

Rotation and vibration of diatomic molecule in the spatially-dependent mass Schrödinger equation with generalized q -deformed Morse potential

Sameer M. Ikhdaire^{1,*}

¹*Physics Department, Near East University, Nicosia, Cyprus, Turkey*

(Dated: April 28, 2009)

Abstract

The analytic solutions of the spatially-dependent mass Schrödinger equation of diatomic molecules with the centrifugal term $l(l+1)/r^2$ for the generalized q -deformed Morse potential are obtained approximately by means of a parametric generalization of the Nikiforov-Uvarov (NU) method combined with the Pekeris approximation scheme. The energy eigenvalues and the corresponding normalized radial wave functions are calculated in closed form with a physically motivated choice of a reciprocal Morse-like mass function, $m(r) = m_0 / (1 - \delta e^{-a(r-r_e)})^2$, $0 \leq \delta < 1$, where a and r_e are the range of the potential and the equilibrium position of the nuclei. The constant mass case when $\delta \rightarrow 0$ is also studied. The energy states for H_2 , LiH , HCl and CO diatomic molecules are calculated and compared favourably well with those obtained by using other approximation methods for arbitrary vibrational n and rotational l quantum numbers.

Keywords: Deformation theory, generalized q -deformed Morse potential, spatially-dependent mass, Pekeris approximation, NU method

PACS numbers: 03.65.Ge, 03.65.Pm, 03.65.-w

*E-mail: sikhdaire@neu.edu.tr; sameer@neu.edu.tr

I. INTRODUCTION

It is well known that a reasonable potential to describe the molecular vibrational spectra of diatomic and even polyatomic molecules successfully is the Morse potential [1-3]. There has been considerable current interest in the use and application of the Morse oscillator model to the investigation of local vibrational modes, with a particular emphasis on those highly excited vibrational levels which are accessible by laser spectroscopy [2]. An effective potential, which is the sum of the centrifugal potential term that depends on the angular momentum l and the Morse potential, has been used as a model for such interactions. It is referred to as the rotational potential. The radial non-relativistic and relativistic wave equations with this potential are exactly solvable for $l = 0$ case [1]. However, for $l \neq 0$ analytic exact solution cannot be determined, only numerical solutions are possible where several approximation techniques have been proposed and extensively used with varying degrees of accuracy and stability [4-17]. The most widely known approximation was devised by Pekeris [5] and used to obtain the semiclassical solutions [6-17]. This approximation [10,13] is based on the expansion of the centrifugal part in exponential terms with exponents that depend on an inter-nuclear distance parameter. This is why the Pekeris approximation is valid only for very small spatial variations from the inter-nuclear separation (i.e., for lower vibrational and rotational energy). Other methods that have also been used include the variational (V) method with the Pekeris approximation [6], supersymmetry (SUSY) using the Pekeris approximation [7], the hypervirial (HV) perturbation method with the effective potential and without the Pekeris approximation [8], the shifted $1/N$ expansion (SE) [9] and the modified shifted large $1/N$ approach (MSE) [9] which is very cumbersome to solve because there are several complex coefficients. There are needs of analytic solutions for these levels in order to be used for static and other applications sometimes using derivatives of this energy level functions. Other methods, which are semi-analytic, have also been used. These include, the Nikiforov-Uvarov (NU) [10] and the asymptotic iteration method (AIM) [12], using the Pekeris approximation, where the energy eigenvalues are obtained by simple transformation of the wave equation and the wave function is calculated iteratively. The exact quantization rule (EQR) [13,14] and the tridiagonal J-matrix representation (TJM) [15] which split original Hamiltonian into two parts as $H = H_0 + V$ where H_0 is the part of the Hamiltonian that could be treated analytically while the remaining part, V , has

to be treated numerically. Recent techniques of approximation denoted as two-point quasi-rational approximation technique (TQA) [16], which is considered as an extension of the Padé procedure, have been used in energy hydrogenic's levels determination of Zeeman effects and Coulomb potential with harmonics and quadratic terms, was used for the hydrogen molecule, the results of Duff and Rabitz (DR) [17] and the Fourier grid Hamiltonian method (FGH) [18], etc.

On the other hand, the studies of the non-relativistic and relativistic wave equations with position-dependent mass (PDM) for central physical potentials have attracted much attentions [18-29]. Such solutions are very useful in different fields of material science and condensed matter physics, such as semiconductors [30], quantum well and quantum dots [31], ^3He clusters [32], quantum liquids [33], graded alloys and semiconductor heterostructures [34], etc.

The NU method [35] and other methods have also been used to solve the Schrödinger equation [27,28], relativistic D -dimensional Klein-Gordon equation [29,36] and Dirac equation [37] with PDM case.

In the last few years, a considerable interest in the use and application of the mass dependence on the inter-nuclear distance in solving the non-relativistic and relativistic wave equations with various central potentials including the Morse potential have been revived. It provides us a reasonable first approximation for vibrational dynamics of diatomic molecules including the effects of anharmonicity and bond dissociation, it's incorrect behavior at large interatomic separations results in a relatively poor description of highly-excited vibrational levels, which are of much concern particularly for laser spectroscopy [2]. In other context, local model descriptions of molecular vibrations are required to understand the behavior of molecules for high overtone and combination levels [2,38]. The development of new experimental methods has unveiled a whole new range of molecular phenomena, including localization, intra-molecular energy redistribution and isomerization [39,40]. Even highly symmetrical molecules can develop localization at higher energy [2], a feature difficult to understand from the point of view of the traditional normal mode models of constant mass. In their pioneering work, Child *et al* have emphasized the need for introducing anharmonicity at the local level as a more natural starting point [2].

Since the realistic diatomic potentials are more accurately modelled by the perturbed or q -deformed Morse potentials, we believe that the present approach will produce much

more accurate information about the structure, dynamics and even the issue of energy resonances while dealing with the diatomic molecules. This is going to be the subject of investigation in the current study. In order to make the treatment very simple, we set out to employ the parametric generalization of the NU method combined with the Pekeris approximation scheme to solve the PDM radial Schrödinger equation for a generalized q -deformed Morse potential with arbitrary rotational angular quantum number. We propose and use a reciprocal Morse-like effective mass distribution function physically derived from the exact pseudo-spin symmetric solution of the Dirac equation [37]. Furthermore, the motivation for the choice is the nature of the field which is supposed to prevail between the interacting nuclei. This suitable choice may result in a solvable PDM Schrödinger equation for its energy eigenvalues and their corresponding wave functions. Besides, it allows one to get a compact analytical expression and transforms the corresponding Morse Hamiltonian into the constant-mass problem.

The present paper is organized as follows. In sect. 2, we briefly outline the basics of the NU method and supplement the parametric generalization of the method to exponential-type potentials in Appendix A. In sect. 3, we calculate the approximate analytic NU bound state energy eigenvalues and normalized wave functions of the PDM Schrödinger equation with the generalized q -deformed Morse potential for any l -state. The Pekeris analytic expansions are cited in Appendix B. In sect. 4, we calculate the numerical energy states for the various vibrational n , rotational l quantum numbers and q deformation parameter for four different diatomic molecules CO , LiH , H_2 and HCl in the constant mass limit ($\delta \rightarrow 0$). Finally, sect. 5 contains the relevant conclusions.

