On the ro–vibrational energies for the lithium dimer; maximum-possible rotational levels

Omar Mustafa

Department of Physics, Eastern Mediterranean University, G. Magusa, north Cyprus, Mersin 10, Turkey

E-mail: omar.mustafa@emu.edu.tr

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Abstract
The Deng–Fan potential is used to discuss the reliability of the improved Greene–Aldrich approximation and the factorization recipe of Badawi et al [17] for the central attractive/repulsive core $\mu J(J + 1)/2r^2$. The factorization recipe is shown to be a more reliable approximation and is used to obtain the rotational–vibrational energies for the $a^3\Sigma^+_u - 7Li_2$ dimer. For each vibrational state only a limited number of the rotational levels are found to be supported by the $a^3\Sigma^+_u - 7Li_2$ dimer.

Keywords: ro–vibrational energies, lithium dimer, maximum-possible rotational levels

1. Introduction

The discovery of Bose–Einstein condensation in some ultracold spin-polarized states of the alkali lithium dimer $^7Li_2$ [1] has encouraged intensive experimental as well as theoretical studies on this system [2–7]. While the Bose–Einstein condensation formation in $^7Li_2$ dimer is found to depend on the interaction potential of the lowest triplet excited $a^3\Sigma^+_u$ state, its stability is observed to be sensitive to the binding energy of the least bound vibrational state (among the 11 vibrational states supported by the $a^3\Sigma^+_u - 7Li_2$ potential) [2–4]. Spectral analysis were carried out to determine vibrational and rotational constants and dissociation energy for this dimer [3, 5, 6]. The transition probabilities, moreover, depend on the molecular rotational–vibrational (ro–vibrational, hereinafter) levels. A general analytical closed-form solution for molecular ro–vibrational energies (with sufficient reliable accuracy in a broad range of the rotational and vibrational quantum numbers) would be of great interest in physics and/or chemistry, for it would allow substantial simplifications of the derivation of molecular transition probabilities [8]. The ro–vibrational energy levels of the $a^3\Sigma^+_u - 7Li_2$ dimer represent the core of the current work.

In the literature, an empirical diatomic molecular potential energy function, $U(r)$, necessarily and desirably satisfies the conditions (see e.g., [9, 10])

$$U(\infty) - U(r_e) = D_e, \quad \left. \frac{dU(r)}{dr} \right|_{r=r_e} = 0,$$

and

$$\left. \frac{d^2U(r)}{dr^2} \right|_{r=r_e} = K_e = \left(2\pi c^2\mu \omega_e^2\right), \quad (1)$$

where $D_e$ is the dissociation energy, $r_e$ is the equilibrium bond length, $c$ is the speed of light, $\mu$ is the reduced mass, and $\omega_e$ is the equilibrium harmonic oscillator vibrational frequency. The introduction of a fourth condition $U(r_e) = 0$ would only shift the potential by a constant at the equilibrium bond length, but never violates the three conditions above [11–19]. For example, the Schöberg [15], and the improved (or the shifted by a constant) Manning–Rosen potentials share the Deng–Fan [14] diatomic molecular potential form

$$U(r) = D_e \left[1 - \frac{e^{\alpha r_e} - 1}{e^{\alpha r_e} - 1}\right]^2. \quad (2)$$

Here $\alpha$ denotes the range of the potential and is obtained using the last condition in (1) to read

$$\alpha = \beta + \frac{1}{r_e} W \left(-r_e\beta e^{-\beta}\right); \quad \beta = \frac{K_e}{2D_e},$$

where $\beta$ is often called the Morse constant [19] and $W(z)$ is the Lambert function. The vibrational spectra of such a model...
is exactly solvable and a closed form solution exists in the literature (e.g., [11, 12]). The main challenge lies, however, in dealing with the central attractive/repulsive core $J(J + 1)/2\mu r^2$ of the radial spherically symmetric Schrödinger equation

$$\frac{\hbar^2}{2\mu} \frac{d^2 u_{\nu\rho}(r)}{dr^2} + \left[ \frac{J(J + 1)\hbar^2}{2\mu r^2} + U(r) \right] \times u_{\nu\rho}(r) = E_{\nu\rho} u_{\nu\rho}(r),$$

(3)

with $\nu$ denoting the vibrational and $J$ denoting the rotational quantum numbers.

