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Abstract
For non-zero ℓ values, we present an analytical solution of the radial Schrödinger equation for the rotating Morse potential using the Pekeris approximation within the framework of the asymptotic iteration method. The bound state energy eigenvalues and corresponding wavefunctions are obtained for a number of diatomic molecules and the results are compared with the findings of the super-symmetry, the hypervirial perturbation, the Nikiforov–Uvarov, the variational, the shifted $1/N$ and the modified shifted $1/N$ expansion methods.

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1. Introduction

The Morse potential has raised a great deal of interest over the years and has been one of the most useful models to describe the interaction between two atoms in a diatomic molecule. It is known that the radial Schrödinger equation for this potential can be solved exactly when the orbital angular quantum number ℓ is equal to zero [1]. On the other hand, it is also known that for $\ell \neq 0$, one has to use some approximations to find analytical or semi-analytical solutions. Several schemes have been presented for obtaining approximate solutions [2]. Among these approximations, the most widely used and convenient one is the Pekeris approximation [3, 4], which is based on the expansion of the centrifugal barrier in a series of exponentials depending on the internuclear distance up to the second order. Other approximations have also been developed to find better analytical formulae for the rotating Morse potential. However, all these approximations other than the Pekeris one require the calculation of a state-dependent internuclear distance through the numerical solutions of transcendental equations [5–8]. In this respect, the rotating Morse potential has so far been solved by the super-symmetry (SUSY) [2, 9], the Nikiforov–Uvarov method (NU) [10, 11], the shifted and modified shifted $1/N$ expansion methods [8, 12] as well as the variational method [13] using Pekeris approximations for $\ell \neq 0$. It is also solved by using the hypervirial perturbation method (HV) [14] with the full potential without Pekeris approximation.

In this paper, our aim is to solve the rotating Morse potential using a different and more practical method called the asymptotic iteration method (AIM) [15, 16] within the Pekeris approximation and to obtain the energy eigenvalues and corresponding eigenfunctions. In the next section, the asymptotic iteration method (AIM) is introduced. Then, in section 3, the Schrödinger equation is solved by the asymptotic iteration method with the non-zero angular momentum quantum numbers for the rotating Morse potential: the exact energy eigenvalues and corresponding wavefunctions are calculated for the H_2, HCl, CO and LiH diatomic molecules and AIM results are compared with the findings of the SUSY [2], the hypervirial perturbation method (HV) [14], the Nikiforov–Uvarov method (NU) [11] and the shifted and modified shifted $1/N$ expansion methods [8, 12] as well as with the variational method [13]. Finally, section 4 is devoted to the summary and conclusion.

2. Basic equations of the asymptotic iteration method (AIM)

We briefly outline the asymptotic iteration method here and the details can be found in [15, 16]. The asymptotic iteration method is proposed to solve the second-order differential equations of the form

$$y'' = \lambda_0(x)y' + s_0(x)y \tag{1}$$

where $\lambda_0(x) \neq 0$ and $s_0(x)$, $\lambda_0(x)$ are in $C_\infty(a, b)$. The variables, $s_0(x)$ and $\lambda_0(x)$, are sufficiently differentiable. The differential equation (1) has a general solution [15]

$$y(x) = \exp\left(-\int^x \alpha(x')\,dx'\right)\left[C_2 + C_1 \int^x \exp\left(\int^{x'}(\lambda_0(x'') + 2\alpha(x''))\,dx''\right)dx'\right] \tag{2}$$

if $k > 0$, for sufficiently large k, we obtain the $\alpha(x)$ values from

$$\frac{s_k(x)}{\lambda_k(x)} = \frac{s_{k-1}(x)}{\lambda_{k-1}(x)} = \alpha(x), \qquad k = 1, 2, 3, \ldots \tag{3}$$

where

$$\begin{aligned}
\lambda_k(x) &= \lambda'_{k-1}(x) + s_{k-1}(x) + \lambda_0(x)\lambda_{k-1}(x) \\
s_k(x) &= s'_{k-1}(x) + s_0(x)\lambda_{k-1}(x), \qquad k = 1, 2, 3, \ldots.
\end{aligned} \tag{4}$$

