Exact solutions for vibrational levels of the Morse potential via the asymptotic iteration method

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Abstract

Exact solutions for vibrational levels of diatomic molecules via the Morse potential are obtained by means of the asymptotic iteration method. It is shown that, the numerical results for the energy eigenvalues of $^7Li_2$ are all in excellent agreement with the ones obtained before. Without any loss of generality, other states and molecules could be treated in a similar way.

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1 Introduction

Since the appearance of the Schrödinger equation in quantum mechanics, there have been continual researches for studying Schrödinger equation with an exactly solvable potentials by using different methods. The range of potentials for which Schrödinger equation can be solved exactly has been extended considerably owing to the investigations inspired, for example, by super-symmetric quantum mechanics [1], shape invariance [2], the factorization method [3-8], and recently the asymptotic iteration method (AIM) [9].

In recent years much attention has been focused on AIM. This method reproduces exact solutions to many differential equations which are important in applications to many problems in physics, such as the equations of Hermite, Laguerre, Legendre, and Bessel [9]. The AIM also gives a complete exact solutions of Schrödinger equation for Pösch-Teller potential, the harmonic oscillator potential, the complex cubic, quartic [10], and sextic anharmonic oscillator potentials [11, 12]. Very recently we applied the AIM and found the exact eigenvalues for the angular spheroidal wave equation [13, 14].

Encouraged by its satisfactory performance through comparisons with the other methods, we feel tempted to extend AIM to solve exactly the one-dimensional Schrödinger equation with the Morse potential [15]. This potential has played an important role in many different fields of physics such as molecular physics, solid state physics, and chemical physics, etc. This potential has been studied by many different approaches such as the standard confluent hypergeometric functions [16], the algebraic method [17], the supersymmetric method [18], the coherent states [19], the controllability [20], the series solutions with the mass distribution [21], laplace
transforms [22], etc.

Fortunately, the one-dimensional Schrödinger equation with the Morse potential can be reduced to a second-order homogenous linear differential equation, and we therefore directly can make use of AIM to formulate an elegant algebraic approach to yield a fairly simple analytic formula which gives rapidly the exact energy eigenvalues with high accuracy. Most importantly, the numerical computation of the Morse potential energy eigenvalues using this method is quite simple, fast, and the energy eigenvalues were satisfying a simple ordering relation. Therefore, one can unambiguously select the correct starting energy eigenvalue. Moreover, this work shows that, the AIM can be a simple alternative approach for computing the vibrational levels of the Morse potential.

In this spirit, this paper is organized as follows. In Sec. 2 the asymptotic iteration method for Schrödinger equation with the Morse potential is outlined. The analytical expressions for asymptotic iteration method are cast in such a way that allows the reader to use them without proceeding into their derivation. In Sec. 3 we present our numerical results compared with other works, and then we conclude and remark therein.

2 Formalism of the asymptotic iteration method for Schrödinger equation with the Morse potential

As an empirical potential, the Morse potential has been one of the most useful and convenient model, which gives an excellent qualitative description of the interaction between two atoms in a diatomic molecule. As we know the rotational energy of a molecule is much smaller than that of its vibrational energy, and therefore, in a pure Morse potential model the rotational energy of a molecule has been omitted.
Hence, the Schrödinger equation for Morse potential with angular momentum $\ell = 0$ is

$$
-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + V(x) \right] \Psi_n(x) = E_n \Psi_n(x),
$$

where $E_n$ are the energy eigenvalues, and $V(x)$ is the Morse potential function

$$
V(x) = D_e \left( e^{-2\beta(x-x_e)} - 2e^{-\beta(x-x_e)} \right).
$$

Equation (1) is called one-dimensional Schrödinger equation, if $x$ is defined on the whole line ($-\infty < x < +\infty$), and the eigenfunctions are normalized $\int_{-\infty}^{+\infty} |\Psi_n(x)|^2 dx = 1$. However, for real diatomic molecules $x$ should ranges from 0 to $\infty$.

$D_e$ is the dissociation energy, $x_e$ is the equilibrium internuclear distance of a diatomic molecules, $\mu$ is the reduced mass, and $\beta$ is an adjustable parameter. Morse potential has a minimum value at $x = x_e$, and it is zero at $x = \infty$. At $x = 0$, $V(0)$ has a finite value of $D_e(e^{2\beta x_e} - 2e^{\beta x_e})$ that is positive when $\beta x_e > ln2$.