In their attempt to obtain the ro–vibrational spectra for the $a^3\Sigma_u^+ - 3\Sigma_g^-$ potential model (2), however, to deal with the central attractive/repulsive core $J(J + 1)/2\mu r^2$ (i.e., the ro–vibrational coupling) they have used the improved Greene–Aldrich approximation [16]

$$\frac{1}{r^2} \approx a^2 \left( \frac{1}{12} + \frac{e^{ar}}{(e^{ar} - 1)^2} \right),$$

(4)

and reported the ro–vibrational energy spectra in a closed analytical form as

$$E_{\nu\rho} = D_\nu + \frac{\hbar^2 a^2}{24\mu} \frac{J(J + 1)\hbar^2 a^2}{2\mu r^2} - \frac{\hbar^2 a^2}{2\mu} \left( \frac{2\mu}{\hbar^2 a^2} D_\nu (e^{ar} - 1) - \frac{a}{4} \right)^2,$$

(5)

with

$$A = 2\nu + 1 + \sqrt{(1 + 2J)^2 + \frac{8\mu}{\hbar^2 a^2} D_\nu (e^{ar} - 1)^2}.$$  

(6)

but never subjected it to a quantitative brute force numerical test for any $J \neq 0$. At this very point, it is obvious that the asymptotic behavior of $e^{ar}/(e^{ar} - 1)^2$ as $ar \to 0$ would manifest the necessary improvement of the Greene–Aldrich approximation

$$\frac{1}{r^2} \approx a^2 \left( \frac{e^{ar}}{(e^{ar} - 1)^2} \right)$$

into the Taylor series expansion

$$\frac{e^{ar}}{(e^{ar} - 1)^2} \approx \frac{1}{12} + O(a^2 r^2);$$

which in turn leads to (4). However, one may wonder as to whether such an approximation is an adequate representation of the ro–vibrational coupling term. Strictly speaking, if such an approximation sacrifices the accuracy for large rotational quantum number $J > 0$ then one should look for an alternative approach and hope for a better and more adequate representation.

In the current proposal, we suggest Badawi et al [17] factorization recipe

$$\frac{r_c^2}{\mu} = C_0 + \frac{C_1}{e^{ar} - 1} + \frac{C_2}{(e^{ar} - 1)^2},$$

(7)

in section 2, as an alternative approach and report a closed form analytical solution for the ro–vibrational energy levels. Although a variant of algebraic approaches are available in the literature (see e.g., Infeld and Hull [20], Wybourne [21], and Iachello and Levine [22, 23]), we recollect (in the same section) the supersymmetric quantization recipe used by Jia et al [18] to obtain the ro–vibrational energies. Moreover, we subject (in section 3) both approaches (4) and (7) into a quantitative brute force numerical test and compare their accuracy performance with those of Roy [19], who have used a generalized pseudospectral (GPS) method to calculate the ro–vibrational energies for six diatomic molecules. We choose the $O_2 (X^2 \Sigma_u^+) - 3\Sigma_g^-$ molecule for the sake of comparison.

In the current proposal, we suggest Badawi et al [17] diatomic molecular potential (2) as

$$U(r) = R + \frac{P_2}{e^{ar} - 1} + \frac{P_3}{(e^{ar} - 1)^2},$$

(8)

where

$$P_1 = D_\nu; P_2 = -2D_\nu (e^{ar} - 1); P_3 = D_\nu (e^{ar} - 1)^2.$$  

(9)

Incorporating (7) and (8) into (3) one would write the effective potential as

$$U_{\text{eff}}(r) = \frac{J(J + 1)\hbar^2}{2\mu r^2} + U(r) = \tilde{R} + \frac{\tilde{R}_2}{e^{ar} - 1} + \frac{\tilde{R}_3}{(e^{ar} - 1)^2},$$

(10)

Section 4 is devoted for our concluding remarks.