II. NU METHOD

The NU method has been used to solve the Schrödinger [28], Klein-Gordon [29] and Dirac [37] wave equations for central and non-central potentials. Let us briefly outline the basic concepts of the method [35]. This method was proposed to solve the second-order linear differential equation of the hypergeometric-type:

$$\sigma^2(z)u''(z) + \sigma(z)\tilde{\tau}(z)u'(z) + \tilde{\sigma}(z)u(z) = 0, \quad (1)$$

where the prime denotes the differentiation with respect to z , $\sigma(z)$ and $\tilde{\sigma}(z)$ are analytic polynomials, at most second-degree, and $\tilde{\tau}(z)$ is a first-degree polynomial. Let us discuss the exact particular solution of Eq. (1) by choosing

$$u(z) = y_n(z)\phi_n(z), \quad (2)$$

resulting in a hypergeometric type equation of the form:

$$\sigma(z)y_n''(z) + \tau(z)y_n'(z) + \lambda y_n(z) = 0. \quad (3)$$

The first part $y_n(z)$ is the hypergeometric-type function whose polynomial solutions are given by the Rodrigues relation

$$y_n(z) = \frac{A_n}{\rho(z)} \frac{d^n}{dz^n} [\sigma^n(z)\rho(z)], \quad (4)$$

where A_n is a normalization factor and $\rho(z)$ is the weight function satisfying the condition

$$[\sigma(z)\rho(z)]' = \tau(z)\rho(z), \quad (5)$$

with

$$\tau(z) = \tilde{\tau}(z) + 2\pi(z), \tau'(z) < 0. \quad (6)$$

Since $\rho(z) > 0$ and $\sigma(z) > 0$, the derivative of $\tau(z)$ has to be negative [35] which is the main essential condition for any choice of particular bound-state solutions. The other part of the wave function is defined as a logarithmic derivative:

$$\frac{\phi'(z)}{\phi(z)} = \frac{\pi(z)}{\sigma(z)}, \quad (7)$$

where

$$\pi(z) = \frac{1}{2} [\sigma'(z) - \tilde{\tau}(z)] \pm \sqrt{\frac{1}{4} [\sigma'(z) - \tilde{\tau}(z)]^2 - \tilde{\sigma}(z) + k\sigma(z)}, \quad (8)$$

with

$$k = \lambda - \pi'(z). \quad (9)$$

The determination of k is the key point in the calculation of $\pi(z)$, for which the discriminant of the square root in the last equation is set to zero. This results in the polynomial $\pi(z)$ which is dependent on the transformation function $z(r)$. Also, the parameter λ defined in Eq. (9) takes the form

$$\lambda = \lambda_n = -n\tau'(z) - \frac{1}{2}n(n-1)\sigma''(z), \quad n = 0, 1, 2, \dots \quad (10)$$

At the end, the energy equation and consequently it's eigenvalues can be obtained by comparing Eqs. (9) and (10).

Let us now construct a parametric generalization of the NU method valid for any central and non-central exponential-type potential. Comparing the following generalized hypergeometric equation

$$[z(1 - c_3z)]^2 u''(z) + [z(1 - c_3z)(c_1 - c_2z)] u'(z) + (-Az^2 + Bz - C) u(z) = 0, \quad (11)$$

with Eq. (1), we obtain

$$\tilde{\tau}(z) = c_1 - c_2z, \quad \sigma(z) = z(1 - c_3z), \quad \tilde{\sigma}(z) = -Az^2 + Bz - C, \quad (12)$$

where the parameters c_1, c_2, c_3, A, B and C are constants to be determined during the solution later. Thus, by following the method, we may obtain all the analytic polynomials and their relevant constants necessary for the solution of a radial wave equation. These analytic expressions are cited in Appendix A.

III. NU SOLUTIONS FOR THE GENERALIZED q -DEFORMED MORSE POTENTIAL

Choosing the separated atoms limit as the zero of energy, the generalized q -deformed Morse potential has the following form [1,41,42]:

$$V_M(r) = D_e [q - \exp(-\alpha x)]^2 = V_1 \exp(-2\alpha x) - V_2 \exp(-\alpha x) + V_3, \quad (13)$$

where $\alpha = ar_e$, $x = (r - r_e)/r_e$, $V_1 = D_e$, $V_2 = 2qD_e$ and $V_3 = q^2D_e$ where subscripts 1 and 2 refer to the repulsive and attractive terms, respectively. The range of the deformation parameter q in the above potential was taken as $q > 0$ by Ref. [43] and has been extended to $-1 \leq q < 0$ or $q > 0$ or even complex by Ref. [44]. The above potential contains three adjustable positive parameters; the parameter D_e corresponds to the depth of the potential well, a is related with the range of the potential and r_e is the equilibrium position of the nuclei. At $r = r_e$, it has a minimum value at $V_M(r_e) = D_e(q - 1)^2$ and approaches qD_e exponentially for large r . If $1/\alpha$ is somewhat smaller than the equilibrium distance r_e , it becomes large (but not infinite) as $r \rightarrow 0$. Here, we refer to the above potential as that applicable to the diatomic molecules. For the case of multiatomic molecules, the

generalization of Morse potentials can be expressed by the Empirical Valence Bond (EVB) approach [45].

We now study the Schrödinger equation with the PDM for the potential form (13), which can be expressed as [20,26,37]

$$\vec{\nabla} \left(\frac{1}{m} \vec{\nabla} \psi(r) \right) + 2 [E_{nl} - V(r)] \psi(\mathbf{r}) = 0, \quad (14)$$

where $m = m(r)$ and E_{nl} are the real mass function and the energy eigenvalues, respectively. For spherical symmetry, the wave function could be separated to the following form [46-49]

$$\psi(\mathbf{r}) = \frac{1}{r} R_l(r) Y_{lm}(\theta, \phi). \quad (15)$$

which gives the following radial wave equation:

$$\left\{ \frac{d^2}{dr^2} + \frac{m'}{m} \left(\frac{1}{r} - \frac{d}{dr} \right) - \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2} [E_{nl} - V(r)] \right\} R_l(r) = 0, \quad (16)$$

where $m' = dm(r)/dr$ and $R_l(r)$ are the radial wave functions. It is worth noting that for $m' = 0$ case, the above equation reduces to the well-known equation with constant mass used in Refs. [49-51]. Furthermore, the above equation with the use of transformation

$$R_l(r) = \sqrt{m} u_l(r), \quad (17)$$

reduces to the Schrödinger-like equation:

$$-\frac{d^2 u_l(r)}{dr^2} + V_{eff}(r) u_l(r) = \frac{2m E_{nl}}{\hbar^2} u_l(r), \quad u_l(0) = 0, \quad (18)$$

$$V_{eff}(r) = -\frac{m''}{2m} + \frac{3}{4} \left(\frac{m'}{m} \right)^2 - \frac{m'}{m} \frac{1}{r} + \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2} V(r),$$

where the interaction potential in the above equation is taken to be the generalized q -deformed Morse potential (13). In addition, for the bound state solutions, i.e., real energy eigenvalues, the wave functions $u_l(r)$ need to be finite near $r = 0$ and $r \rightarrow \infty$.

In order to find an approximation [4] for the centrifugal potential term $l(l+1)/r^2$ and for $1/r$, we apply the Pekeris approximation [5,10]. We further make the appropriate parameter change $r = r_e(1+x)$ and perform the expansion around $x = 0$ ($r = r_e$) to second-order in x (r/r_e) at low-excitation energy (i.e., $r \approx r_e$). Following the approach in Ref. [10], we make the convenient expansions and obtain expansion parameters a_i and b_i ($i = 0, 1, 2$) as demonstrated in Appendix B. Thus, with the Pekeris approximations, the semi-analytic

solution of the Schrödinger equation for the generalized q -deformed Morse potential ($l \neq 0$) has become amenable. For the present potential model, the exponential choice for the PDM allows one to transform the corresponding Morse Hamiltonian into the constant mass problem. Since the field between the two interacting nuclei is a short-range field of which the Morse potential is an example, we are tempted to set the PDM function as a reciprocal Morse-like ansatz having the form [52,53]

$$m = \frac{m_0}{(1 - \delta z)^2}, \quad m' = -\frac{2m_0\delta\alpha z}{(1 - \delta z)^3}, \quad m'' = \frac{2m_0\delta\alpha^2 z}{(1 - \delta z)^3} + \frac{6m_0\delta^2\alpha^2 z^2}{(1 - \delta z)^4}, \quad (19)$$

where $z = \exp(-\alpha x) \in (0, 1)$, and $0 \leq \delta < 1$. The above mass function works well in the present model and it results in a solvable wave equation. However, in this choice, there is no loss of generality when the value of the parameter δ is taken to be small (i.e., $\delta \rightarrow 0$). Then, Eq. (18) with the help of Eq. (19), and the expansions made in Appendix B reduces to,

$$u_l''(z) + \frac{1}{z}u_l'(z) + \frac{1}{z^2(1 - \delta z)^2} \left\{ \frac{2m_0}{\hbar^2 a^2} (E_{nl} - V_3) - \frac{\gamma a_0}{a^2} + \left(\frac{2m_0}{\hbar^2 a^2} V_2 - \frac{\gamma a_1}{a^2} + S\delta \right) z - \left(\frac{2m_0}{\hbar^2 a^2} V_1 + \frac{\gamma a_2}{a^2} + P\delta + Q\delta^2 \right) z^2 \right\} u_l(z) = 0, \quad (20)$$

with

$$S = r_e^2 - \frac{2b_0}{a} + \frac{2\gamma a_0}{a^2}, \quad P = \frac{2b_1}{a} - \frac{2\gamma a_1}{a^2}, \quad Q = r_e^2 - \frac{2b_0}{a} + \frac{\gamma a_0}{a^2}, \quad (21)$$

where a_i and b_i ($i = 0, 1, 2$) are given in Appendix B and $u_l(z) = u_l(r)$. Defining the following parameters

$$\varepsilon_{nl} = \frac{1}{a} \sqrt{\gamma a_0 + \frac{2m_0}{\hbar^2} (V_3 - E_{nl})}, \quad \beta_1 = \frac{1}{a^2} \left(\frac{2m_0}{\hbar^2} V_1 + \gamma a_2 \right) + P\delta + Q\delta^2, \\ \beta_2 = \frac{1}{a^2} \left(\frac{2m_0}{\hbar^2} V_2 - \gamma a_1 \right) + S\delta, \quad (22)$$

reduces Eq. (20) into the form:

$$\frac{d^2 u_l(z)}{dz^2} + \frac{1}{z} \frac{du_l(z)}{dz} + \frac{1}{[z(1 - \delta z)]^2} (-\beta_1 z^2 + \beta_2 z - \varepsilon_{nl}^2) u_l(z) = 0. \quad (23)$$