The energy eigenvalues are obtained from the quantization condition. The quantization condition of the method together with equation (4) can also be written as follows:

$$\delta_k(x) = \lambda_k(x)s_{k-1}(x) - \lambda_{k-1}(x)s_k(x) = 0, \qquad k = 1, 2, 3, \ldots. \tag{5}$$

For a given potential such as the rotating Morse one, the radial Schrödinger equation is converted to the form of equation (1). Then, $s_0(x)$ and $\lambda_0(x)$ are determined and $s_k(x)$ and $\lambda_k(x)$ parameters are calculated. The energy eigenvalues are determined by the quantization condition given by equation (5). However, the wavefunctions are determined by using the following wavefunction generator:

$$y_n(x) = C_2 \exp\left(-\int^x \frac{s_k(x')}{\lambda_k(x')}\,dx'\right). \tag{6}$$

3. Calculation of the energy eigenvalues and eigenfunctions

The motion of a particle with the reduced mass μ is described by the following Schrödinger equation:

$$\frac{-\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] + V(r)\right)\Psi_{n\ell m}(r,\theta,\phi)$$
$$= E\Psi_{n\ell m}(r,\theta,\phi). \tag{7}$$

The terms in the square brackets with the overall minus sign are the dimensionless angular momentum squared operator, $\mathbf{L}^2$. Defining $\Psi_{n\ell m}(r,\theta,\phi) = u_{n\ell}(r)Y_{\ell m}(\theta,\phi)$, we obtain the radial part of the Schrödinger equation:

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)u_{n\ell}(r) - \frac{2\mu}{\hbar^2}\left[V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]u_{n\ell}(r) + \frac{2\mu E}{\hbar^2}u_{n\ell}(r) = 0. \tag{8}$$

It is sometimes convenient to define $u_{n\ell}(r)$ and the effective potential as follows:

$$u_{n\ell}(r) = \frac{R_{n\ell}(r)}{r}, \qquad V_{\text{eff}} = V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}. \tag{9}$$

Since

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\frac{R_{n\ell}(r)}{r} = \frac{1}{r}\frac{d^2}{dr^2}R_{n\ell}(r), \tag{10}$$

the radial Schrödinger equation given by equation (8) follows that

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E - V_{\text{eff}}\right]R_{n\ell}(r) = 0. \tag{11}$$

Instead of solving the partial differential equation (7) in three variables r, θ and ϕ, we now solve a differential equation involving only the variable r, but dependent on the angular momentum parameter ℓ, which makes the solution of this equation difficult for $\ell \neq 0$ or sometimes impossible within a given potential.

The Morse potential we examine in this paper is defined as

$$V_{\text{Morse}}(r) = D(e^{-2\alpha x} - 2e^{-\alpha x}) \tag{12}$$

with $x = (r - r_e)/r_e$ and $\alpha = ar_e$. Here, D and α denote the dissociation energy and Morse parameter, respectively. r_e is the equilibrium distance (bound length) between nuclei and a is a parameter to control the width of the potential well. For the H_2 diatomic molecule, the effective potential, which is the sum of the centrifugal and Morse potentials, is shown in figure 1 for various values of the orbital angular momentum. The superposition of the attractive and repulsive potentials results in the formation of a potential pocket, whose width and depth depend on the orbital angular momentum quantum number for a given molecular potential. The potential pocket becomes shallower as the orbital angular momentum quantum number ℓ increases, which also indicates that the number of states supported by the potential decreases. This pocket is also very important for the scattering case due to the interference of the barrier and internal waves, which creates the oscillatory structure in the cross section. The effect of this pocket can be understood in terms of the interference between the internal and barrier waves that corresponds to a decomposition of the scattering amplitude into two components, the inner and external waves [17–19].