2. Ro–vibrational energies and supersymmetric quantization recipe

In this section we recollect Jia et al [18] work on the 6-parametric exponential-type one-dimensional potential, where a closed form exact energy eigenvalues are obtained. For the sake of our study here, we use a 4-parametric potential and cast the Deng–Fan [14] diatomic molecular potential (2) as

$$U(r) = R + \frac{P_2}{e^{ar} - 1} + \frac{P_3}{(e^{ar} - 1)^2},$$

(8)

where

$$P_1 = D_\nu; P_2 = -2D_\nu (e^{ar} - 1); P_3 = D_\nu (e^{ar} - 1)^2.$$  

(9)

Incorporating (7) and (8) into (3) one would write the effective potential as

$$U_{\text{eff}}(r) = \frac{J(J + 1)\hbar^2}{2\mu r^2} + U(r) = \tilde{R} + \frac{\tilde{R}_2}{e^{ar} - 1} + \frac{\tilde{R}_3}{(e^{ar} - 1)^2},$$

(10)
with
\[ \tilde{P}_1 = P_1 + \gamma C_0 \ ; \ \tilde{P}_2 = P_2 + \gamma C_1 ; \]
\[ \tilde{P}_3 = P_3 + \gamma C_2 , \ \ \ \gamma = \frac{J(J + 1) \hbar^2}{2 \mu r^2} . \] (11)
and the values of the \( C_i \)'s are obtained in the following manner. Let \( y = \alpha (r - r_c) \) then with \( \alpha r = y + u \) and \( u = \alpha r_c \) one implies that
\[ \frac{r_c^2}{r^2} = \frac{1}{(y/u + 1)^2} \text{ and} \]
\[ \frac{r_c^2}{r^2} = C_0 + \frac{C_1}{e^{y/u} - 1} + \frac{C_2}{(e^{y/u} - 1)^2} . \] (12)
Retaining the first three terms of the Taylor's expansion near the equilibrium internuclear distance \( y \to 0 \) (i.e., \( r \to r_c \)) of both expressions in (12) and equating coefficients of same power of \( y \) one obtains
\[ C_0 = 1 - \left( \frac{1 - e^{-u}}{u} \right)^2 \left[ \frac{4u}{1 - e^{-u}} - (3 + u) \right] , \] (13)
\[ C_1 = 2 \left( e^u - 1 \right) \left( \frac{1 - e^{-u}}{u} \right)^2 \left[ \frac{(3 + u)(1 - e^{-u})}{u} - 1 \right] , \] (14)
\[ C_2 = \left( \frac{e^u - 1}{u} \right)^2 \left( 1 - e^{-u} \right)^2 \left[ (3 + u) - \frac{2u}{1 - e^{-u}} \right] . \] (15)
Which are in exact accord with those reported in equation (4) of [17].

Under such potential parametric settings, one would use the supersymmetric quantum recipe used by Jia et al [18] and follow, step-by-step, their procedure for our Schrödinger equation in (3), along with the effective potential in (10). Namely, one should set their equation in (3), along with the effective potential in (10), which, when substituted in (3) along with (10), would result in
\[ 2 \tilde{Q}_1 \tilde{Q}_2 - \alpha \tilde{Q}_2 = \frac{2\mu}{\hbar^2} \tilde{P}_3 \Rightarrow \tilde{Q}_2 = \frac{\alpha}{2} \left( 1 + \frac{1 + 8\mu}{\hbar^2 \alpha^2} \tilde{P}_3 \right) . \] (18)

2. \( \tilde{Q}_1 \tilde{Q}_2 - \alpha \tilde{Q}_2 = \frac{2\mu}{\hbar^2} \tilde{P}_3 \Rightarrow \tilde{Q}_1 \]
\[ = \frac{1}{2 \tilde{Q}_2} \left[ \frac{2\mu}{\hbar^2} (\tilde{P}_1 - \tilde{P}_3) + \tilde{Q}_2^2 \right] \] (19)

and
\[ \tilde{Q}_1^2 = \frac{2\mu}{\hbar^2} (\tilde{P}_1 - E_0) \Rightarrow E_0 \]
\[ = \tilde{P}_1 - \frac{\hbar^2}{2\mu} \left[ \frac{2\mu}{\hbar^2} (\tilde{P}_1 - \tilde{P}_3) + \tilde{Q}_2^2 \right] . \] (20)

