The bound state solution for the Morse potential with a localized mass profile

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We investigate an analytical solution for the Schrödinger equation with a position-dependent mass distribution, with the Morse potential via Laplace transformations. We considered a mass function localized around the equilibrium position. The mass distribution depends on the energy spectrum of the state and the intrinsic parameters of the Morse potential. An exact bound state solution is obtained in the presence of this mass distribution.

Keywords: Schrödinger equation, Morse potential, Laplace transformation method, position-dependent mass

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1. Introduction

The investigations of the analytical solutions of the Schrödinger equation with position-dependent mass is one of the important topics in quantum mechanical sciences. The concept of the local mass has interesting features in the large scale characteristics of the universe and in gravitational field theories.[1–4] The position-dependent mass distribution also has received a great deal of attention in more terrestrial sciences, such as the material science, condensed matter physics, and semiconductors nanosubstructures,[5–7] quantum wells and quantum dots,[8–10] quantum liquids,[11] impurities in crystals,[12] and ^{3}He clusters.[13,14]

The Hermitian Hamiltonian of von Roos with local mass distribution $m = m(\boldsymbol{r})$ is given by,[5]

$$H = \frac{1}{4}\left[m^{\alpha}\boldsymbol{P}m^{\beta}\boldsymbol{P}m^{\gamma} + m^{\gamma}\boldsymbol{P}m^{\beta}\boldsymbol{P}m^{\alpha}\right] + V(r), \qquad (1)$$

where $\boldsymbol{P}$ denotes the momentum operator and $V(r)$ is an arbitrary potential. Also, α, β, and γ are the ambiguity parameters satisfying the dimensional constrain $\alpha+\beta+\gamma=-1$. Several sets of the values of ambiguity parameters are suggested in the literature.[15–19] Here, we apply the ambiguity parameter set suggested by BenDaniel and Duke ($\alpha=\gamma, \beta=-1$).[15] This model ensures the continuities required at the heterojunction boundaries between two crystals.

Amongst the distinct methods that have been applied to solve the Schrödinger equation, one may mention the point-canonical transformation method,[20–23] the factorization scheme,[24,25] the supersymmetry approach,[26–28] the algebraic way,[29] the power series expansion,[30,31] the transfer matrix method,[32,33] the asymptotic iteration method,[34–36] and the Nikiforov–Uvarov approach.[37–40]

One of the most effective methods for solving the Schrödinger equation with different sorts of spherically symmetric potentials is the Laplace transformation method.[41] The advantage of this method is that a second-order differential equation reduces to a first-order differential equation. It was Schrödinger who used this technique for the first time in quantum physics in order to solve the radial eigenfunction of a hydrogen atom.[42] The method has become commonly employed ever since to solve various kinds of spherically symmetric potentials.[43–50]

One of the significant potentials is the Morse potential which is applied for describing the vibrational and rotational movements of the diatomic molecules.[51] Solutions of the Schrödinger equation with the Morse potential are investigated by applying different methods in Refs. [52]–[61].

Here we introduce an analytical bound state solution of the Schrödinger equation with position-dependent mass. We apply the Laplace transformation method to obtain the eigenvalues and the eigenfunctions in a closed form. The point-canonical transformation method also has been applied[56,62] in order to get rid of the first derivative of the wave function. In this way, we can suitably separate the terms contained in the mass function from the terms of the field derivatives. Then, by applying some simple constraints, on the terms included in the mass function, we construct the mass function in such a way that the corresponding equation can be solved via the Laplace transformation method used in Refs. [3] and [46]. The obtained mass distribution is a physical one, that is positive-valued, convergent, and well localized around the equilibrium position of a typical molecule. The mass function depends on the ordinary parameters of the Morse potential. The obtained mass function also depends on the energy spectrum of the Morse oscillator.

The organization of this paper is as follows. In Section 2,

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we firstly introduce the initial form of the mass function with undetermined parameters. Then by considering the desired form of the Schrödinger equation which is most solvable with the Laplace transforms, we setup some constraints on our mass parameters to find the final form of the mass distribution. The parameters of the Morse potential become untouched. Then, in Section 3 we solve the equation and introduce a possible bound state solution of the model. Finally, some results and discussions are presented in Section 4.

