

Exact solution of Schrödinger equation for Pseudoharmonic potential

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Exact solution of Schrödinger equation for the pseudoharmonic potential is obtained for an arbitrary angular momentum. The energy eigenvalues and corresponding eigenfunctions are calculated by Nikiforov–Uvarov method. Wavefunctions are expressed in terms of Jacobi polynomials. The energy eigenvalues are calculated numerically for some values of ℓ and n with $n \leq 5$ for some diatomic molecules.

KEY WORDS: Schrödinger equation, pseudoharmonic potential, diatomic molecules, Nikiforov–Uvarov method

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1. Introduction

The study of anharmonic oscillators in three dimensions has much attention in chemical physics phenomena [1–45]. They have wide applications in molecular physics [1]. The solutions of Schrödinger equation for any ℓ -state for such potentials have also a special interest. The Morse potential is commonly used for an anharmonic oscillator. However, its wavefunction does not vanish at the origin, but the Mie type and the pseudoharmonic potentials do. The Mie type potential

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has the general features of the true interaction energy [1], interatomic and intermolecular and dynamical properties of solids [2]. The pseudoharmonic potential may be used for the energy spectrum of linear and non-linear systems [3]. The Mie type and pseudoharmonic are two exactly solvable potentials other than the Coulombic and harmonic oscillator. This potential may be considered as an intermediate potential between the harmonic oscillator potential and anharmonic potentials, as the Morse oscillator (MO) potential, which is a more realistic potential, in good agreement with the experimental spectroscopical data [47]. A comparative analysis of potentials HO-3D (3-dimensional harmonic oscillator potential) and PHO is performed in Ref. [2].

To solve the Schrödinger equation for the pseudoharmonic potential, the Nikiforov–Uvarov method [46] which is introduced for the solution of the hypergeometric type second order differential equations appeared in the time-independent problems. The method is based on the determination of the solution in terms of special orthogonal functions for any general second-order differential equations [47].

By taking an appropriate $s = s(r)$ coordinate transformation, the Schrödinger equation in spherical coordinates is reduced to a generalized equation of hypergeometric type as

$$\Psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\Psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\Psi(s) = 0, \quad (1)$$

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

The contents of this work is as follows. In section 2, solution of Schrödinger equation for any ℓ -state is introduced. Solutions for Mie-type and pseudoharmonic potential is given. As an example, some numerical values of the energy levels of N_2 , CO , NO , and NH molecules are computed. Section 3 is devoted for the conclusions.

2. Method and solutions

The pseudoharmonic potential has the form Ref. [3]

$$V(r) = V_0 \left(\frac{r}{r_0} - \frac{r_0}{r} \right)^2, \quad (2)$$

where V_0 is the dissociation energy and r_0 is the equilibrium intermolecular separation. The radial part of the Schrödinger equation for a diatomic molecule potential is

$$\left(-\frac{\hbar^2}{2\mu} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + V(r) \right) R_{n\ell}(r) = E_{n\ell} R_{n\ell}(r), \quad (3)$$

where μ is the reduced mass of the diatomic molecules. n denotes the radial quantum number (n and ℓ are named as the vibration-rotation quantum numbers in molecular chemistry), r is the internuclear separation. Substituting the explicit form of $V(r)$, we get

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2}{r} \frac{dR_{n\ell}(r)}{dr} + \frac{2\mu}{\hbar^2} \left(E_{n\ell} - V_0 \left(\frac{r}{r_0} - \frac{r_0}{r} \right)^2 - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right) R_{n\ell}(r) = 0. \quad (4)$$

By defining a coordinate transformation

$$r^2 = s, \quad (5)$$

and the following dimensionless parameters

$$\alpha^2 = \frac{V_0}{r_0^2} \frac{\mu}{2\hbar^2} \quad (6)$$

$$\varepsilon = (E_{n\ell} + 2V_0) \frac{\mu}{2\hbar^2} \quad (7)$$

$$\beta = \left(V_0 r_0^2 + \frac{\ell(\ell+1)\hbar^2}{2\mu} \right) \frac{\mu}{2\hbar^2}, \quad (8)$$

we obtain

$$\frac{d^2 R}{ds^2} + \frac{3/2}{s} \frac{dR}{ds} + \frac{1}{s^2} \left(-\alpha^2 s^2 + \varepsilon s - \beta \right) R(s) = 0. \quad (9)$$

Thus, comparing the equations (1) and (8), we obtain the following polynomials

$$\tilde{\tau}(s) = \frac{3}{2}, \quad \sigma(s) = s, \quad \text{and} \quad \tilde{\sigma}(s) = -\alpha^2 s^2 + \varepsilon s - \beta. \quad (10)$$

To find a particular solution of equation (9), we define the radial wave function as $R_{n\ell}(s) = \phi(s)y(s)$, Schrödinger equation, equation (1) is reduced to an equation of hypergeometric type

$$\sigma(s)y'' + \tau(s)y' + \lambda y = 0, \quad (11)$$

where $\phi(s)$ is a solution of $\phi'(s) \neq \phi(s) = \pi(s)/\sigma(s)$ and $y(s)$ is a hypergeometric type function whose polynomial solutions are given by the well-known Rodrigues relation [46]

$$y(s) = y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s)\rho(s)]. \quad (12)$$

