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Exact solutions for vibrational states with generalized q-deformed Morse potential within the asymptotic iteration method

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Exact eigenvalues and eigenfunctions of the Schrödinger equation with generalized q-deformed Morse potential for diatomic molecules have been derived in the framework of the asymptotic iteration method (AIM). The obtained solutions have been applied to calculate the energies of bound vibrational levels of the lithium molecule in the $A^1\Sigma_u^+$ state. Compared to AIM previous calculations, our results are extremely accurate and are in excellent agreement with those using different approximation techniques.

Key words: q-Deformed Morse potential, asymptotic iteration method.

INTRODUCTION

The solution of the fundamental equation of quantum mechanics, namely the Schrödinger equation has continued to attract interest of physicists and mathematicians. Since solving this equation is always a complicated problem, different methods have been developed to solve this famous equation (Egrifes et al., 1999; Chao and Lin, 1999; Harun et al., 1999; Shi-Hai et al., 1999; Korsch et al., 1982; Rieth et al., 2002; He, 1999). Recently, a new method called "asymptotic iteration method" (AIM) has been developed by Ciftci et al. (2003) which found wide applications in physics, particularly in exploring and understanding some aspects of molecular physics and quantum chemistry (Chabab and Oulne, 2010; Al-Dossary, 2007; Bayrak et al., 2007; Ateser et al., 2007; Durmus and Yasuk, 2007). Its successes in deriving bound states of some diatomic molecules have led to wide acceptance of the AIM as an accurate and easy handling method as compared to the other techniques on the shelf, such as the variational techniques (Utreras-Díaz et al., 1995; Mazziotti, 2002; Kumar, 2009; Mohyud-Din et al., 2010), perturbation

method (Ledoux et al., 2006; Mahasneh and Al-Qararah, 2010; Xue-Ping et al., 2008), Nikiforov- Uvanov method (Cüneyt and Han, 2005; Metin, 2007; Antia et al., 2010), 1/N shifted expansion method (Tang and Chan, 1987; Sinha et al., 2000) and super-symmetry (Cooper et al., 1995; Morales, 2004).

Also, the relevance of several potentials to describe the physics of atoms and molecules and interactions of nuclei has been investigated. Several works have shown that Morse potential proposed in Morse (1929) offers an appropriate model to study bound states of diatomic and even polyatomic molecules. More recently, the vibrational energy levels for the nuclear motion of several diatomic molecules have been examined both analytically and numerically with Morse potential. However, the accuracy of the obtained results seems model or algorithm dependent: it is correlated either to the approximation method used to solve the Schrödinger equation or to the algorithm developed to determine numerical eigenenergies. As an illustration, the vibrational spectrum of $^7\text{Li}_2$ molecule has been computed within distinct methods:

1. Ley-koo et al. (1995) and Taseli (1998) used a confined system in a spherical box of radius l , to examine

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analytically and numerically the eigenenergies. The results of Ley-Koo et al. (1995) were inaccurate because they used too large spherical box, as explained in detail in Taseli (1998) where Taseli presented impressive results which are accurate up to 28 digits.

2. More recently, Barakat et al. (2006), in a comparative study used the AIM method to report the energy levels with accuracy only to about to 14 decimals.

3. Nikiforov-Uvanov method has also been applied to the q-deformed Morse eigenvalue problem in Ikhdair (2009), where an exact solution comes out naturally.

This discrepancy in the accuracy motivates us to revisit this eigenvalue problem for a generalized q-deformed Morse potential. We investigate the bound state energy eigenvalues and the corresponding wave-functions in the framework of the asymptotic iteration method where we derive a q-dependent eigenenergies formula. We also show that, in the case of simple Morse potential where the deformation parameter q is set to 1, our results are recorded to 28 significant figures, as in Taseli (1998), showing that the AIM approach can be equally accurate as the approach used by Taseli, and furthermore, that the limited accuracy in Barakat et al. (2006) is mainly due to the used numerical algorithm in their calculations.

The paper is organized as follows: AIM was applied to the q-deformed Morse potential and the generalized exact solutions of the Schrödinger equation were presented. Finally, the obtained results were discussed and concluded.

