Continuum states of modified Morse potential*

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Using a proper approximation scheme to the centrifugal term, we study any l-wave continuum states of the Schrödinger equation for the modified Morse potential. The normalised analytical radial wave functions are presented, and a corresponding calculation formula of phase shifts is derived. It is shown that the energy levels of the continuum states reduce to those of the bound states at the poles of the scattering amplitude. Some numerical results are calculated to show the accuracy of our results.

Keywords: modified Morse potential, continuum states, approximate analytical solutions
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1. Introduction

It is well known that the Morse potential is one of the important exponential model potentials, and it has been found that the potential function for the lowest electronic states of the actual diatomic molecule can be represented by Morse potential[1] as follows:

$$V_{\rm M}(r) = D\left[1 - \exp(-\alpha(r - r_0))\right]^2, \qquad (1)$$

where D and α are two adjustable positive parameters, and r_0 is the minimum value point, i.e., $V_{\rm M}(r)$ has a minimum value 0 at $r = r_0$. Since the introduction of the Morse potential, numerous advantages and extensive applications of this potential have been made in the fields of diatomic molecule and quantum chemistry.[2−6] Also, the quantum mechanics problems related to this potential have been widely studied within the frameworks of the nonrelativistic and relativistic quantum mechanics separately,[7−12] and it is shown that the eigenvalues and eigenfunction of one-dimensional diatomic molecule represented by Morse potential are not only simple in form, but also practical in calculation. Unfortunately, for the Morse potential, when the distance between the two atoms approaches zero, the interaction between the two atoms represented by Morse potential cannot approach infinity unlike the true interaction. Although this boundary condition seldom brings about a remarkable effect on bound states, it will give rise to some difficulty in solving the collision problem.

In order to overcome the above difficulty of the Morse potential in describing the interaction between the actual diatomic molecules, Deng and Fan,[13] half a century ago, proposed another diatomic molecular potential

$$V(r) = D\left(1 - \frac{d}{{\rm e}^{\alpha r} - 1}\right)^2 \qquad (2)$$

with

$$d = {\rm e}^{\alpha r_e} - 1, \quad (r\forall(0, \infty)), \qquad (3)$$

where parameters D , d and α are three parameters representing the dissociation energy, the position of the minimum r_e and the potential range parameter, respectively. Since this potential has the correct boundary conditions at origin and infinity and can be used to describe the realistic interactions between atoms and molecules, it is called modified Morse potential and widely used in molecular physics and chemical physics.[14,15] Namely, the interaction represented by this potential can approach infinity when the distance between the two atoms approaches zero, and finity when the distance approaches infinity. Thus, it is necessary and considerable interest to systematically study the quantum mechanics problems related to this potential in order to offer some references for molecule physics and quantum chemistry. Recently, the bound states of the Schrödinger equation with this potential have been found by Dong and Gu,[16] and the bound states of the Dirac equation with this potential

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have also been obtained by Zhang *et al.*[17] In addition, other related studies[18−21] have also been carried out within the frameworks of nonrelativistic and relativistic quantum mechanics separately. However, the continuum states of this potential have not been reported up to now. Nevertheless, we should study both of them in order to understand the studied quantum system completely. There are two reasons for us to write this paper. One is that we have not found any reports dealing with the continuum states of this potential, the other is that we intend to investigate the properties of continuum states to show the relations between the energy levels of the continuum states and those of the bound states at the poles of the scattering amplitude.

The remainder of this paper is organised as follows. In Section 2 we derive approximately the analytical continuum states of the modified Morse potential with a centrifugal term. In Section 3 we discuss the analytical properties of scattering amplitude and obtain the bound state energy levels from the poles of scattering amplitude. In Section 4 we show the accuracy of our results by calculating the numerical results of energy eigenvalues with arbitrary quantum numbers n and l. We summarize our conclusions in Section 5.

2. Continuum states

The Schrödinger equation with the modifed Morse potential is given by

$$-\frac{\hbar^2}{2\mu}\nabla^2\Psi(r,\theta,\phi)+V(r)\Psi(r,\theta,\phi)=E\Psi(r,\theta,\phi), \quad (4)$$

where $\mu = m_1m_2/(m_1+m_2)$ is the reduced mass, $\{r,\theta,\phi\}$ is the polar coordinate representation of relative position vector $\boldsymbol{r}$, and $V(r)$ is the potential function of diatomic molecule. Here, the potential is taken as the modified Morse potential, i.e., Eq. (2). Taking $\Psi(r,\theta,\phi)=r^{-1}u(r)Y_{lm}(\theta,\phi)$ and substituting into Eq. (4), we obtain the radial Schrödinger equation as ($\hbar=c=\mu=1$)

$$-\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2}+\left[2E-2D\left(1-\frac{d}{\mathrm{e}^{\alpha r}-1}\right)^2-\frac{l(l+1)}{r^2}\right]u(r)=0. \quad (5)$$

It is shown that Eq. (5) can be solved exactly only for s-wave case due to the centrifugal term. Therefore, we must use a appropriate approximation to the centrifugal term similar to that in the previous work.[22−24] It is noted that for the short-range potential the following formula

$$\frac{1}{r^2}\approx\frac{\alpha^2\,\mathrm{e}^{-\alpha r}}{(1-\mathrm{e}^{-\alpha r})^2} \quad (6)$$

is an appropriate approximation to $1/r^2$. Such an approximation proposed by Greene and Aldrich[25] was for generating pseudo-Hulthén wave functions for arbitrary l-states.

