



# Calculation of the interaction potential energy curve and vibrational levels for the $a^3\Sigma_u^+$ state of ${}^7\text{Li}_2$ molecule



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## ABSTRACT

We solve the Schrödinger equation with the improved expression of the Manning–Rosen empirical potential energy model. The rotation-vibrational energy spectra and the unnormalized radial wave functions have been obtained. The interaction potential energy curve for the  $a^3\Sigma_u^+$  state of  ${}^7\text{Li}_2$  molecule is modeled by employing Manning–Rosen potential model. Favorable agreement for the Manning–Rosen potential is found in comparing with *ab initio* data. The vibrational energy levels predicted by using the Manning–Rosen potential for the  $a^3\Sigma_u^+$  state of  ${}^7\text{Li}_2$  are in good agreement with the RKR data and *ab initio* determinations.

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## 1. Introduction

In 1933, Manning and Rosen [1] proposed a potential function for diatomic molecules,

$$U_{\text{MR}}(r) = \frac{h^2}{8\mu\pi^2b^2} \left[ \frac{\beta(\beta-1)e^{-2r/b}}{(1-e^{-r/b})^2} - \frac{Ae^{-r/b}}{1-e^{-r/b}} \right], \quad (1)$$

in which  $\beta$  and  $A$  are two dimensionless parameters, parameter  $b$  governs the range of the interaction. Conventionally, the range decreases as  $b$  increases. The Manning–Rosen potential can be used to describe the diatomic molecular vibrations [1]. Dong and García-Ravelo [2] investigated the bound state solutions of the  $s$ -wave Schrödinger equation with Manning–Rosen potential in terms of the function analysis method. By using the conventional Greene–Aldrich approximation scheme [3] to deal with the centrifugal term, some authors obtained the bound state solutions and scattering state solutions of the Schrödinger equation with the Manning–Rosen potential in terms of the conventional function analysis method [4,5], Nikiforov–Uvarov method [6], exact quantization rule approach [7], and tridiagonalization program [8]. By employing the Pekeris-like approximation scheme [9–11] to deal

with the centrifugal term, Qiang and Dong [12], and Ikhdaïr [13] investigated the bound state solutions of the Schrödinger equation for the Manning–Rosen potential. By applying the Pekeris-type approximation to the centrifugal term and pseudo-centrifugal term, Wei and Dong [14,15] investigated the bound state solutions of the Dirac equation with the Manning–Rosen potential under the conditions of the spin symmetry and pseudospin symmetry. By using the improved Greene–Aldrich approximation scheme [16] to deal with the centrifugal term, Chen et al. [17] studied the bound state solutions of the Schrödinger equation with the Manning–Rosen potential. Using the  $J$ -matrix approach [18], Nasser et al. [19] investigated the bound state energies for the Manning–Rosen potential energy model. As far as we known, the authors in these works did not reported quantitative tests on real intermolecular potentials and actual vibrational energies of diatomic molecules. Therefore, it is of considerable interest to assess the ability of the Manning–Rosen potential model in fitting actual interaction potentials of diatomic molecules and predicting the vibrational levels.

In recent years, some empirical potential energy functions [20–26] for diatomic molecules have been improved in terms of the dissociation energy and the equilibrium bond length for a diatomic molecule as explicit parameters [27–31]. These empirical potential models include the Rosen–Morse potential [20], Manning–Rosen potential [21], Frost–Musulin potential [22], Tietz potential [23], Schiöberg potential [24], generalized Woods–Saxon potential [25],

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and deformed modified Rosen–Morse potential [26]. The Manning–Rosen potential function given in expression (1) can be expressed in an improved form [27]

$$U_{MR}(r) = D_e \left( 1 - \frac{e^{\alpha r_e} - 1}{e^{\alpha r} - 1} \right)^2, \quad (2)$$

where  $\alpha = 1/b$ ,  $D_e$  is the dissociation energy, and  $r_e$  is the equilibrium bond length. In generating expression (2), we have added one term  $D_e$  to the original Manning–Rosen potential energy function given in expression (1). This change only yields an energy of zero at the potential minimum, i.e.  $U_{MR}(r_e) = 0$ , and does not affect the physical properties of the original potential function. The improved forms of some empirical potential energy functions are more convenient for their applications.