2. A possible mass distribuion

For the BenDaniel–Duke Hamiltonian, the one-dimensional Schrödinger equation, in position representation, is given by

$$\left(-\frac{1}{m}\frac{\mathrm{d}m}{\mathrm{d}r}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\mathrm{d}^2}{\mathrm{d}r^2}\right)\psi(r)=-\frac{2m}{\hbar^2}\left[E-V(r)\right]\psi(r). \quad (2)$$

The first derivative can be eliminated from the right-hand side of Eq. (2) by using the transformation:

$$\psi(r)=\sqrt{m(r)}\phi(r). \quad (3)$$

This technique is based on the point-canonical transformation method.[56,62] Substituting Eq. (3) into Eq. (2), one obtains

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}r^2}+\left[\frac{1}{2m}\frac{\mathrm{d}^2m}{\mathrm{d}r^2}-\frac{3}{4}\left(\frac{1}{m}\frac{\mathrm{d}m}{\mathrm{d}r}\right)^2\right]\phi=-\frac{2m}{\hbar^2}\left[E-V(r)\right]\phi. \quad (4)$$

In the case of the Morse potential,[51] equation (4) turns into the following equation

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}+\left[\frac{m''}{2m}-\frac{3}{4}\left(\frac{m'}{m}\right)^2\right]\phi=-\frac{2mr_0^2}{\hbar^2}\left[E-D\left(\mathrm{e}^{-2\alpha x}-2\mathrm{e}^{-\alpha x}\right)\right]\phi. \quad (5)$$

Here

$$x=\frac{r-r_0}{r_0}, \quad (6)$$

and r_0 is the equilibrium position of the molecules and the prime sign denotes differentiation with respect to x. The parameter D describes the depth of the potential and the dimensionless parameter α characterizes the potential acting range. Applying

$$y=k\mathrm{e}^{-\alpha x}, \qquad k=\frac{r_0\sqrt{8m_0D}}{\hbar\alpha}, \quad (7)$$

where m_0 is a mass dimensional parameter, equation (5) turns into

$$y^2\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2}+y\frac{\mathrm{d}\phi}{\mathrm{d}y}+\left[\frac{y^2}{2m}\frac{\mathrm{d}^2m}{\mathrm{d}y^2}-\frac{3}{4m^2}y^2\left(\frac{\mathrm{d}m}{\mathrm{d}y}\right)^2+\frac{y}{2m}\frac{\mathrm{d}m}{\mathrm{d}y}\right]\phi=\frac{m}{m_0}\left(\frac{1}{4}y^2-\frac{k}{2}y+\beta^2\right)\phi, \quad (8)$$

where

$$\beta^2=-\frac{2Em_0r_0^2}{\alpha^2\hbar^2}. \quad (9)$$

Here, we use the following effective mass distribution

$$\frac{m(y)}{m_0}=\frac{\tau y}{\gamma+\eta y}, \quad (10)$$

where τ, γ, and η are constant parameters. Inserting Eq. (10) into Eq. (8) yields

$$y^2\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2}+y\frac{\mathrm{d}\phi}{\mathrm{d}y}=\left(D_1+D_2y+D_3y^2\right)\phi, \quad (11)$$

with this providing that the constants D_1, D_2, and D_3 must be

$$\begin{aligned} D_1&=\frac{1}{4},\\ D_2&=\frac{1}{16\beta^2}\left(\sqrt{k^2+4\beta^2}-k\right),\\ D_3&=-\frac{k}{32\beta^4}\left(\sqrt{k^2+4\beta^2}-k\right). \end{aligned} \quad (12)$$

Also, the mass parameters in Eq. (10) must be of the following form

$$\tau=\frac{D_2\gamma}{\beta^2}, \qquad \eta=-4\gamma D_2. \quad (13)$$

Substituting the above equations into Eq. (10) leads to

$$m(y)=\frac{m_0y}{4\beta^2(-y+y_\mathrm{c})}, \qquad y_\mathrm{c}=\frac{1}{4D_2}. \quad (14)$$

The mass function (14) is positive and convergent for $y<y_\mathrm{c}$. However, y has an upper limit $y_\mathrm{max}=k\mathrm{e}^{\alpha}$ which can be found for $x_\mathrm{min}=-1$ in Eq. (7). Therefore, this condition is well satisfied for $y_\mathrm{max}<y_\mathrm{c}$.