Now we solve Eq. (5). Inserting transformation $z=1-\mathrm{e}^{-\alpha r}, [r\in(0,\infty), z\in(0,1)]$ into Eq. (5) yields

$$(1-z)^2\frac{\mathrm{d}^2u(z)}{\mathrm{d}z^2}+(z-1)\frac{\mathrm{d}u(z)}{\mathrm{d}z}+\left(\varepsilon+\frac{l(l+1)(z-1)}{z^2}-\frac{k\left[d(z-1)+z\right]^2}{z^2}\right)u(z)=0, \quad (7)$$

where

$$\varepsilon=2E/\alpha^2, \quad k=2D/\alpha^2. \quad (8)$$

Taking the trial wave function of the form

$$u(z)=z^{\lambda}(1-z)^{-\mathrm{i}\delta}f(z), \quad (9)$$

and inserting into Eq. (7), we have

$$(1-z)zf''(z)+[2\lambda-(2\lambda+1-2\mathrm{i}\delta)z]f'(z)+[2dk+2d^2k+l+l^2+\lambda+2\mathrm{i}\delta\lambda-2\lambda^2]f(z)=0 \quad (10)$$

with

$$\lambda=\frac{1}{2}\left[1+\sqrt{1+4d^2k+4l(l+1)}\right],$$
$$\delta=\sqrt{-k+d^2k+l+l^2+\varepsilon+\lambda-\lambda^2}. \quad (11)$$

The solution of Eq. (10) is nothing but the hypergeometric function,[26] whose general expression is given by

$$f(z)=C_1\ {}_2F_1(a;b;c;z)+C_2\ z^{1-c}\ {}_2F_1(a-c+1;b-c+1;2-c;z), \quad (12)$$

where

$$a=\lambda-\mathrm{i}\delta-\sqrt{2dk+2d^2k+l+l^2-\delta^2+\lambda-\lambda^2},$$
$$b=\lambda-\mathrm{i}\delta+\sqrt{2dk+2d^2k+l+l^2-\delta^2+\lambda-\lambda^2},$$
$$c=2\lambda. \quad (13)$$

Considering the boundary condition, i.e., $f(z)$ tending to finity when $z\to0$ ($r\to0$), the allowed solution is

$$f(z)={}_2F_1(a;b;c;z)=\sum_{q=0}^{\infty}\frac{(a)_q(b)_q}{(c)_q}\frac{(z)^q}{q!}, \quad (14)$$

where the Pochhammer symbol is defined as $(z)_q = \Gamma(z+q)/\Gamma(z)$. From Eqs. (9) and (14), we can obtain the analytical radial wave functions of any l-wave continuum states for the modified Morse potential as

$$u(r) = N\left(1-\mathrm{e}^{-\alpha r}\right)^{\lambda}\mathrm{e}^{\mathrm{i}\delta\alpha r}{}_2F_1(a;b;c;1-\mathrm{e}^{-\alpha r}), \tag{15}$$

where N is the normalised constant to be determined later.

Before deriving the phase shifts, we recall a recurrence relation of hypergeometric function, which is used to analyse the asymptotic behaviour of the wave function and present the normalized constant and the phase shifts as follows:

$$\begin{aligned}{}_2F_1(a;b;c;z) = {} & \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\ {}_2F_1(a;b;a+b-c+1;1-z)\\ & + (1-z)^{c-a-b}\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}\ {}_2F_1(c-a;c-b;c-a-b+1;1-z),\end{aligned} \tag{16}$$

with which and the consideration of ${}_2F_1(a;b;c;0)=1$ when $r\to\infty$, we have

$${}_2F_1(a;b;c;1-\mathrm{e}^{-\alpha r}) \underset{r\to\infty}{\longrightarrow} \Gamma(c)\left\{\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} + \mathrm{e}^{-2\mathrm{i}\delta\alpha r}\left[\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right]^*\right\}. \tag{17}$$