Under such settings, the wave function is
\[ \psi (r) = N e^{\frac{\alpha}{4} r} \left( e^{\alpha r} - 1 \right) \tilde{Q}_1^{1/\alpha} \] (21)
and the corresponding eigenvalues are
\[ E_{e,J} = \tilde{P}_1 - \frac{\hbar^2 \alpha^2}{2\mu} \left( \frac{2\mu}{\hbar^2 \alpha^2} (\tilde{P}_1 - \tilde{P}_3) \right) \]
\[ = -1 - 2\nu - \sqrt{1 + \frac{8\mu}{\hbar^2 \alpha^2} \tilde{P}_3} \]
\[ - \frac{1 - 2\nu - \sqrt{1 + \frac{8\mu}{\hbar^2 \alpha^2} \tilde{P}_3}}{4} \] (22)
where
\[ \tilde{P}_1 - \tilde{P}_2 = D_e \left( e^{2\alpha r_c} - 1 \right) + \gamma (C_2 - C_1) \]
and
\[ \tilde{P}_3 = D_e \left( e^{2\alpha r_c} - 1 \right)^2 + \gamma C_2 \]
Hereby, it should be obvious to notice that this result, in (22), is in exact accord with that of Liu and coworkers [11, 12], in (5) and (6), for \( J = 0 \) and hence \( \gamma = 0 \) (i.e., only for the vibrational levels). This is also documented in tables 1–5.

3. Results and discussion

In connection with the central attractive/repulsive core \( J(J + 1)/2\mu r^2 \), we now subject the improved Greene–Aldrich approximation [16], in (4), and the Badawi et al [17] factorization recipe, in (7), to a quantitative brute force numerical test. Hereby, we use the \( O_2 \left( X^3 \Sigma_g^+ \right) \) diatomic spectroscopic molecular parameters \( D_e = 42041 \text{ cm}^{-1} \), \( \omega_e = 1580.2 \text{ cm}^{-1} \), and \( r_c = 1.207 \text{ Å} \) used by Roy [19] and report the results in table 1. In the same table, we show the energy shifts \( \Delta_{\text{Liu}} = E_{\text{Liu}} - E_{\text{Roy}} \) and \( \Delta_{\text{our}} = E_{\text{our}} - E_{\text{Roy}} \) for Liu et al [11] results, in (5), and for our results, in (22), compared with those of Roy’s [19] (GPS), respectively. It is obvious that while the ro–vibrational energies reported by Liu [11] dramatically shift from those of Roy [19] (i.e., \( \Delta_{\text{Liu}} \) grows from \( \sim 11 \text{ cm}^{-1} \) for \( (v, J) = (0, 0) \) to \( \sim 177 \text{ cm}^{-1} \) for
Table 1. Ro-vibrational energies $E_{\nu J}$ (in cm$^{-1}$ units) for $O_2(\Sigma^+ - \Sigma^-)$, where $\Delta_{\text{Liu}}$ and $\Delta_{\text{our}}$ denote the energy shifts for Liu et al [11] in Equation (5) and our results from Equation (22) compared with those of Roy’s [19] (GPS), respectively.

| $\nu$ | $J$ | [11] | Equation (22) | GPS [19] | $\Delta_{\text{Liu}}$ | $\Delta_{\text{our}}$ |
|-------|-----|------|---------------|-----------|----------------|----------------|
| 0     | 0   | 786.380 | 786.380 | 775.074 | 11.306 | 11.306 |
| 1     | 789.941 | 789.153 | 777.848 | 11.562 | 11.305 |
| 2     | 794.699 | 783.395 | 13.671 | 11.304 |
| 10    | 1213.661 | 1118.890 | 1107.634 | 106.027 | 11.256 |
| 15    | 1533.912 | 1367.943 | 1356.714 | 177.198 | 11.229 |
| 5     | 8412.365 | 8366.286 | 8261.257 | 151.108 | 105.029 |
| 10    | 9822.570 | 9388.844 | 927.562 | 54.695 |
| 15    | 1213.661 | 1118.890 | 1107.634 | 106.027 |
| 20    | 1533.912 | 1367.943 | 1356.714 | 177.198 |

Table 2. Ro-vibrational energies $E_{\nu J}$ (in cm$^{-1}$ units) for $^7\text{Li}_2(\Sigma^+ - \Sigma^-)$ with $\nu = 0, 1, 2,$ and 3. Our results from Equation (22) are compared with those of Liu et al [11] in Equation (5) and those of RKR [11] whenever possible.