In comparing Eq. (23) with Eq. (1), we follow Appendix A to obtain the specific values of the parametric constants and hence present them in Table 1 for the currently used potential model. Also, with the aid of Table 1, the key polynomials given in Appendix A now take the following particular analytic forms:

$$\pi(z) = \varepsilon_{nl} - \frac{\delta}{2} (1 + 2\varepsilon_{nl} + \xi) z, \quad (24)$$

$$k = \beta_2 - \delta (2\varepsilon_{nl} + \xi) \varepsilon_{nl}, \quad (25)$$

$$\tau(z) = 1 + 2\varepsilon_{nl} - \delta (2 + 2\varepsilon_{nl} + \xi) z, \quad (26)$$

with $\tau'(z) = -\delta (2 + 2\varepsilon_{nl} + \xi) < 0$, where $\xi = \sqrt{1 + 4\varepsilon_{nl}^2 + \frac{4}{\delta} \left(\frac{\beta_1}{\delta} - \beta_2 \right)}$. We insert the values of the constants given in Table 1 into the energy equation cited in Appendix A to obtain

$$\varepsilon_{nl} = \frac{1}{2} \frac{n(n+1)\delta - 2 \left(n + \frac{1}{2} \right) \sqrt{\beta_1} + \beta_2}{\sqrt{\beta_1} - \left(n + \frac{1}{2} \right) \delta}. \quad (27)$$

The above equation can be written more explicitly for the rotational bound-state energy eigenvalues as

$$E_{nl} = V_3 + \frac{\hbar^2 l(l+1)a_0}{2m_0 r_e^2} - \frac{\hbar^2 a^2}{8m_0} \left[\frac{n(n+1)\delta - 2 \left(n + \frac{1}{2} \right) \sqrt{\beta_1} + \beta_2}{\sqrt{\beta_1} - \left(n + \frac{1}{2} \right) \delta} \right]^2, \quad n, l = 0, 1, 2, \dots, \quad (28)$$

and after substituting the particular values of the parameters β_1 and β_2 from Eq. (22), we finally obtain the energy eigenvalues expressed in terms of the strength parameters V_i ($i = 1, 2, 3$) as

$$E_{nl} = V_3 + \frac{\hbar^2 l(l+1)a_0}{2m_0 r_e^2} - \frac{\hbar^2 a^2}{8m_0} \times \left[\frac{n(n+1)\delta - 2 \left(n + \frac{1}{2} \right) \sqrt{\frac{1}{a^2} \left(\frac{2m_0}{\hbar^2} V_1 + \frac{l(l+1)a_2}{r_e^2} \right) + P\delta + Q\delta^2 + \frac{1}{a^2} \left(\frac{2m_0}{\hbar^2} V_2 - \frac{l(l+1)a_1}{r_e^2} \right) + S\delta}}{\sqrt{\frac{1}{a^2} \left(\frac{2m_0}{\hbar^2} V_1 + \frac{l(l+1)a_2}{r_e^2} \right) + P\delta + Q\delta^2} - \left(n + \frac{1}{2} \right) \delta} \right]^2, \quad (29)$$

where S , P and Q are constant parameters given in Eq. (21). In particular, for the constant mass case, i.e., in the limit $\delta \rightarrow 0$ ($m \rightarrow m_0$), we can easily reduce the above equation to,

$$\varepsilon_{nl} = \frac{\beta_2}{2\sqrt{\beta_1}} - \left(n + \frac{1}{2} \right), \quad (30)$$

or more explicitly as

$$E_{nl} = V_3 + \frac{\hbar^2}{2\mu r_e^2} l(l+1) \left(1 - \frac{3}{ar_e} + \frac{3}{a^2 r_e^2} \right) - \frac{\hbar^2 a^2}{2\mu} \left[\sqrt{\frac{2\mu}{\hbar^2 a^2} \frac{\frac{V_2}{2} - \frac{\hbar^2}{2\mu r_e^2} l(l+1) \left(\frac{2}{ar_e} - \frac{3}{a^2 r_e^2} \right)}{\sqrt{V_1 - \frac{\hbar^2}{2\mu r_e^2} l(l+1) \left(\frac{1}{ar_e} - \frac{3}{a^2 r_e^2} \right)}} - \left(n + \frac{1}{2} \right)} \right]^2, \quad (31)$$

with $\mu = m_1 m_2 / (m_1 + m_2)$ denotes the reduced mass for the diatomic molecule. The above equation represents the energy eigenvalues for the generalized q -deformed Morse potential [42]. The vibrational bound state energy levels for s -waves ($l = 0$) are

$$E_n = V_3 - \frac{1}{4\kappa^2} [1 + 2n - \eta\kappa]^2, \quad (32)$$

with

$$\eta = \frac{V_2}{\sqrt{V_1}}, \quad \kappa = \frac{r_e}{\alpha\hbar} \sqrt{2\mu}, \quad n_{\max} \leq \frac{1}{2} \left(\frac{\sqrt{2\mu}}{\hbar a} \frac{V_2}{\sqrt{V_1}} - 1 \right), \quad (33)$$

where V_i ($i = 1, 2, 3$) are defined after Eq. (13). Therefore, the vibrational quantum number $n = 0, 1, 2, \dots, n_{\max}$, where n_{\max} is the number of bound states for the whole bound spectrum near the continuous zone. Thus, n_{\max} cannot be infinite, which is reflected in the above condition. Therefore, the Morse eigenfunctions for real systems do not form an infinite-dimensional Lie algebra.

Let us now turn to the calculations of the corresponding wave functions in the varying mass case. Referring to Appendix A and Table 1, we find the explicit form of the weight function as

$$\rho(z) = z^{2\varepsilon_{nl}} (1 - \delta z)^\xi, \quad (34)$$

where ε_{nl} is given in Eq. (27). The above weight function gives the first part of the wave functions:

$$y_n(z) \rightarrow P_n^{(2\varepsilon_{nl}, \xi)} (1 - 2\delta z), \quad (35)$$

and hence the second part of the wave functions can be found as

$$\phi(z) \rightarrow z^{\varepsilon_{nl}} (1 - \delta z)^{\frac{1}{2} + \frac{1}{2}\xi}. \quad (36)$$

Hence, the unnormalized wave functions are being expressed in terms of the Jacobi polynomials as

$$u_l(z) = \mathcal{N}_n z^{\varepsilon_{nl}} (1 - \delta z)^{\frac{1}{2}(1+\xi)} P_n^{(2\varepsilon_{nl}, \xi)} (1 - 2\delta z), \quad 0 < \delta < 1, \quad (37)$$

where the normalization constant is being calculated using the formulas placed in Appendix A as

$$\begin{aligned} \mathcal{N}_n = & \left[\frac{\Gamma(2\varepsilon_{nl} + 1) \Gamma(\xi + 2)}{\alpha \delta^{\varepsilon_{nl}} \Gamma(n)} \sum_{p=0}^{\infty} \frac{(-1)^p \Gamma(n+p) (n+1+2\varepsilon_{nl}+\xi)_p}{p! (p+2\varepsilon_{nl}) \Gamma(p+2\varepsilon_{nl}+\xi+2)} \right. \\ & \left. \times {}_3F_2(p+2\varepsilon_{nl}, -n, n+2\varepsilon_{nl}+\xi+1; p+2\varepsilon_{nl}+\xi+2; 1+2\varepsilon_{nl}; 1) \right]^{-1/2}, \end{aligned} \quad (38)$$

with ε_{nl} and ξ defined in Eq. (27) and after Eq. (26), respectively. $(x)_p$ is the Pochhammer symbols defined as

$$(x)_p = \frac{\Gamma(x+p)}{\Gamma(x)}. \quad (39)$$

Thus, the total radial part of the wave functions of the generalized q -deformed potential is

$$\begin{aligned} \psi_l(r) = \mathcal{N}_n \frac{1}{r} [\exp[-a(r-r_e)]]^{\varepsilon_{nl}} (1 - \delta \exp[-a(r-r_e)])^{-\frac{1}{2} + \frac{1}{2}\xi} \\ \times P_n^{(2\varepsilon_{nl}, \xi)}(1 - 2\delta \exp[-a(r-r_e)]), \quad 0 < \delta < 1, \end{aligned} \quad (40)$$

where \mathcal{N}_n is defined in Eq. (38).