Starting with Morse’s substitution $u = e^{-\beta(x-x_e)}$, we rewrite equation (1) in the form

$$
-\frac{d^2\Psi_n(u)}{du^2} - \frac{1}{u} \frac{d\Psi_n(u)}{du} + \frac{8\mu D_e}{\beta^2 \hbar^2} [u^2 - 2] \Psi_n(u) = \frac{8\mu E_n}{\beta^2 \hbar^2} u^2 \Psi_n(u).
$$

Furthermore, we remove the first derivative by proposing the ansatz

$$
\Psi_n(u) = \Phi_n(u) \exp(-p(r)/2); \quad p(r) = \frac{1}{u},
$$

Which in turn implies

$$
-\frac{d^2\Phi_n(u)}{du^2} + \frac{\epsilon_n(\epsilon_n + 1)}{u^2} \Phi_n(u) + \gamma^2 u^2 \Phi_n(u) = 2\gamma^2 \Phi_n(u),
$$

where

$$
\epsilon_n(\epsilon_n + 1) = -\frac{1}{4} - \frac{8\mu E_n}{\beta^2 \hbar^2}, \quad \gamma^2 = \frac{8\mu D_e}{\beta^2 \hbar^2}.
$$
If we further introduce the frequency

$$\omega_0 = \beta \sqrt{2D_e/\mu}$$  \hspace{1cm} (7)

of classical small vibrations about the equilibrium position $x = x_e$, and express the energy parameters in unit $\hbar \omega_0$; that is,

$$D_e = \Delta \hbar \omega_0; \quad E_n = \varepsilon_n \hbar \omega_0; \quad \varepsilon_n = -\frac{(\epsilon_n + \frac{1}{2})^2}{16\Delta^2},$$  \hspace{1cm} (8)

it is now more convenient to write the eigenvalue problem in the re-scaled form

$$-\frac{d^2\Phi_n(u)}{du^2} + \frac{\epsilon_n(\epsilon_n + 1)}{u^2}\Phi_n(u) + 16\Delta^2 u^2 \Phi_n(u) = 32\Delta^2 \Phi_n(u).$$  \hspace{1cm} (9)

In order to guarantee the asymptotic behaviour of this eigenvalue problem when $u \to \infty$, and $u \to 0$ we found that this asymptotic behaviour suggests that $\Phi_n(u)$ should look like

$$\Phi_n(u) = u^{(\epsilon_n+1)}e^{-2\Delta u^2}f_n(u).$$  \hspace{1cm} (10)

This implies that the function $f_n(u)$ will satisfy a second-order homogenous linear differential equation of the form

$$\frac{d^2f_n(u)}{du^2} - (8\Delta u - 2\epsilon_n + 2)\frac{df_n(u)}{du} - (12\Delta + 8\Delta \epsilon_n - 32\Delta^2)f_n(u) = 0.$$  \hspace{1cm} (11)

The systematic procedure of the asymptotic iteration method begins now by rewriting equation (11) in the following form

$$f_n''(u) = \lambda_0(u)f_n'(u) + s_0(u)f_n(u),$$  \hspace{1cm} (12)

where

$$\lambda_0(u) = (8\Delta u - 2\epsilon_n + 2), \quad \text{and} \quad s_0(u) = (12\Delta + 8\Delta \epsilon_n - 32\Delta^2).$$  \hspace{1cm} (13)
The primes of $f_n(u)$ in equation (12) denote derivatives with respect to $u$.

Now, in order to find a general solution to this equation we rely on the symmetric structure of the right hand side of equation (12). Thus, if we differentiate equation (12) with respect to $u$, we obtain

$$f'''_n(u) = \lambda_1(u)f'_n(u) + s_1(u)f_n(u),$$

(14)

where

$$\lambda_1(u) = \lambda'_0(u) + s_0(u) + \lambda^2_0(u), \quad \text{and} \quad s_1(u) = s'_0(u) + s_0(u)\lambda_0(u).$$

Likewise, the calculations of the second derivative of equation (14) yield

$$f''''_n(u) = \lambda_2(u)f'_n(u) + s_2(u)f_n(u),$$

(15)

where

$$\lambda_2(u) = \lambda'_1(u) + s_1(u) + \lambda_0(u)\lambda_1(u), \quad \text{and} \quad s_2(u) = s'_1(u) + s_0(u)\lambda_1(u).$$