The effective potential together with the Morse potential for $\ell \neq 0$ can be written as

$$V_{\text{eff}}(r) = V_\ell(r) + V_{\text{Morse}}(r) = \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + D(e^{-2\alpha x} - 2e^{-\alpha x}). \tag{13}$$
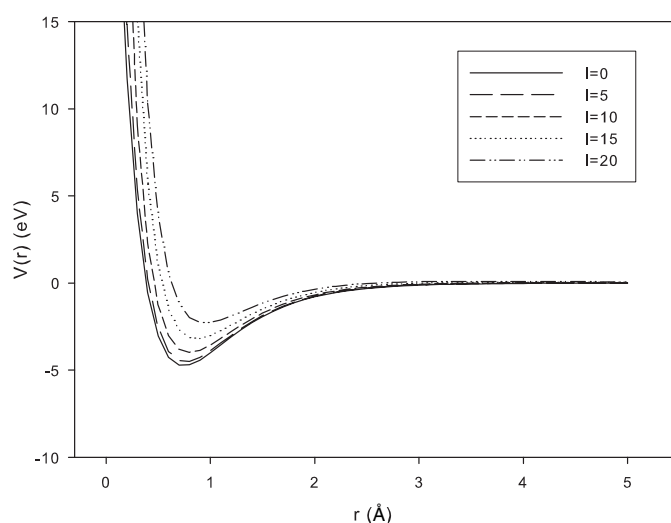
Figure 1. The shape of the rotating Morse potential for H_2 diatomic molecule is plotted against the separation r for different orbital angular momentum quantum numbers.

It is known that the Schrödinger equation cannot be solved exactly for this potential for $\ell \neq 0$ by using the standard methods such as SUSY and NU. As it is seen from equation (13), the effective potential is a combination of the exponential and inverse square potentials, which cannot be solved analytically. Therefore, an approximation has to be made: the most widely used and convenient one is the Pekeris approximation. This approximation is based on the expansion of the centrifugal barrier in a series of exponentials depending on the internuclear distance, keeping terms up to second order, so that the effective ℓ-dependent potential keeps the same form as the potential with $\ell = 0$ [2]. It should be pointed out, however, that this approximation is valid only for low vibrational energy states. In the Pekeris approximation, by change of the coordinates $x = (r - r_e)/r_e$, the centrifugal potential is expanded in a series around $x = 0$

$$V_\ell(x) = \frac{\ell(\ell + 1)\hbar^2}{2\mu r_e^2} \frac{1}{(1 + x)^2} = \gamma(1 - 2x + 3x^2 - 4x^3 + \cdots) \tag{14}$$

where $\gamma = \frac{\ell(\ell+1)\hbar^2}{2\mu r_e^2}$. Taking up to the second-order degrees in this series and writing them in terms of exponentials, we get

$$\widetilde{V}_\ell(x) = \gamma(c_0 + c_1 \, e^{-\alpha x} + c_2 \, e^{-2\alpha x}). \tag{15}$$

In order to determine the constants c_0, c_1 and c_2, we also expand this potential in a series of x

$$\widetilde{V}_\ell(x) = \gamma \left(c_0 + c_1 + c_2 - (c_1 + 2c_2)\alpha x + \left(\frac{c_1}{2} + 2c_2 \right) \alpha^2 x^2 + \cdots \right). \tag{16}$$

Comparing equal powers of equations (14) and (16), we obtain the constants c_0, c_1 and c_2 as

$$c_0 = 1 - \frac{3}{\alpha} + \frac{3}{\alpha^2}, \qquad c_1 = \frac{4}{\alpha} - \frac{6}{\alpha^2}, \qquad c_2 = -\frac{1}{\alpha} + \frac{3}{\alpha^2}. \tag{17}$$

Now, the effective potential with Pekeris approximation becomes

$$\widetilde{V}_{\text{eff}}(x) = \gamma(c_0 + c_1 \, e^{-\alpha x} + c_2 \, e^{-2\alpha x}) + D(e^{-2\alpha x} - 2 \, e^{-\alpha x}). \tag{18}$$