The constant mass case should be treated separately. To avoid repetition, we can use our previous calculations to find an explicit form for the weight function as [50,51]

$$\rho(z) = z^{2\varepsilon_{nl}} \exp\left[-2\sqrt{\beta_1}z\right], \quad (41)$$

which gives the Laguerre polynomials:

$$y_n(z) \rightarrow z^{-2\varepsilon_{nl}} \exp\left[2\sqrt{\beta_1}z\right] \frac{d^n}{dz^n} (z^{n+2\varepsilon_{nl}} \exp\left[-2\sqrt{\beta_1}z\right]) \rightarrow L_n^{2\varepsilon_{nl}}(y), \quad (42)$$

where $y = 2\sqrt{\beta_1}z$. The second part of the wave functions can be found as

$$\phi(z) \rightarrow z^{\varepsilon_{nl}} \exp\left[-\sqrt{\beta_1}z\right], \quad (43)$$

Hence, the un-normalized wave functions expressed in terms of the Laguerre polynomials read

$$R_l(r) = N_n \left(2\sqrt{\beta_1}\right)^{-\varepsilon_{nl}} y^{\varepsilon_{nl}} \exp\left(-\frac{y}{2}\right) L_n^{2\varepsilon_{nl}}(y), \quad (44)$$

where ε_{nl} is given in Eq. (27) and $y = 2\sqrt{\beta_1} \exp[-a(r-r_e)]$ [10].

To demonstrate the importance of adjusting the three potential strength parameters V_i ($i = 1, 2, 3$) and α for real and/or complex values in any possible numerical calculation, we now discuss four special cases of the Morse potential given in (13) which are of much concern to the readers [41,54,55].

A. Generalized Vibrational Morse potential

We consider the generalized vibrational Morse potential defined by [41,54,55]

$$V_M(x) = V_1 e^{-2\alpha x} - V_2 e^{-\alpha x} + V_3, \quad V_1 = D, \quad V_2 = 2qD, \quad V_3 = 0, \quad (45)$$

and find the vibrational bound state energy spectrum as

$$E_n = -\alpha^2 E_0 \left[\lambda q - n - \frac{1}{2} \right]^2, \quad n = 0, 1, 2, \dots, n_{\max} \quad (46)$$

$$\lambda^2 = \frac{D}{\alpha^2 E_0}, \quad n_{\max} \leq \frac{1}{2} (2\lambda q - 1), \quad (47)$$

where the derived quantity $E_0 = \frac{\hbar^2}{2\mu r_e^2}$ (eV) with the following condition on the deformation parameter $q = \frac{1}{2\lambda}$ for the final vibrational bound-state. The above result is identical to Eq. (30) of Ref. [55]. Also, the wave functions are calculated as

$$R_n(x) = A_n \exp \left\{ -\alpha \left(\lambda q - n - \frac{1}{2} \right) x - \lambda e^{-\alpha x} \right\} L_n^{2(\lambda q - n - \frac{1}{2})} (2\lambda e^{-\alpha x}). \quad (48)$$

where A_n is a normalizing factor.

B. Non-PT Symmetric and Non-Hermitian Morse Case

Following Refs. [54,55], let us assume the potential strength parameters $V_1 = (A_1 + iB_1)^2$, $V_2 = (2C_1 + 1)(A_1 + iB_1)$, $V_3 = 0$ and $\alpha = 1$ where A_1 , B_1 and C_1 are real constants and $i = \sqrt{-1}$. Under appropriate changes of parameters, the potential (13) turns to become a complex Morse-like potential:

$$V(x) = -D \left[e^{-2x} + i\hat{D}e^{-x} \right]. \quad (49)$$

Hence, we can get the vibrational real bound state energy spectrum given by

$$E_n = -E_0 \left[\frac{1}{2} \hat{D} \kappa_1 - n - \frac{1}{2} \right]^2, \quad n = 0, 1, 2, \dots, n_{\max}, \quad (50)$$

with

$$\kappa_1 = \frac{r_e}{\hbar} \sqrt{2\mu D}, \quad n_{\max} \leq \frac{1}{2} \left(\frac{r_e}{\hbar} \hat{D} \sqrt{2\mu D} - 1 \right), \quad (51)$$

which is similar to Eq. (41) of Ref. [55] and the wave functions as

$$R_n(x) = B_n (2\kappa_1)^{-\left(\frac{1}{2}\hat{D}\kappa_1 - \frac{1}{2} - n\right)} (2\kappa_1 e^{-x})^{\left(\frac{1}{2}\hat{D}\kappa_1 - \frac{1}{2} - n\right)} e^{-\kappa_1 \exp(-x)} L_n^{2\left(\frac{1}{2}\hat{D}\kappa_1 - \frac{1}{2} - n\right)} (2\kappa_1 e^{-x}), \quad (52)$$

where B_n is a normalizing factor.

C. The First Type of PT-Symmetric and Non-Hermitian Morse case

We consider the same strength parameters as in the previous case but $\alpha = i$, the potential (43) becomes

$$V(x) = -D \left[e^{-2ix} + i\hat{D}e^{-ix} \right]. \quad (53)$$

Following the same procedure as before, we get no real spectrum for this kind of potentials:

$$E_n = E_0 \left[\frac{1}{2} \hat{D} \kappa_2 - n - \frac{1}{2} \right]^2, \quad n = 0, 1, 2, \dots, n_{\max}, \quad (54)$$

with

$$\kappa_2 = \frac{r_e}{i\hbar} \sqrt{2\mu D}, \quad n_{\max} \leq \frac{1}{2} \left(\frac{r_e}{i\hbar} \hat{D} \sqrt{2\mu D} - 1 \right). \quad (55)$$

Also, this gives the wave functions as

$$R_n(x) = C_n (2\kappa_2)^{-\left(\frac{1}{2}\hat{D}\kappa_2 - \frac{1}{2} - n\right)} (2\kappa_2 e^{-ix})^{\left(\frac{1}{2}\hat{D}\kappa_2 - \frac{1}{2} - n\right)} e^{-\kappa_2 \exp(-ix)} L_n^{2\left(\frac{1}{2}\hat{D}\kappa_2 - \frac{1}{2} - n\right)} (2\kappa_2 e^{-ix}), \quad (56)$$

where C_n is a normalizing factor.

D. The Second Type of PT-Symmetric and Non-Hermitian Morse case

We consider the strength parameters $V_1 = \omega^2$, $V_2 = D$, $V_3 = 0$ and $\alpha \rightarrow i\alpha$ where ω and D are real constants. The potential takes the form:

$$V(x) = -\omega^2 e^{-2i\alpha x} + D e^{-i\alpha x}, \quad (57)$$

we get real spectrum for this kind of potentials:

$$E_n = E_0 \left[\frac{1}{2} \frac{\sqrt{D}}{\omega} \kappa_3 - n - \frac{1}{2} \right]^2, \quad n = 0, 1, 2, \dots, n_{\max}, \quad (58)$$

with

$$\kappa_3 = \frac{r_e}{\hbar} \sqrt{2\mu D}, \quad n_{\max} \leq \frac{1}{2} \left(\frac{r_e}{\hbar} \frac{\sqrt{D}}{\omega} \sqrt{2\mu D} - 1 \right). \quad (59)$$

Also, this gives the wave functions as

$$R_n(x) = D_n (2\kappa_3)^{-\left(\frac{1}{2} \frac{\sqrt{D}}{\omega} \kappa_3 - \frac{1}{2} - n\right)} (2\kappa_3 e^{-i\alpha x})^{\left(\frac{1}{2} \frac{\sqrt{D}}{\omega} \kappa_3 - \frac{1}{2} - n\right)} e^{-\kappa_3 \exp(-i\alpha x)} \\ \times L_n^{2\left(\frac{1}{2} \frac{\sqrt{D}}{\omega} \kappa_3 - \frac{1}{2} - n\right)} (2\kappa_3 e^{-i\alpha x}), \quad (60)$$

where D_n is a normalizing factor.