| $\nu$ | $J$ | [11] | Equation (22) | RKR [11] | $\nu$ | [11] | Equation (22) | RKR [11] |
|-------|-----|------|---------------|----------|-------|------|---------------|----------|
| 0     | 0   | 31.7694 | 31.7694 | 31.857 | 2   | 0   | 142.3939 | 142.3939 |
| 1     | 32.4900 | 32.3035 | 144.4101 | 143.7867 |
| 2     | 33.9311 | 33.3714 | 144.4101 | 143.7867 |
| 3     | 36.0919 | 34.9720 | 146.2555 | 145.1782 |
| 4     | 38.9717 | 37.1038 | 149.1115 | 147.0311 |
| 5     | 42.5692 | 39.7651 | 152.4668 | 149.3436 |
| 10    | 71.2648 | 60.9108 | 179.2270 | 167.6973 |
| 15    | 117.5735 | 94.7215 | 223.5620 | 211.4519 |
| 0     | 90.3292 | 90.3292 | 90.453 | 3   | 0   | 188.0375 | 188.240 |
| 1     | 91.0254 | 90.8283 | 90.453 | 3   | 0   | 188.0375 | 188.240 |
| 2     | 92.4177 | 91.8260 | 93.3215 | 90.6159 |
| 3     | 94.5054 | 93.3215 | 93.3215 | 90.6159 |
| 4     | 97.2877 | 95.3132 | 95.3132 | 92.3315 |
| 5     | 100.7635 | 97.7991 | 102.4686 | 94.4724 |
| 10    | 128.4858 | 117.5415 | 223.5620 | 211.4519 |
| 15    | 173.2177 | 149.0671 | 265.1939 | 238.4792 |

Table 3. Ro-vibrational energies $E_{\nu J}$ (in cm$^{-1}$ units) for $^7\text{Li}_2(\Sigma^+ - \Sigma^-)$ with $\nu = 4, 5, 6,$ and 7. Our results from Equation (22) are compared with those of Liu et al [11] in Equation (5) and those of RKR [11] whenever possible.

| $\nu$ | $J$ | [11] | Equation (22) | RKR [11] | $\nu$ | [11] | Equation (22) | RKR [11] |
|-------|-----|------|---------------|----------|-------|------|---------------|----------|
| 4     | 0   | 227.332 | 227.332 | 227.679 | 6   | 0   | 287.160 | 287.665 |
| 1     | 227.9573 | 227.7287 | 287.160 | 287.4898 |
| 2     | 229.2066 | 228.5206 | 288.955 | 288.1480 |
| 3     | 231.0799 | 229.7072 | 290.6299 | 289.1341 |
| 4     | 233.5763 | 231.2870 | 292.9411 | 290.4465 |
| 5     | 236.6949 | 233.2580 | 295.8281 | 292.0833 |
| 10    | 261.5633 | 248.8779 | 318.8468 | 305.0266 |
| 20    | 301.6712 | 273.6914 | 355.9576 | 325.4829 |
| 5     | 0   | 260.350 | 260.350 | 260.837 | 7   | 0   | 307.832 | 308.098 |
| 1     | 260.9517 | 260.7128 | 308.377 | 308.1285 |
| 2     | 262.1544 | 261.4374 | 309.4988 | 308.7209 |
| 3     | 263.9578 | 262.5233 | 311.1647 | 309.6083 |
| 4     | 266.3611 | 263.9687 | 313.3849 | 310.7892 |
| 5     | 269.3633 | 265.7717 | 316.1581 | 312.2614 |
| 10    | 293.3016 | 280.0462 | 338.2671 | 323.8878 |
| 15    | 331.9027 | 302.6694 | 355.9576 | 325.4829 |
Table 4. Ro–vibrational energies $E_{ν,J}$ (in cm$^{-1}$ units) for $^7$Li$_2$($^3Σ_u^+$) with $ν = 8, 9$ and 10. Our results from Equation (22) are compared with those of Liu et al [11] in Equation (5) and those of RKR [11] whenever possible.