Instead of solving the radial Schrödinger equation for the effective potential given by equation (13), we solve the radial Schrödinger equation for the new effective potential given by equation (18) obtained by using the Pekeris approximation. Inserting this effective potential equation (18) into equation (11) and using the following ansätze

$$-\varepsilon^2 = \frac{2\mu r_e^2}{\hbar^2}(E - \gamma c_0), \qquad \beta_1^2 = \frac{2\mu r_e^2}{\hbar^2}(2D - \gamma c_1), \qquad \beta_2^2 = \frac{2\mu r_e^2}{\hbar^2}(\gamma c_2 + D). \quad (19)$$

The radial Schrödinger equation takes the following form:

$$\frac{d^2 R_{n\ell}(x)}{dx^2} + \left(-\varepsilon^2 + \beta_1^2 e^{-\alpha x} - \beta_2^2 e^{-2\alpha x}\right) R_{n\ell}(x) = 0. \quad (20)$$

If we rewrite equation (20) by using a new variable of the form $y = e^{-\alpha x}$, we obtain

$$\frac{d^2 R_{n\ell}(y)}{dy^2} + \frac{1}{y}\frac{d R_{n\ell}(y)}{dy} + \left[-\frac{\varepsilon^2}{\alpha^2}\frac{1}{y^2} + \frac{\beta_1^2}{\alpha^2}\frac{1}{y} - \frac{\beta_2^2}{\alpha^2}\right] R_{n\ell}(y) = 0. \quad (21)$$

In order to solve this equation with AIM for $\ell \neq 0$, we should transform this equation to the form of equation (1). Therefore, the reasonable physical wavefunction we propose is as follows:

$$R_{n\ell}(y) = y^{\frac{\varepsilon}{\alpha}} e^{-\frac{\beta_2}{\alpha} y} f_{n\ell}(y). \quad (22)$$

If we insert this wavefunction into equation (21), we have the second-order homogeneous linear differential equations in the following form:

$$\frac{d^2 f_{n\ell}(y)}{dy^2} = \left(\frac{2\beta_2\alpha y - 2\varepsilon\alpha - \alpha^2}{y\alpha^2}\right)\frac{d f_{n\ell}(y)}{dy} + \left(\frac{2\varepsilon\beta_2 + \alpha\beta_2 - \beta_1^2}{y\alpha^2}\right) f_{n\ell}(y) \quad (23)$$

which is now amenable to an AIM solution. By comparing this equation with equation (1), we can write the $\lambda_0(y)$ and $s_0(y)$ values and by means of equation (4) we may calculate $\lambda_k(y)$ and $s_k(y)$. This gives (the subscripts are omitted)

$$\lambda_0 = \left(\frac{2\beta_2 y - 2\varepsilon - \alpha}{\alpha y}\right)$$

$$s_0 = \left(\frac{2\varepsilon\beta_2 + \alpha\beta_2 - \beta_1^2}{\alpha^2 y}\right)$$

$$\lambda_1 = \frac{-3\beta_2\alpha y + 6\alpha\varepsilon + 2\alpha^2 - 6y\varepsilon\beta_2 - y\beta_1^2 + 4\beta_2^2 y^2 + 4\varepsilon^2}{\alpha^2 y^2} \quad (24)$$

$$s_1 = 2\frac{\left(2\varepsilon\beta_2 + \alpha\beta_2 - \beta_1^2\right)(-\alpha + \beta_2 y - \varepsilon)}{\alpha^3 y^2}$$

$$\ldots\ldots$$

Combining these results with the quantization condition given by equation (5) yields

$$\frac{s_0}{\lambda_0} = \frac{s_1}{\lambda_1} \quad \Rightarrow \quad \varepsilon_0 = -\frac{1}{2}\frac{\alpha\beta_2 - \beta_1^2}{\beta_2}$$

$$\frac{s_1}{\lambda_1} = \frac{s_2}{\lambda_2} \quad \Rightarrow \quad \varepsilon_1 = -\frac{1}{2}\frac{3\alpha\beta_2 - \beta_1^2}{\beta_2} \quad (25)$$

$$\frac{s_2}{\lambda_2} = \frac{s_3}{\lambda_3} \quad \Rightarrow \quad \varepsilon_2 = -\frac{1}{2}\frac{5\alpha\beta_2 - \beta_1^2}{\beta_2}.$$

$$\ldots\ldots$$

Table 1. For the H_2 diatomic molecule, the comparison of the energy eigenvalues (in eV) obtained by using AIM with other methods for different values of n and ℓ. Potential parameters are $D = 4.7446$ eV, $a = 1.9425$ (Å)$^{-1}$, $r_e = 0.7416$ Å, $\hbar c = 1973.29$ eV Å and $\mu = 0.503\,91$ amu.