IV. RESULTS

Firstly, in the constant mass limit, the numerically generated vibrational bound state energies of the original Morse potential ($q = 1$, $V_3 = 0$ case) for H_2 , LiH , HCl and CO molecules are found to be identical to those given in Table 2 of Ref. [15] (available from the author upon request). These numerical computations were performed using the model parameters [6,10,13,14,16] shown in Table 2 with the order of the eigenvalues represented by n (the vibrational quantum number). It is found that NU method, in the present study, can generate results similar to the tridiagonal J-matrix representation [15] which is relatively cumbersome in solving a matrix of dimension $N = 100$ for H_2 , LiH and HCl molecules to even $N = 200$ for CO molecule. We have also calculated the total number of bound states $n_{\max} = 17, 24, 29$ and 83 along with the whole vibrational bound-state spectrum near the continuous zone for the above molecules, respectively [56]. The bound state energy for the last state is found to be $E_{n_{\max}} = -1.231 \times 10^{-4}, -1.303 \times 10^{-3}, -1.270 \times 10^{-3}$ and $-5.533 \times 10^{-7} eV$ for H_2, HCl, LiH and CO molecules, respectively. The relative accuracy can be of order 10^{-5} or less (up to five significant figures) for LiH, HCl and CO molecules and 10^{-4} - 10^{-5} for H_2 molecule (up to four-five significant figures).

In addition, the known spectroscopic values in Table 2 are used to produce the energy states for selected different arbitrary values of the vibrational n and rotational l angular momentum as shown in Table 3. We also list analogous results obtained before by other methods (using the Pekeris scheme) such as the NU [10], AIM [12], variational [6], SUSY [7] and EQR [13,14] methods together with perturbative and variational quantum mechanical methods like the tridiagonal J-matrix representation (TJM) [15], the shifted $1/N$ expansion (SE) [9], the modified shifted $1/N$ expansion (MSE) [9], the results of Duff and Rabitz (DR) [17], the hyper-virial perturbation (HV) [8], the two-point quasi-rational approximation technique (TQA) [16] and the Fourier grid Hamiltonian method (FGH) [18]. The quality of the results is reassuring with the agreement between our numerical results and those generated by other methods reaching up to four-five significant digits. The current NU approximations to the ro-vibrational energy bound-states are slightly improved from the previous NU approximations probably for two simple reasons. The present calculations are given to four significant digits and if they rounded off to three-significant figures would coincide with those given before in Ref. [10]. Throughout this numerical study, the parameter

conversions in Table 1 into energy units (eV) might be the second reason. The conversions used are $1 \text{ amu} = 931.502 \text{ MeV}/c^2$, $1 \text{ cm}^{-1} = 1.23985 \times 10^{-4} eV$ and $\hbar c = 1973.29 \text{ eV} \times \text{\AA}$ (cf. pp. 791 in [57]). A first look at Table 3 shows that the present approximations give results of identical accuracy like the other well-known semi-analytic variational, EQR, AIM and SUSY methods using the same Pekeris approximation for those fairly small rotational quantum numbers l . This is simply due to the Pekeris approximation [5] where the centrifugal term is being approximated to second-order in r/r_e (i.e., at lower rotational energy, where $r \approx r_e$). This is why the Pekeris approximation is valid only for very small spatial variations from the inter-nuclear separation. The method loses its accuracy for these higher ro-vibrational states. Nonetheless, our calculated vibrational energy states are in higher agreement with the recently calculated energy states (cf. Table 2 in Ref. [15]) for lower- and higher-excitation energy states. Overmore, the ro-vibrational energy states generated by non-perturbative NU, EQR, SUSY, AIM and variational methods are nearly same and slightly different from those given by the cumbersome perturbative and variational methods like HV, TJM, SE, MSE, TQA, FGH and DR, which are not using Pekeris approximation, particularly for higher-excitation ro-vibrational levels.

The further numerical calculations of the ro-vibrational energy states for various quantum numbers n and l on the CO , LiH , H_2 and HCl molecules [55] are also calculated (available from the author upon request) using the generalized q -deformed Morse potential ($V_3 = 0$ case). The variation of the deformation parameter q in our model will produce much more accurate information throughout these spectra about the structure and dynamics of such diatomic molecules. For the case of multi-atomic molecules, the generalization of Morse potentials can be expressed by the Empirical Valence Bond (EVB) approach [45]. Connections of potential functions have been extensively established for various combinations of pair potentials, these have been largely confined to simple potentials such as the harmonic [58], Leonard-Jones [59], Morse [1], Rydberg [60] and Buckingham [61] potential functions (cf. Ref. [62]). For example, parametric connections between the generalized Morse and Extended-Rydberg (ER) potential functions have been attained. Since the number of parameters for ER exceeds those of generalized Morse by 1, therefore only V_i ($i = 1, 2$) are required for converting the ER parameters into generalized Morse parameters but both the Morse indices are needed to obtain V_1 , V_2 and V_3 [45,63]. The present potential functions have greater flexibility consisting of more parameters. There are two sets of relationship

between the Generalized Morse and the ER parameters: (i) for the case where $V_2 < 0$, and (ii) for the case where $V_2 > 0$. For example, the choice of low deformation [43] $q = -1$ provides $V_2 < 0$, i.e., Morse-like potential, $V_M(r) = D_e (e^{-2a(r-r_e)} + 2e^{-a(r-r_e)})$ with the position of a minimum value approaching at $V_M(r_e) = 3D_e$ and strength ratio $\frac{V_2}{V_1} = -2$. Whereas the high deformations $q = \pm 5$ provide the two mentioned cases for the potential $V_M(r) = D_e (e^{-2a(r-r_e)} \mp 10e^{-a(r-r_e)})$ of minima values approaching at $V_M(r_e) = -9D_e$ and $11D_e$, strength ratios $\frac{V_2}{V_1} = \pm 10$, respectively. Some other numerical energy calculations can be estimated including the generalized q -deformed Morse potential ($V_3 \neq 0$ case) [42] (available from the author upon the request). For example, the choice of low deformations $q = \pm 1$ provide a solution for a Morse-like potential, $V_M(r) = D_e (\pm 1 - e^{-a(r-r_e)})^2$ with a minimum value approaching at $V_M(r_e) = 0$ and $4D_e$, respectively. By this choice of parameters $V_2 < 0$ and $V_2 > 0$ for Be-S and H-Na potentials, respectively, we can optimize the generalized Morse potential to ER where good correlation is seen at and near equilibrium [45,62]. This wide range of spectra for various deformed potential models might be necessary in fitting the true experimental one. This approach could be also useful to study further Ar_2 , O_2 , I_2 and NO molecules and others.

V. FINAL REMARKS

To summarize, we have used a parametric generalization of the NU method derived for any exponential-type potential to obtain the bound state solutions of the spatially-dependent mass Schrödinger equation with any rotational angular momentum quantum number l for the generalized q -deformed Morse potential. In this paper, a suitable choice of a mass function has also been proposed. The present calculations include energy equation and the normalized wavefunctions expressed in terms of the Jacobi and Laguerre polynomials. We find a general equation for the ro-vibrational bound-state energy eigenvalues true for the currently proposed mass function given in (22) and in terms of three potential strength parameters V_i (where $i = 1, 2, 3$). Hence, with selected values of the parameter δ , we can obtain a family of solutions. The non-relativistic limit of the solution is being obtained by an appropriate choice of the parameter $\delta \rightarrow 0$ in the mass function. Obviously, we can generate non-relativistic bound state solutions for the rotating Morse potential when the deformation parameters $q = 1$. The numerical application of the method to diatomic

molecules demonstrates that the values obtained are in high agreement with other methods and numerical data at low-rotational excitation energy. This provides an alternative systematic procedure to calculate the energy eigenvalues with a reasonable accuracy and also considered as a suitable method in the treatment of such potentials with a varying mass functions as well. It is worth noting that the analytical results presented here allow one calculating the energy eigenvalues as well as wavefunctions in a very simple way, with very high accuracy for lower-excitation rotational levels and for lower- and higher-excitation vibrational levels, probably enough for most of the applications known until now. The real advantages of our semi-analytic method are systematic, highly accurate, handy, easily implemented and not cumbersome as most of the other well-known methods mentioned before in this paper. We believe that the procedures could be easily extended to other short-range as well as long-range potentials.