For $(k+1)^{th}$, and $(k+2)^{th}$ derivatives, $k = 1, 2, \ldots$, one can obtain

$$f^{(k+1)}_n(u) = \lambda_{k-1}(u)f'_n(u) + s_{k-1}(u)f_n(u),$$

(16)

and

$$f^{(k+2)}_n(u) = \lambda_k(u)f'_n(u) + s_k(u)f_n(u),$$

(17)

respectively, where

$$\lambda_k(u) = \lambda'_{k-1}(u) + s_{k-1}(u) + \lambda_0(u)\lambda_{k-1}(u), \quad \text{and} \quad s_k(u) = s'_{k-1}(u) + s_0(u)\lambda_{k-1}(u).$$

The ratio of the $(k+2)^{th}$, and $(k+1)^{th}$ derivatives, can be expressed as:

$$\frac{d}{du}\ln(f^{(k+1)}_n(u)) = \frac{f^{(k+2)}_n(u)}{f^{(k+1)}_n(u)} = \frac{\lambda_k(f'_n(u) + \frac{s_k(u)}{\lambda_k(u)}f_n(u))}{\lambda_{k-1}(f'_n(u) + \frac{s_{k-1}(u)}{\lambda_{k-1}(u)}f_n(u)).}$$

(19)
For sufficiently large $k$, we can now introduce the "asymptotic" aspect of the method; that is,

$$\frac{s_k(u)}{\lambda_k(u)} = \frac{s_{k-1}(u)}{\lambda_{k-1}(u)} \equiv \varrho(u). \tag{20}$$

Thus equation (19) can be reduced to

$$\frac{d}{du} \ln(f_{n+1}^{(k)}(u)) = \frac{\lambda_k(u)}{\lambda_{k-1}(u)}, \tag{21}$$

which yields

$$f_{n+1}^{(k)}(u) = C_1 \exp \left( \int \frac{\lambda_k(u)}{\lambda_{k-1}(u)} du \right) = C_1 \lambda_{k-1}(u) \exp \left( \int (\varrho(u) + \lambda_0(u)) du \right), \tag{22}$$

where $C_1$ is the integration constant, and the right hand side of equation (22) follows from equation (18), and the definition of $\varrho$. Substituting equation (22) into equation (16) we obtain a first-order differential equation

$$f_n'(u) + \varrho(u)f_n(u) = C_1 \exp \left( \int (\varrho(u) + \lambda_0(u)) du \right), \tag{23}$$

which, in turn, yields the general solution to equation (12)

$$f_n(u) = \exp \left( -\int^u \varrho(u') du' \right) \left[ C_2 + C_1 \int^u \exp \left( \int^{u'} \{ \lambda_0(u'') + 2\varrho(u'') \} du'' \right) du' \right]. \tag{24}$$

Here, it should be noted that one can construct the eigenfunctions $f_n(u)$ from the knowledge of $\varrho$.

### 3 Numerical results for the vibrational levels of the Morse potential

Within the framework of the AIM mentioned in the above section, the energy eigenvalues of the Morse potential $\varepsilon_n$ are calculated by means of equation (20). To obtain the energy eigenvalues $\varepsilon_n$, first equation (20) is solved for $\varepsilon_n$ where the
iterations should be terminated by imposing a condition \( \delta_n(u) = 0 \) as an approximation to equation (20). On the other hand, for each iteration, the expression \( \delta_n(u) = s_n(u)\lambda_{n-1}(u) - s_{n-1}(u)\lambda_n(u) \) depends on two variables: \( \epsilon_n \), and \( u \). The calculated \( \epsilon_n \) by means of this condition should, however, be independent of the choice of \( u \). Nevertheless, the choice of \( u \) is observed to be critical only to speed of the convergence to \( \epsilon_n \), as well as for the stability of the process. In this work it is observed that, the best starting value for \( u \) is the value at which the effective potential of equation (9) takes its minimum value, that is when \( u = 1 \). Therefore, at the end of the iterations we put \( u = 1 \).

