. Theor. Phys.* **49**, 1302 (2010)
21. C.S. Jia, J.Y. Liu, P.Q. Wang, X. Lin, *Int. J. Theor. Phys* **48**(9), 2633 (2009)
22. C.L. Pekeris, *Phys. Rev.* **45**, 98 (1934)
23. R.L. Greene, C. Aldrich, *Phys. Rev. A.* **143**(6), 2363 (1976)
24. M. Aktas, R. Sever, *J. Mol. Struct. THEOCHEM* **710**, 223 (2004)
25. C. Berkdemir, J. Han, *Chem. Phys. Lett.* **409**, 203 (2005)
26. S.M. Ikhdair, *J. Math. Phys.* **52**, 052303 (2011a)
27. S.M. Ikhdair, *Phys. Scr.* **83**, 015010 (2011b)
28. A. Durmus, *J. Phys. A. Math. Theor.* **44**, 155205 (references therein, 2011)
29. O. Mustafa, M. Odeh, *Eur. Phys J. B.* **15**, 143 (2000)
30. E. Castro, J.L. Paz, P. Martin, *J. Mol. Struct. THEOCHEM* **769**, 15 (2006)
31. I. Nasser, M.S. Abdelmonem, H. Bahlouli, A.D. Alhaidari, *J. Phys. B. A. Mol. Opt. Phys.* **40**, 4245 (2007)
32. S.M. Ikhdair, *Chem. Phys.* **361**, 9 (2009)
33. W.C. Qiang, S.H. Dong, *Phys. Lett. A.* **363**, 169 (2007)
34. D.A. Morales, *Chem. Phys. Lett.* **394**, 68 (2004)
35. L.H. Zhang, X.P. Li, C.S. Jia, *Phys. Lett. A.* **372**, 2201 (2008)
36. F.R. Silva, E.D. Filho, *Chem. Phys. Lett.* **498**, 198 (2010)
37. P.M. Morse, *Phys. Rev.* **34**, 57 (1929)
38. S.H. Dong, *Commun. Theor. Phys.* **55**, 969 (2011)
39. G.F. Wei, W.L. Chen, *Chin. Phys. B* **19**(9), 090308 (2010)
40. L.H. Zhang, X.P. Li, C.S. Jia, *Phys. Scr.* **80**, 035003 (2009)
41. C. Berkdemir, R. Sever, *J. Math. Chem.* **46**, 1122 (2009)
42. W.A. Yahya, K.J. Oyewumi, C.O. Akoshile, T.T. Ibrahim, *J. Vect. Rel.* **5**(3), 27 (2010)
43. A.F. Nikiforov, V.B. Uvarov, *Special Functions of Mathematical Physics.* (Birkhäuser, Basel, 1988)
44. M. Eshghi, *Adv. Stud. Theor. Phys* **5**(12), 559 (2011)
45. H. Hassanabadi, E. Maghsoodi, S. Zarrinkamar, H. Rahimov, *J. Math. Phys.* **53**, 022104 (references therein, 2012)
46. M. Eshghi, M. Hamzavi, *Commun. Theor. Phys.* **57**, 355 (2012)
47. M. Hamzavi, A.A. Rajabi, H. Hassanabadi, *Few Body Syst.* **52**(1–2), (2012)
48. S.I. Grashsteyn, I.M. Ryzhik, *Table of Integrals, Series, and Products*, 7th edn. (Elsevier Academic Press, USA, 2007)
49. J.F. Harrison, *Chem. Rev.* **100**(2), 679 (2000)
50. Y.P. Vashni, *Chem. Phys.* **353**(1–3), 32 (2008)
51. S.M. Ikhdair, *Mol. Phys.* **110**(13), 1415 (2012)
52. J. Beringer, et al. (Particle Data Group), *Phys. Rev. D* **86**, 010001 (2012)
53. W. Lucha, F.F. Schöberl, *Int. Mod. Phys. C* **10**, 607 (1999)