Acknowledgments

The author thanks the anonymous kind referees for the constructive comments and suggestions that have improved the paper greatly. He is also grateful for the partial support provided by the Scientific and Technological Research Council of Turkey (TÜBİTAK).

APPENDIX A: PARAMETRIC GENERALIZATION OF THE NU METHOD

We complement the theoretical formulation of the NU method in presenting the essential polynomials, energy equation and wave functions together with their relevant constants as follows.

(i) The key polynomials:

$$\pi(z) = c_4 + c_5 z - [(\sqrt{c_9} + c_3 \sqrt{c_8}) z - \sqrt{c_8}], \quad (\text{A1})$$

$$k = -(c_7 + 2c_3 c_8) - 2\sqrt{c_8 c_9}. \quad (\text{A2})$$

$$\tau(z) = 1 - (c_2 - 2c_5) z - 2[(\sqrt{c_9} + c_3 \sqrt{c_8}) z - \sqrt{c_8}], \quad (\text{A3})$$

$$\tau'(z) = -2c_3 - 2(\sqrt{c_9} + c_3 \sqrt{c_8}) < 0, \quad (\text{A4})$$

(ii) The energy equation:

$$(c_2 - c_3) n + c_3 n^2 - (2n + 1) c_5 + (2n + 1) (\sqrt{c_9} + c_3 \sqrt{c_8}) + c_7 + 2c_3 c_8 + 2\sqrt{c_8 c_9} = 0. \quad (\text{A5})$$

(iii) The wave functions:

$$\rho(z) = z^{c_{10}}(1 - c_3 z)^{c_{11}}, \quad (\text{A6})$$

$$\phi(z) = z^{c_{12}}(1 - c_3 z)^{c_{13}}, \quad (\text{A7})$$

$$y_n(z) = P_n^{(c_{10}, c_{11})}(1 - 2c_3 z), \quad (\text{A8})$$

$$u(z) = \mathcal{N}_n z^{c_{12}}(1 - c_3 z)^{c_{13}} P_n^{(c_{10}, c_{11})}(1 - 2c_3 z), \quad (\text{A9})$$

where $P_n^{(\alpha, \beta)}(1 - 2s)$ are the Jacobi polynomials with

$$P_n^{(\alpha, \beta)}(1 - 2s) = \frac{(\alpha + 1)_n}{n!} {}_2F_1(-n, 1 + \alpha + \beta + n; \alpha + 1; s), \quad (\text{A10})$$

and \mathcal{N}_n is a normalizing factor. Also, the above wavefunctions can be expressed in terms of the hypergeometric function as

$$u(z) = \mathcal{N}_n z^{c_{12}}(1 - c_3 z)^{c_{13}} {}_2F_1(-n, 1 + c_{10} + c_{11} + n; c_{10} + 1; c_3 z), \quad (\text{A11})$$

where ${}_2F_1(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{p=0}^{\infty} \frac{\Gamma(a+p)\Gamma(b+p)}{\Gamma(c+p)} \frac{z^p}{p!}$. We can determine the normalization constant using the condition $\int_0^1 u^2(r) dr = 1$ and [64]

$$\int_0^1 (1 - s)^{\mu-1} s^{\nu-1} {}_2F_1(\alpha, \beta; \gamma; as) dz = \frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu + \nu)} {}_3F_2(\nu, \alpha, \beta; \mu + \nu; \gamma; a). \quad (\text{A12})$$

(iv) The relevant constants:

$$\begin{aligned} c_4 &= \frac{1}{2}(1 - c_1), \quad c_5 = \frac{1}{2}(c_2 - 2c_3), \quad c_6 = c_5^2 + A, \\ c_7 &= 2c_4c_5 - B, \quad c_8 = c_4^2 + C, \quad c_9 = c_3(c_7 + c_3c_8) + c_6, \\ c_{10} &= c_1 + 2c_4 + 2\sqrt{c_8} - 1, \quad c_{11} = 1 - c_1 - 2c_4 + \frac{2}{c_3}\sqrt{c_9}, \\ c_{12} &= c_4 + \sqrt{c_8}, \quad c_{13} = -c_4 + \frac{1}{c_3}(\sqrt{c_9} - c_5). \end{aligned} \quad (\text{A13})$$

APPENDIX B: THE PEKERIS APPROXIMATION FOR THE ROTATIONAL MORSE POTENTIAL

In this appendix, we present the Pekeris approximation [5,10] performed up to the second order term in r/r_e . We get started by making the change of parameters and coordinates as follows: $x = (r - r_e)/r_e$ and expanding around $x = 0$ ($r = r_e$) to obtain:

$$V_{rot}(x) = \frac{\gamma}{(1+x)^2} = \gamma_1 [1 - 2x + 3x^2 + O(x^3)], \quad \gamma = \frac{l(l+1)}{r_e^2}, \quad (\text{B1})$$

where the first few terms are sufficient for the lower-excitation rotational states since $r \approx r_e$. The corresponding rotational term expressed in the exponential form up to the second order is

$$\tilde{V}_{rot}(x) = \gamma (a_0 + a_1 e^{-\alpha x} + a_2 e^{-2\alpha x}), \quad (\text{B2})$$

$$\begin{aligned} \tilde{V}_{rot}(x) &= \gamma \left[a_0 + a_1 \left(1 - \alpha x + \frac{(\alpha x)^2}{2!} - O(x^3) \right) + a_2 \left(1 - 2\alpha x + \frac{(2\alpha x)^2}{2!} - O(x^3) \right) \right], \\ &= \gamma \left[\sum_{i=0}^2 a_i - \alpha (a_1 + 2a_2) x + \alpha^2 \left(\frac{a_1}{2} + 2a_2 \right) x^2 - O(x^3) \right], \end{aligned} \quad (\text{B3})$$

where a_i ($i = 1, 2, 3$) are the expansion coefficients. Comparing (B.1) with (B.4), we obtain specific values for the expansion coefficients as

$$a_0 = 1 - \frac{3}{\alpha} \left(1 - \frac{1}{\alpha} \right), \quad a_1 = \frac{2}{\alpha} \left(2 - \frac{3}{\alpha} \right), \quad a_2 = -\frac{1}{\alpha} \left(1 - \frac{3}{\alpha} \right), \quad \alpha = ar_e. \quad (\text{B4})$$

On the other hand, we repeat similar procedures to obtain an exponential expansion for the term $1/r$ around $x = 0$ ($r = r_e$) as follows:

$$\frac{1}{r} = \frac{1}{r_e(1+x)} = \frac{1}{r_e} [1 - x + x^2 - O(x^3)], \quad (\text{B5})$$

or equivalently in the exponential expansion:

$$\begin{aligned} \frac{1}{r} &= \frac{1}{r_e} (b_0 + b_1 e^{-\alpha x} + b_2 e^{-2\alpha x}), \\ &= \frac{1}{r_e} \left[\sum_{i=0}^2 b_i - \alpha (b_1 + 2b_2) x + \alpha^2 \left(\frac{b_1}{2} + 2b_2 \right) x^2 - O(x^3) \right], \end{aligned} \quad (\text{B6})$$

Thus, comparing (B.5) with (B.6), we obtain the following expansion coefficients as

$$b_0 = 1 - \frac{1}{\alpha} \left(\frac{3}{2} - \frac{1}{\alpha} \right), \quad b_1 = \frac{2}{\alpha} \left(1 - \frac{1}{\alpha} \right), \quad b_2 = -\frac{1}{\alpha} \left(\frac{1}{2} - \frac{1}{\alpha} \right), \quad \alpha = ar_e. \quad (\text{B7})$$