In the above derivation, we have used the following relations:

$$\begin{aligned} & c-a-b = 2\mathrm{i}\delta = (a+b-c)^*,\\ & c-a = \lambda+\mathrm{i}\delta+\sqrt{2dk+2d^2k+l+l^2-\delta^2+\lambda-\lambda^2} = b^*,\\ & c-b = \lambda+\mathrm{i}\delta-\sqrt{2dk+2d^2k+l+l^2-\delta^2+\lambda-\lambda^2} = a^*. \end{aligned} \tag{18}$$

By taking

$$\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} = \left|\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right|\mathrm{e}^{\mathrm{i}\theta}, \tag{19}$$

and inserting into Eq. (17), we have

$${}_2F_1(a;b;c;1-\mathrm{e}^{-\alpha r}) \underset{r\to\infty}{\longrightarrow} \Gamma(c)\left|\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right|\mathrm{e}^{-\mathrm{i}\delta\alpha r}\left[\mathrm{e}^{\mathrm{i}(\delta\alpha r+\theta)}+\mathrm{e}^{-\mathrm{i}(\delta\alpha r+\theta)}\right]. \tag{20}$$

Inserting Eq. (20) into Eq. (15), we have the asymptotic form of formula (15) for $r\to\infty$,

$$u(r) \underset{r\to\infty}{\longrightarrow} 2N\Gamma(c)\left|\frac{\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\right|\sin\left(\delta\alpha r+\frac{\pi}{2}+\theta\right). \tag{21}$$

Comparing Eq. (21) with the boundary condition[27] $r\to\infty \Rightarrow u(\infty)\to 2\sin(\delta\alpha r + l\pi/2+\theta_l)$, we can obtain the phase shifts and the normalised constant as follows:

$$\theta_l = \frac{\pi}{2}(l+1)+\theta = \frac{\pi}{2}(l+1)+\arg\Gamma(c-a-b)-\arg\Gamma(c-a)-\arg\Gamma(c-b), \tag{22}$$

$$N = \frac{1}{\Gamma(c)}\left[\frac{\Gamma(c-a)\Gamma(c-b)}{\Gamma(c-a-b)}\right]. \tag{23}$$

The substitution of Eqs. (13) and (18) into Eqs. (22) and (23) allows us to give the expressions of the phase shifts and normalised constant as follows:

$$\begin{aligned}\theta_l = {} & \frac{\pi}{2}(l+1)+\theta\\ = {} & \frac{\pi}{2}(l+1)+\arg\Gamma(2\mathrm{i}\delta)-\arg\Gamma(\lambda+\mathrm{i}\delta+\sqrt{2dk+2d^2k+l+l^2-\delta^2+\lambda-\lambda^2})\\ & -\arg\Gamma(\lambda+\mathrm{i}\delta-\sqrt{2dk+2d^2k+l+l^2-\delta^2+\lambda-\lambda^2}),\end{aligned} \tag{24}$$

$$\begin{aligned}N = {} & \frac{\left|\Gamma(\lambda+\mathrm{i}\delta+\sqrt{2dk+2d^2k+l+l^2-\delta^2+\lambda-\lambda^2})\right|}{\Gamma(2\lambda)}\\ & \times\left|\frac{\Gamma(\lambda+\mathrm{i}\delta-\sqrt{2dk+2d^2k+l+l^2-\delta^2+\lambda-\lambda^2})}{\Gamma(2\mathrm{i}\delta)}\right|.\end{aligned} \tag{25}$$

3. Analytical properties of scattering amplitude

In this section we study the analytical properties of the scattering amplitude. It is well known that the discrete energy levels of the bound states correspond to the single pole of the scattering amplitude.[27] This suggests that we discuss the properties of the Gamma function $\Gamma(\lambda + \mathrm{i}\delta + \sqrt{2dk + 2d^2k + l + l^2 - \delta^2 + \lambda - \lambda^2})$ based on Eq. (24). From the definition of the Gamma function

$$\begin{aligned}\Gamma(z) &= \frac{\Gamma(z+1)}{z} \\ &= \frac{\Gamma(z+2)}{z(z+1)} \\ &= \frac{\Gamma(z+3)}{z(z+1)(z+2)} \\ &= \ldots, \end{aligned} \tag{26}$$

we know that $z = 0, -1, -2, \ldots$ are the first order poles of function $\Gamma(z)$. Therefore, the first order poles of $\Gamma(\lambda + \mathrm{i}\delta + \sqrt{2dk + 2d^2k + l + l^2 - \delta^2 + \lambda - \lambda^2})$ are situated at

$$\begin{aligned}&\lambda + \mathrm{i}\delta + \sqrt{2dk + 2d^2k + l + l^2 - \delta^2 + \lambda - \lambda^2} \\ &= 0, -1, -2, -3, \ldots = -n, (n = 0, 1, 2 \ldots). \end{aligned} \tag{27}$$

At the poles of the scattering amplitude, the corresponding energy levels are determined by the following energy equation:

$$\begin{aligned}&\left(2dk + 2d^2k + l + l^2 - n^2 + \lambda - 2n - 2\lambda^2\right)^2 \\ &+ 4\delta^2(n + \lambda)^2 = 0. \end{aligned} \tag{28}$$

It is not difficult to find that the energy levels determined by Eq. (28) coincide with those expressed by Eq. (17) of Ref. [16], that is to say, the energy levels of the continuum states reduce to those of the bound states at the poles of the scattering amplitude.