ASYMPTOTIC ITERATION METHOD

The radial Schrödinger equation for the central field motion of a diatomic molecule (in a spherical potential $V(r)$) is given by:

$$\left[-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) - \frac{\ell(\ell+1)}{r^2} + V(r) \right] R(r) = ER(r) \quad (1)$$

where m is the reduced mass of the diatomic molecule, \hbar the reduced Planck's constant and ℓ the angular momentum quantum number with $\ell = 0, 1, 2, \dots$. To study the purely vibrational states of diatomic molecules, one has to solve Equation 1 where $\ell = 0$ using a model potential like generalized Morse one:

$$V(r) = V_1 e^{-2c(r-r_0)} + V_2 e^{-c(r-r_0)} + V_3 \quad (2)$$

where the parameter $V_1 = D_s$ is the energy dissociation parameter in Morse (1929) potential which can be expressed in units $\hbar \omega_0$, the parameters $V_2 < 0$ and V_3 are related to V_1 , hence, to the energy dissociation parameter D_s and c is a parameter related to

the frequency of classical vibrations about the equilibrium position γ_0 (Ley-Koo et al., 1995).

In this case, we can simplify Equation 1 by changing the radial function $R(r)$ into $\frac{u(r)}{r}$. Equation 1 becomes:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V(r) \right] u(r) = Eu(r) \quad (3)$$

Equation 3 could also be simplified by substituting $x = e^{-(r'-r'_0)}$ into the relation (Equation 2) where $r' = cr$ and $r'_0 = cr'_0$. It transforms into the following form:

$$\left[-\frac{1}{2} \left(\frac{d^2}{dx^2} + \frac{1}{x} \frac{d}{dx} - \frac{\mu^2}{x^2} \right) - \frac{\lambda}{x} \right] u(x) = \gamma u(x) \quad (4)$$

with,

$$\mu^2 = \frac{V_3 - E}{c^2}, \lambda = -\frac{V_2}{2c^2}, \gamma = -\frac{V_1}{2c^2} \quad (5)$$

where we took $\hbar = 2m = 1$ for commodity.

Equation 4 looks like the Schrödinger equation for the hydrogen atom. Therefore, the eigenfunctions of this equation must satisfy the boundary conditions:

$$u(0) = 0 \text{ and } u(x \rightarrow \infty) = 0 \quad (6)$$

To solve Equation 4 using the asymptotic iteration method as proposed in Ciftci et al. (2003), we propose the following ansatz for the wave function which undergoes the limits conditions (Equation 6):

$$u(x) = x^\mu e^{-\sqrt{-2\gamma}x} f(x) \quad (7)$$

where $f(x)$ is an asymptotic iteration function to be determined. After inserting the relation (Equation 7) into Equation 4, we get the differential equation for the function $f(x)$:

$$\frac{d^2}{dx^2} f(x) = \lambda_0(x) \frac{d}{dx} f(x) + s_0(x) f(x) \quad (8)$$

with

$$\lambda_0(x) = \frac{-2\mu + 2\sqrt{-2\gamma}x - 1}{x} \quad (9)$$

and

$$s_0(x) = \frac{2\sqrt{-2\gamma}\mu + \sqrt{-2\gamma} - 2\lambda}{x} \quad (10)$$

The differential Equation 8 has a general solution given in Ciftci et al. (2003) of the form:

$$f(x) = e^{\int^x \delta(t) dt} \left[C_2 + C_1 \int^x e^{\int^t (\lambda_0(\tau) + 2\delta(\tau)) dt} dt \right] \quad (11)$$

where the $\delta(x)$ values are obtained from:

$$\frac{s_n(x)}{\lambda_n(x)} = \frac{s_{n-1}(x)}{\lambda_{n-1}(x)} \equiv \delta(x) \quad (12)$$

for sufficiently large $n > 0$ and for,

$$\lambda_n(x) = \lambda'_{n-1}(x) + s_{n-1}(x) + \lambda_0(x)\lambda_{n-1}(x) \quad (13a)$$

$$s_n(x) = s'_{n-1}(x) + s_0(x)\lambda_{n-1}(x), n=1,2,3,\dots \quad (13b)$$

Equation 12 could be solved iteratively for a given starting value of x as explained in Ciftci et al. (2003). The obtained solutions define the eigenvalues of Equation 4. For $n = 20$ iterations, the obtained solutions are:

$$\mu_0 = -\frac{1}{2} - \frac{\sqrt{-2\gamma}}{2\gamma} \lambda, \mu_1 = -\frac{3}{2} - \frac{\sqrt{-2\gamma}}{2\gamma} \lambda, \mu_2 = -\frac{5}{2} - \frac{\sqrt{-2\gamma}}{2\gamma} \lambda, \dots \quad (14)$$