-
- [1] P.M. Morse, Phys. Rev. 34 (1929) 57; A. Lopez Piñeiro and B. Moreno, J. Chem. Phys. 87 (1987) 520; D. Popov, Phys. Scr. 63 (2001) 257; S.H. Dong *et al*, Int. J. Quantum Phys. 86 (2002) 433.
- [2] M.S. Child and L. Halonen, Advan. Chem. Phys. 57 (1984) 1; L. Pauling and E.B. Wilson Jr., Introduction to Quantum Mechanics with Applications to Chemistry (Dover, New York, 1985).
- [3] S. Flügge, P. Walgner and A. Weiguny, J. Mol. Spectra 23 (1967) 243; R.N. Kesarwani and Y.P. Varshni, Can. J. Phys. 58 (1980) 363; H. Konwent *et al.*, J. Phys. A: Math. Gen. 31 (1998) 7541; E.D. Davis, Phys. Rev. A 70 (2004) 032101.
- [4] S.M. Ikhdair, Eur. Phys. J. A 39 (3) (2009) 307.
- [5] C.L. Pekeris, Phys. Rev. 45 (1934) 98; S. Flügge, Practical Quantum Mechanics, Vol. 1 (Springer-Verlag, Berlin, 1994).
- [6] E.D. Filho and R.M. Ricotta, Phys. Lett. A 269 (2000) 269.
- [7] D.A. Morales, Chem. Phys. Lett. 161 (1989) 253; Chem. Phys. Lett. 394 (2004) 68.
- [8] J.P. Killingbeck, Grosjean and G. Jolicard, J. Chem. Phys. 116 (2002) 447.
- [9] T.D. Imbo and U.P. Sukhatme, Phys. Rev. Lett. 54 (1985) 2184; M. Bag, M.M. Panja and R. Dutt, Phys. Rev. A 46 (1992) 6059.
- [10] C. Berkdemir and J. Han, Chem. Phys. Lett. 409 (2005) 203; C. Berkdemir, Nucl. Phys. A 770 (2006) 32.
- [11] J.R. Elsum and G. Gordon, J. Chem. Phys. 76 (1982) 5452.
- [12] O. Bayrak and I. Boztosun, J. Phys. A: Math. Gen. 39 (2006) 6955.
- [13] W.C. Qiang and S.H. Dong, Phys. Lett. A 363 (2007) 169.
- [14] S.M. Ikhdair and R. Sever, J. Math. Chem. 42 (2007) 461.
- [15] I. Nasser *et al*, J. Phys. B: At. Mol. Opt. Phys. 40 (2007) 4245.
- [16] E. Castro, J.L. Paz and P. Martin, J. Mol. Struct.: Theochem 769 (2006) 15.
- [17] M. Duff and H. Rabitz, Chem. Phys. Lett. 53 (1978) 152.
- [18] C.C. Marston and G.G. Balint-Kurti, J. Chem. Phys. 91 (1989) 3571.
- [19] B. Gönül *et al.*, Mod. Phys. Lett. A 17 (2002) 2057; *ibid.*, Mod. Phys. Lett. A 17 (2002) 2453.

- [20] A.D. Alhaidari, Phys. Rev. A 66 (2002) 042116; *ibid.*, Int. J. Theor. Phys. 42 (2003) 12; *ibid.*, Phys. Lett. A 322 (2004) 72.
- [21] J. Yu, S.H. Dong and G.H. Sun, Phys. Lett. A 322 (2004) 290; J. Yu and S.H. Dong, Phys. Lett. A 325 (2004) 194; A. de Souza Dutra and G. Chen, Phys. Lett. A 349 (2006) 297; G. Chen, Z.D. Chen and P.E. Xuan, Phys. Scr. 74 (2006) 367.
- [22] A. de Souza Dutra and C.A.S. Almeida, Phys. Lett. A 275 (2000) 25.
- [23] R. Koç and M. Koca, J. Phys. A: Math. Gen. 36 (2003) 8105.
- [24] C.S. Jia and A. de Souza Dutra, Annals of Phys. 323 (2008) 566; C.S. Jia *et al*, Int. J. Theor. Phys. 47 (2008) 2513.
- [25] Y. Xu, S. He and C.S. Jia, J. Phys. A: Math. Theor. 41 (2008) 255302.
- [26] L. Dekar *et al.*, J. Math. Phys. 39 (1998) 2551; Phys. Rev. A 59 (1998) 107; G. Chen and Z.D. Chen, Phys. Lett. A 331 (2004) 312.
- [27] R. Sever and C. Tezcan, Int. J. Mod. Phys. E 17 (2008) 1327.
- [28] S.M. Ikhdair and R. Sever, Int. J. Mod. Phys. C 20(3) (2009) 361.
- [29] S.M. Ikhdair, Eur. Phys. J. A 40 (2009) [arXiv:0903.3841] (at press); S.M. Ikhdair and R. Sever, Phys. Scr. 79 (2009) 035002; S.M. Ikhdair and R. Sever, Ann. Phys. (Berlin) 18(4) (2009) 189.
- [30] G. Bastard, Wave Mechanics Applied to Semiconductor Heterostructure, Les Editin de Physique, Les Ulis, 1988.
- [31] P. Harison, Quantum Wells, Wires and Dots, Wiley, New York, 2000; L. Serra and E. Lipparin, Europhys. Lett. 40 (1997) 667.
- [32] M. Barranco *et al.*, Phys. Rev. B 56 (1997) 8997.
- [33] F. Arias *et al.*, Phys. Rev. B 50 (1997) 4248.
- [34] C. Weisbuch, B. Vinter, Quantum Semiconductor Heterostructure, Academic Press, New York, 1993.
- [35] A.F. Nikiforov and V.B. Uvarov, Special Functions of Mathematical Physics (Birkhauser, Bassel, 1988).
- [36] A. Arda, R. Sever and C. Tezcan, Phys. Scr. 79 (2009) 015006.
- [37] S.M. Ikhdair, "Solution of the spatially dependent mass Dirac equations with the spin and pseudospin symmetry for a Coulomb potential", submitted to J. Phys. A (2009); G. Chen, Phys. Lett. A 329 (2004) 22.

- [38] I.A. Watson, B.R. Henry and I.G. Ross, *Spectrochim. Acta* 37 A (1981) 857.
- [39] M.S. Child and R.T. Lawton, *Chem. Phys. Lett.* 87 (1982) 217.
- [40] L. Halonen and M.S. Child, *Mol. Phys.* 46 (1982) 239.
- [41] H. Taşeli, *J. Phys. A* 31 (1998) 779; M. Znojil, *Phys. Lett. A* 264 (1999) 108; Ö. Yeşiltaş *et al*, *Phys. Scr.* T67 (2003) 472; G. Lévai and M. Znojil, *J. Phys. A.* 35 (2002) 8793.
- [42] J. Lu, *Phys. Scr.* 72 (2005) 349; J. Lu *et al*, *Chinese Phys.* 14 (2005) 2402; C.-S. Jia *et al*, *Phys. Scr.* 75 (2007) 388.
- [43] H. Eğrişes, D. Demirhan, F. Büyükkılıç, *Phys. Scr.* 60 (1999) 195.
- [44] C.S. Jia, X.L. Zeng and L.T. Sun, *Phys. Lett. A* 294 (2002) 185; C.S. Jia *et al*, *Phys. Lett. A* 311 (2003) 115.
- [45] T.-C. Lim, *Acta Chim. Slov.* 52 (2005) 149; A. Warshel, *Computer Modeling of Chemical Reactions in Enzymes and Solutions*, John Wiley and Sons, New York, 1991.
- [46] S.M. Ikhdair and R. Sever, *Z. Phys. C* 56 (1992) 155; *ibid.* C 58 (1993) 153; *ibid.* D 28 (1993) 1; *ibid.* *Int. J. Mod. Phys. A* 18 (2003) 4215; *ibid.* A 20 (2005) 4035; *ibid.* A 21 (2006) 2191, 6699.
- [47] S.M. Ikhdair and R. Sever, *Int. J. Mod. Phys. A* 19 (2004) 1771; *ibid.*, A 20 (2005) 6509.
- [48] S.M. Ikhdair and R. Sever, *Int. J. Mod. Phys. E* 17 (2008) 669.
- [49] M.N. Nieto, *Am. J. Phys.* 47 (1979) 1067.
- [50] S.M. Ikhdair and R. Sever, *Ann. Phys. (Leibzig)* 16 (2007) 218; *ibid.*, *Int. J. Theor. Phys.* 46 (2007) 1643, 2384; S.M. Ikhdair and R. Sever, *J. Math. Chem.* 42 (2007) 461.
- [51] S.M. Ikhdair, *Int. J. Mod. Phys. C* 20 (2009) 25; S.M. Ikhdair, *Chin. J. Phys.* 46 (2008) 291; S.M. Ikhdair and R. Sever, *Ann. Phys. (Berlin)* 17 (2008) 897; *ibid.*, *Cent. Eur. J. Phys.* 6 (2008) 141, 685; *ibid.*, *Int. J. Mod. Phys. C* 19 (2008) 221, 1425.
- [52] B. Bagchi, P.S. Gorain and C. Quesne, *Mod. Phys. Lett. A* 21 (2006) 2703.
- [53] S.M. Ikhdair, 'Approximate solution of the Klein-Gordon equation of diatomic molecules with a generalized deformed empirical scalar and vector potentials', to be published in *Int. J. Mod. Phys. C* (2009).
- [54] G. Faridfathi, R. Sever and M. Aktaş, *J. Math. Chem.* 38 (2005) 533.
- [55] M. Aktaş and R. Sever, *Mod. Phys. Lett. A* 19 (2004) 2871.
- [56] S.M. Ikhdair and R. Sever, *J. Math. Chem.* 45(4) (2009) 1137.
- [57] B.H. Bransden and C.J. Joachain, *Quantum Mechanics*, 2nd edn., Pearson Education Ltd.,

England.