n	ℓ	AIM results	SUSY results	HV results	Variational results	Modified shifted $1/N$ expansion results	Shifted $1/N$ expansion results
0	0	−4.476 01	−4.476 01	−4.476 01	−4.4758	−4.4760	−4.4749
	5	−4.258 80	−4.258 80	−4.259 01	−4.2563	−4.2590	−4.2590
	10	−3.721 93	−3.721 93	−3.724 73	−3.7187	−3.7247	−3.7247
5	0	−2.220 52	−2.220 51	−2.220 51	–	−2.2205	−2.2038
	5	−2.043 55	−2.043 53	−2.052 85	–	−2.0530	−2.0525
	10	−1.603 91	−1.603 89	−1.652 65	–	−1.6535	−1.6526
7	0	−1.537 44	−1.537 43	−1.537 43	–	−1.5374	−1.5168
	5	−1.376 56	−1.376 54	−1.392 63	–	−1.3932	−1.3887
	10	−0.975 81	−0.975 78	−1.052 65	–	−1.0552	−1.0499

Table 2. For the HCl diatomic molecule, the comparison of the energy eigenvalues (in eV) obtained by using AIM with other methods for different values of n and ℓ. Potential parameters are $D = 37\,255$ cm^{-1}, $a = 1.8677$ (Å)$^{-1}$, $r_e = 1.2746$ Å, $\hbar c = 1973.29$ eV Å and $\mu = 0.980\,1045$ amu.

n	ℓ	AIM results	Variational results	Modified shifted $1/N$ expansion results	Shifted $1/N$ expansion results
0	0	−4.4356	−4.4360	−4.4355	−4.4352
	5	−4.3968	−4.3971	−4.3968	−4.3967
	10	−4.2941	−4.2940	−4.2940	−4.2939
5	0	−2.8051	–	−2.8046	−2.7727
	5	−2.7721	–	−2.7718	−2.7508
	10	−2.6847	–	−2.6850	−2.6712
7	0	−2.2570	–	−2.2565	−2.2002
	5	−2.2263	–	−2.2262	−2.1874
	10	−2.1451	–	−2.1461	−2.1194

When the above expressions are generalized, the eigenvalues turn out as

$$\varepsilon_{n\ell} = \frac{\beta_1^2 - (2n+1)\alpha\beta_2}{2\beta_2}, \qquad n = 0, 1, 2, 3, \ldots. \tag{26}$$

Using equation (19), we obtain the energy eigenvalues $E_{n\ell}$ as

$$E_{n\ell} = -\frac{\hbar^2}{2\mu r_e^2}\left[\frac{\beta_1^2}{2\beta_2} - \left(n + \frac{1}{2}\right)\alpha\right]^2 + \gamma c_0. \tag{27}$$

As it is seen that the energy eigenvalue equation is easily obtained by using AIM. This is the advantage of the AIM that it gives the eigenvalues directly by transforming the radial Schrödinger equation into a form of $y'' = \lambda_0(r)y' + s_0(r)y$. In order to test the accuracy of equation (27), we calculate the energy eigenvalues of the H_2, HCl, CO and LiH diatomic molecules. The AIM results are compared with those obtained by SUSY method [2] using original Pekeris approximation, the hypervirial perturbation method (HV) [14], the shifted $1/N$ and modified shifted $1/N$ expansion methods [8] for the H_2 diatomic molecule in table 1. In table 2, we show the same comparison for the HCl diatomic molecule. Furthermore, the