4. Numerical results

To show the accuracy of our results, the numerical results of energy eigenvalues calculated from Eq. (28) that we give in the present study are compared with those obtained by a MATHEMATICA package programmed by Lucha and Schöberl[28] as shown in Table 1. It is shown that our results are in good agreement with the numerical ones for short-range potentials. However, the difference between them will appear for long-range potentials, i.e., large α. This means that Eq. (6) is not a good approximation to the centrifugal term when the value of potential parameter α becomes large.

Table 1. Eigenvalues E as a function of α for 2p, 3p, 3d, 4p, 4d, 4f, 5p, 5d, 5f, 5g, 6p, 6d, 6f and 6g states with $r_e = 0.4, 0.8$ and $D = 15$ ($\hbar = \mu = c = 1$).

states	α	$r_e = 0.4$		$r_e = 0.8$	
		present	Lucha *et al.*	present	Lucha *et al.*
2p	0.02	7.804927573	7.805035114	4.093831415	4.093913555
	0.03	7.823529313	7.823677540	4.109468205	4.109586239
	0.04	7.842085474	7.842294216	4.125083988	4.125258923
	0.35	8.395287973	8.405532360	4.599633298	4.609816074
	0.40	8.480630573	8.493963718	4.674614104	4.687861919
3p	0.02	10.89735466	10.89746332	7.416823416	7.416943073
	0.03	10.93089625	10.93104887	7.455489448	7.455652714
	0.04	10.96429624	10.96450567	7.494076029	7.494293690
	0.35	11.92989316	11.93998861	8.651133793	8.661256313
	0.40	12.07305127	12.08612394	8.830681405	8.843792243
3d	0.02	10.13249146	10.13260889	5.675481908	5.675610065
	0.03	10.160234555	10.16047812	5.696794273	5.697050571
	0.04	10.187855719	10.18827868	5.718008889	5.718439579
	0.06	10.242733499	10.24365664	5.760146761	5.761071682
4p	0.02	12.374390454	12.37448931	9.448063366	9.448194981
	0.03	12.415713303	12.41585112	9.503210496	9.503384113
	0.04	12.456714547	12.45691252	9.558124407	9.558358669

Table 1 *continued*

states	α	$r_e = 0.4$		$r_e = 0.8$	
		present	Lucha *et al.*	present	Lucha *et al.*
	0.06	12.537751828	12.53811693	9.667251179	9.667655468
4d	0.02	11.983590726	11.98371935	8.363478492	8.363629818
	0.03	12.021880454	12.02212858	8.406735249	8.407017231
	0.04	12.059905175	12.06033182	8.449815048	9.558358669
	0.06	12.135161098	12.13608599	8.535461568	8.450275898
4f	0.02	11.712597477	11.71280336	7.342280028	7.342493534
	0.03	11.748485503	11.74893808	7.372873857	7.373341084
	0.04	11.784131547	11.78493547	7.403265489	7.404077053
5p	0.04	13.283129883	13.28330755	10.91278491	10.91301584
	0.06	13.371479666	13.37182474	11.04418628	11.04458570
5d	0.04	13.05400296	13.05442144	10.175651589	10.17611647
	0.06	13.13937882	13.14030504	10.291041363	10.29201365
5f	0.04	12.899043568	12.89985037	9.500259209	9.501092434
	0.06	12.981995479	12.98380136	9.5986306396	9.600467205
5g	0.04	12.791374387	12.79270792	8.9033811012	8.904723644
	0.06	12.872464381	12.87546587	8.9848401415	8.987842083
6d	0.06	13.733593820	13.73451090	11.4700252632	11.47099257
6f	0.06	13.636950744	13.63874960	10.9978268429	10.99967051
6g	0.06	14.0491839294	14.05097723	11.9627070491	11.96454477

5. Conclusions

In this work we study approximately the analytical continuum states of the l-wave Schrödinger equation with the modified Morse potential. The normalised analytical radial wave functions are obtained and the corresponding calculation formula of phase shifts is presented. In addition, we obtain the bound state energy levels at the poles of the scattering amplitude of the continuum states. Finally, to show the accuracy of our results, we calculate the numerical results for the energy eigenvalues with arbitrary quantum numbers n and l. It is obvious to show that our presented results are in good agreement with those obtained by a MATHEMATICA package programmed by Lucha and Schöberl.

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