Here, $\sigma(s)$ is a polynomial of degree at most one, $\rho(s)$ is a weight function and B_n is a normalization constant. It satisfies the condition

$$(\sigma\rho)' = \tau\rho. \tag{13}$$

The function π and parameter λ are defined as

$$\pi = \left(\frac{\sigma' - \tilde{\tau}}{2}\right) \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma}, \tag{14}$$

and

$$\lambda = k + \pi'. \tag{15}$$

Here $\pi(s)$ is a polynomial with the parameter s . Determination of k is the essential point in the calculation of $\pi(s)$. k is determined by setting the square root as the square of a polynomial. Thus a new eigenvalue equation for the Schrödinger equation becomes

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma''; \quad n = 0, 1, 2, \dots, \tag{16}$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s), \tag{17}$$

and it will have a negative derivative. Therefore, the polynomial of $\pi(s)$ is found in four positive values

$$\begin{aligned} \pi(s) &= -\frac{1}{4} \pm \left(\alpha s + \sqrt{\beta + \frac{1}{16}}\right), \quad k_+ = \varepsilon + \gamma \\ &= -\frac{1}{4} \pm \left(\alpha s - \sqrt{\beta + \frac{1}{16}}\right), \quad k_- = \varepsilon - \gamma, \end{aligned} \tag{18}$$

where $\gamma = 2\alpha\sqrt{\beta + \frac{1}{16}}$. By following equation (17), we get

$$\tau(s) = \frac{3}{2} + 2 \begin{cases} -\frac{1}{4} \pm \left(\alpha s + \sqrt{\beta + \frac{1}{16}}\right), & \text{for } k_+ = \varepsilon + \gamma \\ -\frac{1}{4} \pm \left(\alpha s - \sqrt{\beta + \frac{1}{16}}\right), & \text{for } k_- = \varepsilon - \gamma. \end{cases} \tag{19}$$

To have a negative derivative of $\tau(s)$ and a physical eigenfunction, we take the following substitution: for $k_- = \varepsilon - \gamma$, we have

$$\pi(s) = -\frac{1}{4} - \left(\alpha s - \sqrt{\beta + \frac{1}{16}}\right), \tag{20}$$

and

$$\tau(s) = 1 - 2 \left(\alpha s - \sqrt{\beta + \frac{1}{16}} \right). \quad (21)$$

Thus, using equation (16) we obtain

$$\lambda = \lambda_n = 2n\alpha, \quad (22)$$

and using equations (22) and (15) we obtain the following energy eigenvalues,

$$\varepsilon = \left(2n + 1 + 2\sqrt{\beta + \frac{1}{16}} \right) \alpha. \quad (23)$$

Substituting equation (23) into equation (7), the energy eigenvalue becomes

$$E_{n\ell} = -2V_0 + \frac{\hbar}{r_0} \sqrt{\frac{2V_0}{\mu}} \left[(2n + 1) + 2\sqrt{\frac{\mu}{2\hbar^2} \left(V_0 r_0^2 + \frac{\ell(\ell + 1)\hbar^2}{2\mu} \right) + \frac{1}{16}} \right]. \quad (24)$$

In order to calculate the wave function, the weight function ρ can be obtained by using equation (13) as

$$\rho(s) = s^{2\sqrt{\beta + \frac{1}{16}}} e^{-2\alpha s}, \quad (25)$$

and using equation (12) which is Rodrigues relation, we can get the function y ,

$$y_n(s) = s^{1+2\sqrt{\beta + \frac{1}{16}}} e^{-2\alpha s}. \quad (26)$$

Finally the wave function is obtained as

$$R_{n\ell} = s^{-\frac{1}{4} + \sqrt{\beta + \frac{1}{16}}} e^{-\alpha s} L_n^{2\sqrt{\beta + \frac{1}{16}}}(2\alpha s). \quad (27)$$

3. Conclusions

We have studied analytical solution of Schrödinger equation for a pseudo-harmonic potential. Energy eigenvalues and the corresponding wave functions are calculated for a diatomic system with any angular momentum ℓ . The NU method is used in the computations. Numerical values of energy for N_2 , CO , NO , and NH molecules are calculated for different values of principal and angular quantum numbers n and ℓ . Results are listed in Table 1. The potential parameters are obtained from Ref. [10].

Table 1
Energy eigenvalues (in eV) of pseudoharmonic potential for N_2 , CO, NO, and CH diatomic molecules with different values of n and ℓ . Necessary parameters are given in Ref. [8].

n	ℓ	N_2	CO	NO	CH
0	0	0.10915590	0.10193061	0.08248827	0.16863440
1	0	0.32734304	0.30567217	0.24735916	0.50500718
	1	0.32784167	0.30615078	0.24778171	0.50859034
2	0	0.54553018	0.50941373	0.41223005	0.84137996
	1	0.54602881	0.50989234	0.41265260	0.84496312
	2	0.54702603	0.51084953	0.41349768	0.85212458
4	0	0.98190446	0.91689685	0.74197183	1.51412550
	1	0.98240309	0.91737546	0.74239438	1.51770870
	2	0.98340031	0.91833265	0.74323946	1.52487010
	3	0.98489606	0.91976835	0.74450700	1.53560020
	4	0.98689026	0.92168247	0.74619689	1.54988430
5	0	1.20009160	1.12063840	0.90684272	1.85049830
	1	1.20059020	1.12111700	0.90726527	1.85408150
	2	1.20158750	1.12207420	0.90811035	1.86124290
	3	1.20308320	1.12350990	0.90937789	1.87197290
	4	1.20507740	1.12542400	0.91106778	1.88625710
	5	1.20756990	1.12781650	0.91317990	1.90407610

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