| $ν$ | $J$ | Equation (22) | RKR [11] |
|-----|-----|---------------|-----------|
| 8   | 0   | 322.432       | 322.432   |
|     | 1   | 322.9654      | 322.6962  |
|     | 2   | 324.0314      | 323.2236  |
|     | 3   | 325.6298      | 324.0134  |
|     | 4   | 327.7599      | 325.0640  |
|     | 5   | 330.4205      | 327.9394  |
|     | 6   | 333.6105      | 327.9394  |
|     | 7   | 337.3283      | 329.7585  |
|     | 8   | 341.5722      | 331.8272  |
| 9   | 0   | 331.027       | 331.027   |
|     | 1   | 331.5383      | 331.2592  |
|     | 2   | 332.5598      | 331.7222  |
|     | 3   | 334.0913      | 332.4154  |
|     | 4   | 336.1322      | 333.3373  |
| 10  | 0   | 333.683       | 333.683   |

($ν, J) = (0, 20)$ and from $\sim 151$ cm$^{-1}$ for $(ν, J) = (5, 10)$ to $\sim 289$ cm$^{-1}$ for $(ν, J) = (5, 20)$) as $J$ increases, our energies remain at an almost constant shift from Roy’s results (i.e., $Δ_{\text{out}} \sim 11$ cm$^{-1}$ for $(ν, J) = (0, 0)$ to $(ν, J) = (0, 20)$ and $Δ_{\text{out}} \sim 105$ cm$^{-1}$ for $(ν, J) = (5, 10)$ to $(ν, J) = (5, 20)$). This observation would in turn imply that the factorization recipe (7) of Badawi et al [17] is more stable and more adequate than that of Greene–Aldrich approximation [16] used by Liu et al [11]. Of course one should expect such energy shifts because of the different forms of the interaction potentials used. Roy [19] have used Tietz–Hua potential whereas the Deng–Fan [14] is used here and also used by Liu [11]. Nevertheless, the Deng–Fan potential is shown to be equivalent to the improved Manning–Rosen potential [12, 13].

We now safely proceed with our calculations for the ro–vibrational energies using the ‘reliable’ factorization recipe (7) of Badawi et al [17]. In tables 2, 3 and 4 we report the ro–vibrational energy levels for the $a^3Σ_u^+ –$Li$_2$ dimer. Here, we have used the $a^3Σ_u^+ –$Li$_2$ dimer spectroscopic molecular parameters $D_0 = 333.690$ cm$^{-1}$, $ω_ν = 65.130$ cm$^{-1}$, and $r_ν = 4.173$ Å as used by Liu et al [11]. In table 3, nevertheless, one observes that the energies are listed up to $J = 10$ for $ν = 7$. Limited similar numbers of the ro–vibrational energies are also observed in table 4. The binding energy is known to satisfy the condition

$$E_{\text{binding}} = E_{ν,J} - D_0 < 0.$$  \hspace{1cm} (23)

Therefore, when the energies $E_{ν,J}$ approach the dissociation energy $D_0 = 333.690$ cm$^{-1}$ they would in fact signal the very existence of a maximum possible rotational quantum number, $J_{\text{max}}$, associated with a corresponding vibrational quantum number, $ν$. That is, for each of the only available 11 vibrational states there is a maximum possible number of rotational levels for the $a^3Σ_u^+ –$Li$_2$ molecular dimer.

In table 5, we report the feasible ‘maximum-possible’ ro–vibrational energy levels. For example, we observe that for $ν = 0$ the ‘maximum-possible’ ro–vibrational energy level is $J_{\text{max}} = 34$, for $ν = 1$ is $J_{\text{max}} = 32$, for $ν = 2$ is $J_{\text{max}} = 29$, for $ν = 3$ is $J_{\text{max}} = 26$, and so on. $J_{\text{max}}$ gradually decreases as $ν$ grows up to the 11th vibrational state where only one rotational level is obtained at $J_{\text{max}} = 1$. Of course, in judging on the ‘maximum-possible’ ro–vibrational energy level we have taken into account the stability patterns of our energy shifts discussed above for the $O_2(X^2Σ_u^+)$ diatomic molecule (in table 1) and projected such stability patterns for the $a^3Σ_u^+ –$Li$_2$ dimer (by comparing our results for $ν = 0$ with the RKR (Rydberg–Klein–Rees) ones reported in [11]). We may very clearly observe that the improved Greene–Aldrich approximation [16], in (4), used by Liu et al [11] ceases to satisfy condition (23) at lower values of the rotational quantum number $J$ (documented in tables 3, 4 and 5). Indeed, the the Deng–Fan [14] potential (2) (used here) may not be the best interaction potential to describe the $a^3Σ_u^+ –$Li$_2$ molecular dimer. It had, nevertheless, shown intuitive consistency with the common sense contemplation on that each of the only available 11 vibrational states may, very well, accommodate a limited number of rotational states.