Table 3. For the CO diatomic molecule, the comparison of the energy eigenvalues (in eV) obtained by using AIM with other methods for different values of n and ℓ. Potential parameters are $D = 90\,540$ cm^{-1}, $a = 2.2994$ (Å)$^{-1}$, $r_e = 1.1283$ Å, $\hbar c = 1973.29$ eV Å and $\mu = 6.860\,6719$ amu.

n	ℓ	AIM results	NU results	Variational results	Modified shifted $1/N$ expansion results	Shifted $1/N$ expansion results
0	0	−11.0915	−11.091	−11.093	−11.092	−11.091
	5	−11.0844	−11.084	−11.085	−11.084	−11.084
	10	−11.0653	−11.065	−11.066	−11.065	−11.065
5	0	−9.7952	−9.795	–	−9.795	−9.788
	5	−9.7883	−9.788	–	−9.788	−9.782
	10	−9.7701	−9.769	–	−9.770	−9.765
7	0	−9.2992	−9.299	–	−9.299	−9.286
	5	−9.2925	−9.292	–	−9.292	−9.281
	10	−9.2745	−9.274	–	−9.274	−9.265

Table 4. For the LiH diatomic molecule, the comparison of the energy eigenvalues (in eV) obtained by using AIM with other methods for different values of n and ℓ. Potential parameters are $D = 20\,287$ cm^{-1}, $a = 1.1280$ (Å)$^{-1}$, $r_e = 1.5956$ Å, $\hbar c = 1973.29$ eV Å and $\mu = 0.880\,1221$ amu.

n	ℓ	AIM results	NU results	Variational results	Modified shifted $1/N$ expansion results	Shifted $1/N$ expansion results
0	0	−2.4289	−2.4287	−2.4291	−2.4280	−2.4278
	5	−2.4013	−2.4012	−2.4014	−2.4000	−2.3999
	10	−2.3288	−2.3287	−2.3287	−2.3261	−2.3261
5	0	−1.6477	−1.6476	–	−1.6402	−1.6242
	5	−1.6238	−1.6236	–	−1.6160	−1.6074
	10	−1.5607	−1.5606	–	−1.5525	−1.5479
7	0	−1.3776	−1.3774	–	−1.3682	−1.3424
	5	−1.3550	−1.3549	–	−1.3456	−1.3309
	10	−1.2958	−1.2957	–	−1.2865	−1.2781

AIM results are compared with those obtained by NU method [11], shifted $1/N$ and modified shifted $1/N$ expansion methods [8] for the CO and LiH diatomic molecules in tables 3 and 4, respectively. As it can be seen from the results presented in these tables that the AIM results are in good agreement with the findings of the other methods.

After we find the energy eigenvalues, the following wavefunction generator can be used to find $f_n(y)$ functions by using AIM

$$f_n(y) = \exp\left(-\int^y \frac{s_k}{\lambda_k}\, \mathrm{d}y'\right) \tag{28}$$

where n represents the radial quantum number and k shows the iteration number. Below, the first few $f(y)$ functions can be seen:

$$f_0(y) = 1 \tag{29}$$

$$f_1(y) = \left(2\alpha\beta_2 - \beta_1^2\right)\left(1 - \frac{2\beta_2 y}{\alpha\left(\frac{\beta 1^2 - 3\alpha\beta_2}{\alpha\beta_2} + 1\right)}\right) \tag{30}$$

$$f_2(y) = \left(\beta_1^2 - 4\alpha\beta_2\right)\left(\beta_1^2 - 3\alpha\beta_2\right)\left(1 - \frac{4\beta_2 y}{\alpha\left(\frac{\beta_1^2 - 5\alpha\beta_2}{\alpha\beta_2} + 1\right)} + \frac{4\beta_2^2 y^2}{\alpha^2\left(\frac{\beta_1^2 - 5\alpha\beta_2}{\alpha\beta_2} + 1\right)\left(\frac{\beta_1^2 - 5\alpha\beta_2}{\alpha\beta_2} + 2\right)}\right)$$