In general form, we have:

$$\mu_n = -\frac{2n+1}{2} - \frac{\sqrt{-2\gamma}}{2\gamma} \lambda \quad (15)$$

After substituting γ and λ by their values given in Equation 5, we obtain:

$$\mu_n = \frac{1}{2} \left[\frac{|V_2|}{c\sqrt{V_1}} - (2n+1) \right] \quad (16)$$

and finally we get the exact eigenvalues of Equation 4,

$$E_n = -\frac{1}{4V_1} \left[|V_2| - c\sqrt{V_1}(2n+1) \right]^2 + V_3 \quad (17)$$

For $V_3 = 0$, the relation (Equation 17) coincides with the exact eigenvalues formula as obtained in the quantum mechanics book of Bagrov and Gitman (1990).

To study the classical small vibrations about the equilibrium position $r = r_e$, we introduce the frequency:

$$\omega_0 = c \sqrt{\frac{2V_1}{m}} \quad (18)$$

The energy dissociation parameter in Morse potential can be expressed in units $\hbar \omega_0$ as:

$$D_e = \Delta \hbar \omega_0 \quad (19)$$

The parameter V_2 in the potential presented in Equation 2 is chosen to be equal to $-2qV_1$, where q is a deformation parameter and the parameter V_3 is taken in the form $\frac{q^2-1}{2}V_1$. For $q = 1$, we

will deal with the simple Morse potential. With these parameters, we get from Equation 17 the energies of vibrational levels of diatomic molecules depending on the q deformation parameter:

$$E_n = -\frac{1}{16\Delta} [-(2n+1) + 4q\Delta]^2 + \frac{q^2-1}{2} \Delta \quad (20)$$

in units $\hbar \omega_0$.

The direct solution of the differential Equation 8 gives:

$$f(x) = CL_n^{2\mu} (2\sqrt{-2\gamma}x) = CL_n^{2\mu} (4\Delta x) \quad (21)$$

where $L_n^{2\mu}$ are Laguerre polynomials. Then, we obtain the exact eigenfunctions of the Equation 4:

$$u(x) = Cx^\mu e^{-\sqrt{-2\gamma}x} L_n^{2\mu} (2\sqrt{-2\gamma}x) = Cx^\mu e^{-\sqrt{-2\gamma}x} L_n^{2\mu} (4\Delta x) \quad (22)$$

where C is the normalization constant.

DISCUSSION

Morse potential has shown a great ability in the description of diatomic interactions and proven successful in molecular physics and laser physics. A review of Morse potential problems may be found in Ikhdaier (2009) work. In this note, we have reanalyzed the energy levels and the corresponding vibrational states of diatomic molecule Li_2 via a q -deformed Morse potential. For this, we have solved the radial Schrödinger equation by making use of the asymptotic iteration method. In Table 1, we show the vibrational spectra of ${}^7\text{Li}_2$ obtained in the frame by different authors and compared them to this present work. We see clearly that the calculation performed in Ley-Koo et al. (1995) is surprisingly inaccurate. As to the recently computed eigenenergies in Barakat et al. (2006) via AIM method up to 14 digits, they are far from being as accurate as Taseli (1998) spectra. Besides, the authors of Barakat et al. (2006) based their work on a comparative study to Ley-Koo et al. (1995) which is inconsistent since it used a too large spherical box as explained in Taseli (1998). On the other hand, our AIM calculations are extremely precise and present the energy levels up to 28 decimals with a full agreement with Taseli (1998). One may consider such accuracy as being extreme in nowadays molecular spectroscopy, but it is an important criterion to discriminate between the approximations methods used in the literature.

Finally, we would like to notice that, although, the AIM and the confined spherical box methods are equally highly accurate, the latter technique requires a lot of computational time, and may even fail for levels close to dissociation as the spherical box is increased in size to accommodate more energetic vibrations. In fact, unlike the AIM, it would seem that a method using such a confined spherical box is bound to become inapplicable

Table 1. Energy levels of ${}^7\text{Li}_2$ computed by Morse (1929), Ley-Koo et al. (1995), Barakat et al. (2006), Taseli (1998) and the present work in the $A^1\Sigma_u^+$ state with the parameters values $\Delta = 34.997$, $r_e = 3.10821$ and $c = 0.616$.