- [58] R. Hooke, The True Theory of Elasticity and Springiness, 1676.
- [59] J.E. Leonard-Jones, Proc. Roy. Soc. Lond. A 106 (1924) 463.
- [60] R. Rydberg, Z. Phys. 73 (1931) 376.
- [61] R.A. Buckingham, Proc. Roy. Soc. Lond. A 169 (1938) 264.
- [62] T.C. Lim, J. Math. Chem. 34 (2003) 221; J. Math. Chem. 36 (2004) 261; Z. Naturforsch. A 58 (2003) 615; Phys. Scr. 70 (2004) 347; Chin. J. Phys. 43 (2005) 43.
- [63] P. Huxley and J.N. Murrell, J. Chem. Soc. Faraday Trans II 79 (1983) 323.
- [64] I.S. Gradshteyn and I.M. Ryzhik, Tables of Integrals, Series and Products, 5th edn. (Academic, New York, 1994).

TABLE I: The specific values for the parametric constants necessary for the present potential.

Constant Value		Constant Value	
c_1	1	c_2	δ
c_3	δ	c_4	0
c_5	$-\frac{1}{2}\delta$	c_6	$\frac{1}{4}(\delta^2 + 4\beta_1)$
c_7	$-\beta_2$	c_8	ε_{nl}^2
c_9	$\frac{1}{4}\delta^2\xi^2$	c_{10}	$2\varepsilon_{nl}$
c_{11}	ξ	c_{12}	ε_{nl}
c_{13}	$\frac{1}{2}(1 + \xi)$	A	β_1
B	β_2	C	ε_{nl}^2

TABLE II: Model parameters for CO , LiH , H_2 and HCl diatomic molecules in our study as obtained from the cited sources.

Parameters	CO [13]	LiH [13]	H_2 [16]	HCl [13]
D_0 (cm^{-1})	90540	20287	38266	37255
a (A°) ⁻¹	2.2994	1.1280	1.9426	1.8677
r_0 (A°)	1.1283	1.5956	0.7416	1.2746
μ (amu)	6.8606719	0.8801221	0.50391	0.9801045

TABLE III: Bound-state energy eigenvalues ($-E_{nl}$) for the H_2 , LiH , CO and HCl molecules (in eV) for different values of the vibrational n and rotational l quantum numbers in the usual Morse potential ($q = 1$, $V_3 = 0$).

n	l	This work	SUSY [7]	AIM [12]	HV [8]	DR [17]	MSE [9]	TJM [15]	SE [9]	V [6]	TQA [16]
H_2											
0	0	4.47601	4.47601	4.47601	4.47601	4.4762	4.4760	4.4760131	4.4749	4.4758	4.4760084
	5	4.25880	4.25880	4.25880	4.25901	4.2592	4.2590	4.2590180	4.2589	4.2563	4.2590038
	10	3.72194	3.72193	3.72193	3.72473	3.7251	3.7247	3.7247471	3.7247	3.7187	3.7247181
5	0	2.22052	2.22051	2.22052	2.22051	2.218	2.2205	2.2205369			
	5	2.04355	2.04353	2.04355	2.05285	2.050	2.0430	2.0528808			
	10	1.60391	1.60389	1.60391	1.65265	1.650	1.6535	1.6526902			
7	0	1.53744	1.53743	1.53744	1.53743		1.5374	1.5374552			
	5	1.37656	1.37654	1.37656	1.39263		1.3932	1.3926614			
	10	0.97581	0.97578	0.97581	1.05265		1.0552	1.0526836			
n	l	This work	NU [10]	EQR [13]	SUSY [7]	AIM [12]	MSE [9]	TJM [15]	FGH [18]	SE [9]	V [6]
LiH											
0	0	2.42886	2.4287	2.42886	2.42886	2.4289	2.4280	2.4288627	2.42886	2.4278	2.4291
	5	2.40133	2.4012	2.40133	2.40133	2.4013	2.4000	2.4013352	2.40133	2.3999	2.4014
	10	2.32884	2.3287	2.32883	2.32883	2.3288	2.3261	2.3288530	2.32885	2.3261	2.3287
5	0	1.64771	1.6476	1.64772	1.64772	1.6477	1.6402	1.6477149	1.64772	1.6242	
	5	1.62377	1.6236	1.62377	1.62377	1.6238	1.6160	1.6239497	1.62395	1.6074	
	10	1.56074	1.5606	1.56074	1.56074	1.5607	1.5525	1.5615114	1.56152	1.5479	
7	0	1.37756	1.3774	1.37757	1.37756	1.3776	1.3862	1.3775588	1.37756	1.3424	
	5	1.35505	1.3549	1.35505	1.35505	1.3550	1.3456	1.3553770	1.35538	1.3309	
	10	1.29580	1.2956	1.29581	1.29580	1.2958	1.2865	1.2971612	1.29715	1.2781	

TABLE IV: Continue.

n	l	This work	SUSY [7]	AIM [12]	NU [10]	EQR [13]	MSE [9]	TJM [15]	SE [9]	FGH [18]	V [6]
<i>CO</i>											
0	0	11.0915	11.0915	11.0915	11.091	11.0915	11.092	11.0915353	11.091	11.0915	11.093
	5	11.0844	11.0844	11.0845	11.084	11.0844	11.084	11.0843875	11.084	11.0844	11.084
	10	11.0653	11.0653	11.0653	11.065	11.0653	11.065	11.0653334	11.065	11.0653	11.0653
5	0	9.79518	9.79519	9.7952	9.795	9.79519	9.795	9.7951838	9.788	9.79519	
	5	9.78833	9.78834	9.7883	9.788	9.78835	9.788	9.7883443	9.782	9.78835	
	10	9.77009	9.77010	9.7701	9.769	9.77011	9.770	9.7701124	9.765	9.77011	
7	0	9.29918	9.29920	9.2992	9.299	9.29920	9.299	9.2991935	9.286	9.29920	
	5	9.29246	9.29248	9.2925	9.292	9.29248	9.292	9.2924786	9.281	9.29248	
	10	9.27455	9.27458	9.2745	9.274	9.27457	9.274	9.2745791	9.265	9.27458	
n	l	This work	V [6]	EQR [13]	SUSY [7]	AIM [12]	MSE [9]	TJM [15]	FGH [18]	SE [9]	
<i>HCl</i>											
0	0	4.43556	4.4360	4.43556	4.43556	4.4356	4.4355	4.4355522	4.43556	4.4352	
	5	4.39682	4.3971	4.39681	4.39681	4.3968	4.3968	4.3968066	4.39682	4.3967	
	10	4.29408	4.2940	4.28407	4.28408	4.2841	4.2940	4.2940628	4.28409	4.2939	
5	0	2.80506		2.80507	2.80508	2.8051	2.8046	2.8049687	2.80508		
	5	2.77209		2.77210	2.77211	2.7721	2.7718	2.7721880	2.77230		
	10	2.68471		2.68472	2.68473	2.6847	2.6850	2.6853673	2.68549		
7	0	2.25701		2.25702	2.25703	2.2570	2.2565	2.2568924	2.25703		
	5	2.22634		2.22636	2.22636	2.2263	2.2262	2.2265969	2.22673		
	10	2.14511		2.14512	2.14513	2.1451	2.1461	2.1464148	2.14656		