(31)

$$f_3(y) = \left(-4\alpha\beta_2 + \beta_1^2\right)\left(\beta_1^2 - 5\alpha\beta_2\right)\left(\beta_1^2 - 6\alpha\beta_2\right)\left(1 - \frac{6\beta_2 y}{\alpha\left(\frac{\beta_1^2 - 7\alpha\beta_2}{\beta_2\alpha} + 1\right)}\right.$$

$$\left. + \frac{12\beta_2^2 y^2}{\alpha^2\left(\frac{\beta_1^2 - 7\alpha\beta_2}{\alpha\beta_2} + 1\right)\left(\frac{\beta_1^2 - 7\alpha\beta_2}{\alpha\beta_2} + 2\right)} - \frac{8\beta_2^3 y^3}{\alpha^3\left(\frac{\beta_1^2 - 7\alpha\beta_2}{\alpha\beta_2} + 1\right)\left(\frac{\beta_1^2 - 7\alpha\beta_2}{\alpha\beta_2} + 2\right)\left(\frac{\beta_1^2 - 7\alpha\beta_2}{\alpha\beta_2} + 3\right)}\right)$$

$$\cdots$$

(32)

It can be understood from the results given above that we can write the general formula for $f_n(y)$ as follows:

$$f_n(y) = (-1)^n \left(\prod_{k=n}^{2n-1}\left(\beta_1^2 - (k+1)\alpha\beta_2\right)\right) {}_1F_1\left(-n, \frac{2\varepsilon_n}{\alpha} + 1; \frac{2\beta_2 y}{\alpha}\right).$$

(33)

Thus, we can write the total radial wavefunction as follows:

$$R_{n\ell} = (-1)^n \left(\prod_{k=n}^{2n-1}\left(\beta_1^2 - (k+1)\alpha\beta_2\right)\right) y^{\frac{\varepsilon_n}{\alpha}} e^{-\frac{\beta_2}{\alpha}y} {}_1F_1\left(-n, \frac{2\varepsilon_n}{\alpha} + 1; \frac{2\beta_2 y}{\alpha}\right).$$

(34)

When the hypergeometric function is written in terms of the Laguerre polynomials, we get

$$R_{n\ell} = N y^{\frac{\varepsilon_n}{\alpha}} e^{-\frac{\beta_2}{\alpha}y} L_n^{\frac{2\varepsilon_n}{\alpha}}\left(\frac{2\beta_2}{\alpha}y\right)$$

(35)

where N is the normalization constant and can be obtained from $N^2 \int_0^\infty y^{\frac{2\varepsilon_n}{\alpha}}$ $e^{-\frac{2\beta_2}{\alpha}y}\left[L_n^{\frac{2\varepsilon_n}{\alpha}}\left(\frac{2\beta_2}{\alpha}y\right)\right]^2 dy = 1$ as follows:

$$N = \frac{1}{n!}\left(\frac{2\beta_2}{\alpha}\right)^{\frac{\xi+1}{2}}\sqrt{\frac{(n-\xi)!}{n!}}$$

(36)

where $\xi = \frac{2\varepsilon_n}{\alpha}$.

4. Conclusion

We have shown an alternative method to obtain the energy eigenvalues and corresponding eigenfunctions of the rotating Morse potential using Pekeris approximation within the framework of the asymptotic iteration method. The main results of this paper are the energy eigenvalues and eigenfunctions, which are given by equations (27) and (35), respectively. The energy eigenvalues are obtained for the H_2, HCl, CO and LiH diatomic molecules. Our AIM results are compared with the findings of the other methods such as the SUSY [2], the hypervirial perturbation method (HV) [14], the Nikiforov–Uvarov method (NU) [11] and the shifted and modified shifted $1/N$ expansion methods [8, 12] as well as the variational method [13] in tables 1–4. The advantage of the asymptotic iteration method is that it gives the eigenvalues directly by transforming the radial Schrödinger equation into a form of $y'' = \lambda_0(r)y' + s_0(r)y$. The wavefunctions are easily constructed by iterating the values of $s_0(r)$ and $\lambda_0(r)$. The method presented in this study is a systematic one and it is very efficient and practical. It is worth extending this method to the solution of other interaction problems.

Acknowledgments

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