4. Concluding remarks

In this study, we have considered the Deng–Fan [14] potential (2) and discussed the reliability of two available approximations for the central attractive/repulsive core $J(J + 1)/2μr^2$ (i.e., the improved Greene–Aldrich approximation [16], in (4), and the Badawi et al [17] factorization recipe, in (7)). We have studied and analyzed the numerical outcomes of both approximations for $J > 0$ using the $O_2(X^2Σ_u^+)$ diatomic molecule and compared the results with those of Roy [19]. As long as the rotational quantum number $J > 0$ (especially for $J \gg 0$) is in point, such a comparison suggested that the factorization recipe (7) of Badawi et al [17] is more reliable than that of Greene–Aldrich approximation [16] used by Liu et al [11]. The stability and reliability of which is documented in the almost constant energy shifts $Δ_{\text{out}}$ (obtained and listed in table 1). That is, $Δ_{\text{out}} \sim 11$ cm$^{-1}$ for $(ν, J) = (0, 0)$–$(ν, J) = (0, 20)$ and $Δ_{\text{out}} \sim 105$ cm$^{-1}$ for $(ν, J) = (5, 10)$–$(ν, J) = (5, 20)$, whereas $Δ_{\text{in}}$ grows up from $\sim 11$ cm$^{-1}$ for $(ν, J) = (0, 0)$ to $\sim 177$ cm$^{-1}$ for $(ν, J) = (0, 20)$ and from $\sim 151$ cm$^{-1}$ for $(ν, J) = (5, 10)$ to $\sim 289$ cm$^{-1}$ for $(ν, J) = (5, 20)$.

On the other hand, we have used the same potential to study the ro–vibrational energies for the $a^3Σ_u^+ –$Li$_2$ molecular dimer. We have shown that only a limited number of the rotational levels is supported by the $a^3Σ_u^+ –$Li$_2$ dimer. That is, the $ν = 0$ vibrational state accommodates only 34 rotational levels, $ν = 1$ accommodates 32, $ν = 2$ accommodates 29, $ν = 3$ accommodates 26, $ν = 4$ accommodates 23, $ν = 5$ accommodates 20, $ν = 6$ accommodates 16, $ν = 7$...
accommodates 11, $\nu = 8$ accommodates 9, $\nu = 9$ accommodates 5, and $\nu = 10$ accommodates only one rotational level. To the best of our knowledge, this has never been reported elsewhere.

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### Table 5.

| $\nu$ | $J$   | Equation (22) | $\nu$ | $J$   | Equation (22) |
|------|------|---------------|------|------|---------------|
| 0    | 20   | 181.0396      | 4    | 20   | 356.5889      |
| 25   | 261.0387 | 196.7792       | 23   | 396.4097 | 330.3157     |
| 30   | 356.7841 | 262.3569       | 5    | 20   | 384.7428      |
| 34   | 444.0906 | 320.1449       | 6    | 16   | 365.0368      |
| 1    | 20   | 234.5100      | 7    | 11   | 344.3232      |
| 25   | 311.7476 | 243.8808       | 8    | 9    | 346.3401      |
| 30   | 404.1552 | 304.4789       | 9    | 5    | 338.6815      |
| 34   | 445.1631 | 330.6137       | 10   | 1    | 334.1715      |
| 2    | 20   | 281.5434      | 2    | 20   | 284.6083      |
| 25   | 356.0508 | 328.6431       |
| 29   | 426.2105 |              |
| 3    | 20   | 322.2125      | 3    | 20   | 324.7310      |
| 25   | 394.0204 | 319.0345       |
| 26   | 410.0931 | 328.7317       |

Table 5. Ro-vibrational energies $E_{\nu J}$ (in cm$^{-1}$ units) for $^7$Li$_2(a^3\Sigma_u^+)$.

Our results from equation (22) are compared with those of Liu et al [11] in equation (5). For each value of $\nu$ we show the ‘maximum-possible’ rotational quantum number $J$ (i.e., $J_{\text{max}}$ is the last value of $J$ for each $\nu$).