Most recently, one of the present authors and collaborators [32] investigated the bound state solutions of the Klein–Gordon equation with the improved expression of the Manning–Rosen empirical potential energy model, and studied the relativistic vibrational transition frequencies for the  $a^3\Sigma_u^+$  state of  ${}^7\text{Li}_2$  molecule. The lithium dimer,  ${}^7\text{Li}_2$ , has received a great deal of attention, following the discovery by Bradley and co-workers [33] of Bose–Einstein condensation for this system. The stability of the  ${}^7\text{Li}_2$  Bose–Einstein condensation is sensitive to the binding energy of the least bound vibrational level [34]. For the  $a^3\Sigma_u^+$  state of  ${}^7\text{Li}_2$ , many works have been done on the vibrational levels and the interaction potential in terms of the Rydberg–Klein–Rees (RKR) method [35] and ab initio approach [36,37]. In this Letter, we investigate the bound state solutions of the Schrödinger equation with the improved expression of the Manning–Rosen potential energy model. We also compute the vibrational energy spectra for the  $a^3\Sigma_u^+$  state of  ${}^7\text{Li}_2$  molecule and compared the calculated values with the RKR data and *ab initio* data.

## 2. Rotation-vibrational energy spectrum

In the presence of a spherical symmetric potential model  $U(r)$ , the time-independent Schrödinger equation reads

$$\left[ -\frac{\hbar^2}{2\mu} \nabla^2 + U(r) \right] \Psi(r, \theta, \varphi) = E \Psi(r, \theta, \varphi), \quad (3)$$

where  $r$  is the internuclear separation,  $\mu$  is the reduced mass of a diatomic molecule, and  $\hbar$  denotes the Planck constant. Expressing the wave function as  $\Psi(r, \theta, \varphi) = \frac{u(r)}{r} Y_{Jm}(\theta, \varphi)$  and substituting expression (2) into Eq. (3), where  $Y_{Jm}(\theta, \varphi)$  is the spherical harmonic function, we obtain the following differential equation describing the radial motion of a diatomic molecule by separating the angular and radial variables in the Schrödinger equation (3),

$$-\frac{\hbar^2}{2\mu} \frac{d^2 u_{vJ}(r)}{dr^2} + \left[ D_e \left( 1 - \frac{e^{\alpha r_e} - 1}{e^{\alpha r} - 1} \right)^2 + \frac{J(J+1)\hbar^2}{2\mu r^2} \right] u_{vJ}(r) = E_{vJ} u_{vJ}(r), \quad (4)$$

where  $E_{vJ}$  denotes the rotation-vibrational energy of the diatomic molecule system,  $v$  and  $J$  are the vibrational and rotational quantum numbers, respectively. Eq. (4) can be solved exactly only for the case of  $J = 0$ . We employ the improved Greene–Aldrich approximation scheme to deal with the centrifugal term [16],

$$\frac{1}{r^2} \approx \alpha^2 \left( \frac{1}{12} + \frac{e^{\alpha r}}{(e^{\alpha r} - 1)^2} \right). \quad (5)$$

This improved Greene–Aldrich approximation scheme has been widely used to deal with the centrifugal term and pseudo-centrifugal term [38–40]. Substituting expression (5) into Eq. (4) leads us to obtain the following equation

$$\begin{aligned} & -\frac{d^2 u_{vJ}(r)}{dr^2} + \left( \frac{2\mu D_e (e^{\alpha r_e} - 1)^2 + J(J+1)\alpha^2}{(e^{\alpha r} - 1)^2} e^{\alpha r} \right. \\ & \quad \left. - \frac{2\mu D_e (e^{2\alpha r_e} - 1)}{\hbar^2} \frac{1}{e^{\alpha r} - 1} \right) u_{vJ}(r) \\ & = \frac{1}{\hbar^2} \left( 2\mu E_{vJ} - \frac{1}{12} J(J+1)\hbar^2 \alpha^2 - 2\mu D_e \right) u_{vJ}(r). \end{aligned} \quad (6)$$