N	Morse (1929)	Ley-Koo et al. (1995)	Barakat et al. (2006)	Taseli (1998)	Present work
0	-34.4987858673600594	-34.4987858673604677	-34.4987858673600556	-34.4987858673600594336657427779/8	-34.4987858673600594336657427778
1	-33.5130728062405349	-33.5130728062414320	-33.5130728062405367	-33.5130728062405349029916850016/5	-33.5130728062405349029916850015
2	-32.5416466840014858	-32.5416466840021528	-32.5416466840014849	-32.5416466840014858416435694488/7	-32.5416466840014858416435694487
3	-31.5845075006429122	-31.5845075006434506	-31.5845075006429106	-31.5845075006429122496213961197/6	-31.5845075006429122496213961196
4	-30.6416552561648141	-30.6416552561655102	-30.6416552561648174	-30.6416552561648141269251650141/0	-30.6416552561648141269251650140
5	-29.7130899505671914	-29.7130899505676886	-29.7130899505671913	-29.7130899505671914735548761322/1	-29.7130899505671914735548761321
6	-28.7988115838500442	-28.7988115838512790	-28.7988115838500462	-28.7988115838500442895105294738/7	-28.7988115838500442895105294739
7	-27.8988201560133725	-27.8988201560141817	-27.8988201560133717	-27.898820156013372574792125038/7	-27.8988201560133725747921250392
8	-27.0131156670571763	-27.0131156670575088	-27.0131156670571784	-27.0131156670571763293996628282/1	-27.0131156670571763293996628282
9	-26.1416981169814555	-26.1416981169820595	-26.1416981169814555	-26.1416981169814555533331428407	-26.1416981169814555533331428407
10	-25.2845675057862102	-25.2845675057870984	-25.2845675057862103	-25.2845675057862102465925650769	-25.2845675057862102465925650769
11	-24.4417238334714404	-24.4417238334716096	-24.4417238334714426	-24.4417238334714404091779295367	-24.4417238334714404091779295367
12	-23.6131671000371460	-23.6131671000377494	-23.6131671000371455	-23.6131671000371460410892362202	-23.6131671000371460410892362202
13	-22.7988973054833271	-22.7988973054838091	-22.7988973054833259	-22.7988973054833271423264851272	-22.7988973054833271423264851272
14	-21.9989144498099837	-21.9989144498102718	-21.9989144498099840	-21.9989144498099837128896762579	-21.9989144498099837128896762579
15	-21.2132185330171157	-21.2132185330174288	-21.2132185330171161	-21.2132185330171157527788096122	-21.2132185330171157527788096122
16	-20.4418095551047232	-20.4418095551052090	-20.4418095551047223	-20.4418095551047232619938851901	-20.4418095551047232619938851901
17	-19.6846875160728062	-19.6846875160729802	-19.6846875160728061	-19.6846875160728062405349029916	-19.6846875160728062405349029916
18	-18.9418524159213646	-18.9418524159217014	-18.9418524159213639	-18.9418524159213646884018630168	-18.9418524159213646884018630168
19	-18.2133042546503986	-18.2133042546505699	-18.2133042546503994	-18.2133042546503986055947652655	-18.2133042546503986055947652655
20	-17.4990430322599079	-17.4990430322602215	-17.4990430322599053	-17.4990430322599079921136097379	-17.4990430322599079921136097379
21	-16.7990687487498928	-16.7990687487502584	-16.7990687487498924	-16.7990687487498928479583964339	-16.7990687487498928479583964339
22	-16.1133814041203531	-16.1133814041206413	-16.1133814041203536	-16.1133814041203531731291253535	-16.1133814041203531731291253535
23	-15.4419809983712889	-15.4419809983712994	-15.4419809983712888	-15.4419809983712889676257964968	-15.4419809983712889676257964968
24	-14.7848675315027002	-14.7848675315028206	-14.7848675315027016	-14.7848675315027002314484098637	-14.7848675315027002314484098637

in the vicinity of the dissociation limit.

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