The results of the AIM for \( \epsilon_n \) with different values of \( n \), yield

\[
\epsilon_0 = \frac{-3 + 8\Delta}{2}, \quad \epsilon_1 = \frac{-7 + 8\Delta}{2}, \quad \epsilon_2 = \frac{-11 + 8\Delta}{2}, \quad \ldots \quad \ldots
\]

(25)

respectively, that means

\[
\epsilon_n = \frac{-4n - 3 + 8\Delta}{2}, \quad \text{for} \quad n = 0, 1, 2, \ldots
\]

(26)

The parameters \( \epsilon_n \) were calculated by means of 18 iterations only. Therefore, the exact energy eigenvalues of the Morse potential \( \epsilon_n \) are

\[
\epsilon_n = -\frac{(-2(2n + 1) + 8\Delta)^2}{64\Delta}, \quad \text{for} \quad n = 0, 1, 2, \ldots
\]

(27)

For numerical illustration, in table I we calculate the vibrational energies of the \( ^7Li_2 \) molecule in the \( A^1\Sigma_u^+ \) electronic state. The parameters of the respective Morse potential are explicitly indicated, with the dissociation energy parameter in both units \( cm^{-1} \), and \( \hbar\omega_0 \); the later is better suited to compare with the unit separation of the corresponding levels of the harmonic oscillator and appreciate
the decreasing separations in the Morse potential. The table includes the energy eigenvalues according to Morse’s exact solution, E. Ley-Koo et al. [23], and to the calculations of this work using AIM. One can also compare the results of this work with those of H. Taşeli [24], and can easily judge the accuracy of the AIM.

Finally, we would like to emphasize that, within the framework of the AIM, we have easily obtained the exact bound state solutions for the one-dimensional Schrödinger equation for the Morse potential.
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Table 1: Energy eigenvalues of Morse potential for $^7Li_2$ in the $A^1\Sigma_u^+$ state with $D_e = 8940 \text{ cm}^{-1} = 34.997 \hbar \omega_0$, $x_0 = 3.10821$, and $\beta = 0.616$.

| $n$ | $\varepsilon_n$(Morse) [15] | $\varepsilon_n$ [23] | $\varepsilon_n$(AIM) |
|-----|-----------------------------|------------------------|---------------------|
| 0   | -34.4987869262695313        | -34.4987858673604677  | -34.4987858673600556 |
| 1   | -33.5130744534329139        | -33.5130728062414320  | -33.5130728062405367 |
| 2   | -32.5416483298483712        | -32.5416466840021528  | -32.5416466840014849 |
| 3   | -31.5845091444715536        | -31.584507506434506   | -31.584507506429106  |
| 4   | -30.6416568973024646        | -30.6416552561655102  | -30.6416552561648174  |
| 5   | -29.7130915883411006        | -29.7130899505676886  | -29.7130899505671913  |
| 6   | -28.7988132175874689        | -28.7988115838512790  | -28.7988115838500462  |
| 7   | -27.8988217850415658        | -27.8988201560141817  | -27.8988201560133717  |
| 8   | -27.0131172907033879        | -27.0131156670575088  | -27.0131156670571784  |
| 9   | -26.1416997345729385        | -26.1416981169820595  | -26.1416981169814555  |
| 10  | -25.2845691166502178        | -25.2845675057870984  | -25.2845675057862103  |
| 11  | -24.4417254369352221        | -24.4417238334716096  | -24.4417238334714426  |
| 12  | -23.6131686954279552        | -23.6131671000377494  | -23.6131671000371455  |
| 13  | -22.7988988921284204        | -22.7988973054838091  | -22.7988973054833259  |
| 14  | -21.9989160270366071        | -21.9989144498102718  | -21.9989144498099840  |
| 15  | -21.2132201001525260        | -21.2132185330174288  | -21.2132185330171161  |
| 16  | -20.44181111114761700       | -20.4418095551052090  | -20.4418095551047223  |
| 17  | -19.6846890610075462        | -19.6846875160729802  | -19.6846875160728061  |
| 18  | -18.94185394874666475       | -18.9418524159217014  | -18.9418524159213639  |
| 19  | -18.2133057746934739        | -18.2133042564505699  | -18.2133042564503994  |
| 20  | -17.4990445388480325        | -17.4990430326202215  | -17.4990430322599053  |
| 21  | -16.7990702412103161        | -16.7990687487502584  | -16.7990687487498924  |
| 22  | -16.1133828817803284        | -16.1133814041206413  | -16.1133814041203536  |
| 23  | -15.4419824605580693        | -15.4419809983712994  | -15.4419809983712888  |
| 24  | -14.7848689773435389        | -14.7848675315028206  | -14.7848675315027016  |