Defining a new variable of the form  $z = e^{-\alpha r}$  and substituting it into Eq. (6), we can generate the following second-order differential equation

$$\begin{aligned} & z^2 \frac{d^2 u_{vJ}(z)}{dz^2} + z \frac{du_{vJ}(z)}{dz} \\ & + \left[ -\varepsilon^2 - \frac{\beta z}{(1-z)^2} + \frac{\gamma}{1-z} + \frac{\gamma z}{1-z} \right] u_{vJ}(z) = 0, \end{aligned} \quad (7)$$

where the parameters  $\varepsilon$ ,  $\beta$  and  $\gamma$  are defined as follows:

$$\begin{aligned} \varepsilon &= \left[ \frac{1}{\hbar^2 \alpha^2} \left( 2\mu D_e + \frac{1}{12} J(J+1)\hbar^2 \alpha^2 - 2\mu E_{vJ} \right) \right. \\ & \quad \left. + \frac{\mu D_e}{\hbar^2 \alpha^2} (e^{2\alpha r_e} - 1) \right]^{\frac{1}{2}}, \end{aligned} \quad (8)$$

$$\beta = \frac{2\mu D_e}{\hbar^2 \alpha^2} (e^{\alpha r_e} - 1)^2 + J(J+1), \quad (9)$$

$$\gamma = \frac{\mu D_e}{\hbar^2 \alpha^2} (e^{2\alpha r_e} - 1). \quad (10)$$

We analyze the asymptotic solutions of Eq. (7). When  $r \rightarrow 0$  ( $z \rightarrow 1$ ), we obtain a solution  $u_{vJ}(z) = (1-z)^\delta$  for Eq. (7), where the parameter  $\delta$  is given by

$$\delta = \frac{1}{2} \left( 1 + \sqrt{(1+2J)^2 + \frac{8\mu D_e (e^{\alpha r_e} - 1)^2}{\hbar^2 \alpha^2}} \right). \quad (11)$$

When  $r \rightarrow \infty$  ( $z \rightarrow 0$ ), solving Eq. (7) yields an asymptotic solution of  $u_{vJ}(z) = z^\eta$ , where

$$\eta = \sqrt{\varepsilon^2 - \gamma}. \quad (12)$$

Taking the asymptotic solutions of Eq. (7) into account, we write the function  $u_{vJ}(z)$  as  $u_{vJ}(z) = (1-z)^\delta z^\eta f(z)$ . Substitute this expression into Eq. (7), we obtain the following equation

$$\begin{aligned} & (1-z)z \frac{d^2 f(z)}{dz^2} + [1+2\eta - (1+2\delta+2\eta)z] \frac{du_{vJ}(z)}{dz} \\ & - (\delta^2 + 2\delta\eta - 2\gamma) u_{vJ}(z) = 0. \end{aligned} \quad (13)$$

This equation is just a hypergeometric equation, and its solution is the hypergeometric function

$$\begin{aligned} f(z) &= {}_2F_1(a, b; 1+2\eta; z) \\ &= \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{k=0}^{\infty} \frac{\Gamma(a+k)\Gamma(b+k)}{\Gamma(c+k)} \frac{z^k}{k!}, \end{aligned} \quad (14)$$

where the parameters  $a$  and  $b$  are given by

$$a = \delta + \eta - \sqrt{\varepsilon^2 + \gamma}, \quad (15)$$

$$b = \delta + \eta + \sqrt{\varepsilon^2 + \gamma}. \quad (16)$$

When either  $a$  or  $b$  equals to a negative integer  $-v$ , the hypergeometric function  $f(z)$  turns to a polynomial of degree  $v$ . This tells us that the hypergeometric function  $f(z)$  approaches finite in the following quantum condition

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