3. Bound state solutions

In the presence of the mass function (14) our Schrödinger equation turns into Eq. (11). In order to have finite solutions at large values of y, we should apply the following ansatz

$$\phi=y^{-\sqrt{D_1}}f(y)=y^{-1/2}f(y), \quad (15)$$

then equation (11) becomes

$$\left[y\frac{\mathrm{d}^2}{\mathrm{d}y^2}-\left(D_2+D_3y\right)\right]f=0. \quad (16)$$

Here we use the Laplace transformation method to solve Eq. (16),[3,46] By applying Laplace transform[41]

$$F(s)=\mathscr{L}[f(y)]=\int_0^\infty \mathrm{e}^{-sy}f(y)\,\mathrm{d}y,$$

the following equation can be obtained

$$\left(s^2+D_4^2\right)\frac{\mathrm{d}}{\mathrm{d}s}F(s)+[2s+D_2]F(s)=0, \tag{17}$$

where $D_4=\sqrt{-D_3}$ and from Eq. (12) $D_3<0$. Equation (17) is a first-order differential equation and its solutions are in the form

$$F(s)=N'\left(1-\frac{2\mathrm{i}D_4}{s+\mathrm{i}D_4}\right)^{[(\mathrm{i}/2)(D_2/D_4)-1]}(s+\mathrm{i}D_4)^{-2}, \tag{18}$$

where N' is a constant. Here the term

$$(1-2\mathrm{i}D_4/(s+\mathrm{i}D_4))^{[(\mathrm{i}2)(D_2/D_4)-1]}$$

is a multi-valued function. In order to have a single valued wave function we impose the condition

$$\frac{D_2}{D_4}=2n,\quad n=0,1,2,3,\ldots. \tag{19}$$

Now inserting Eqs. (7), (9), and (12) into Eq. (19), the eigenvalues of the bound states can be obtained as

$$E_n=-64Dn^2\left(1+16n^2\right). \tag{20}$$

In order to find the eigenfunctions, we should apply inverse Laplace transforms to Eq. (18). However, in order to do so, it needs to be expanded in power series. This leads to

$$F=N'\sum_{j=0}\frac{(-1)^j(in-1)!}{j!(in-1-j)!}(s+\mathrm{i}D_4)^{-(j+2)}(2\mathrm{i}D_4)^j. \tag{21}$$

After applying the inverse Laplace transform, we find

$$f(y)=N'\sum_{j=0}^{m}\frac{(-1)^j(in-1)!}{j!(in-1-j)!}\frac{y^{j+1}\,\mathrm{e}^{-\mathrm{i}D_4y}}{\Gamma(j+2)}(2\mathrm{i}D_4)^j. \tag{22}$$

The series expansion of the confluent hypergeometric functions is given as

$$\mathrm{F}(-m,\gamma,z)=\sum_{j=0}^{m}\frac{(-1)^j(m)!}{j!(m-j)!}\frac{\Gamma(\gamma)}{\Gamma(\gamma+j)}z^j. \tag{23}$$

Comparing Eq. (22) with Eq. (23) yields

$$f(y)=N'y\mathrm{e}^{-\mathrm{i}D_4y}\frac{\mathrm{F}(-\mathrm{i}n+1,2,\mathrm{i}D_4y)}{\Gamma(2)}. \tag{24}$$

Inserting Eq. (24) into Eq. (15) and then Eq. (3) and using Eq. (14), leads to

$$\psi_n(y)=N_n\frac{y\exp\left(-\mathrm{i}\dfrac{kn}{\beta_n^2}y\right)}{\left(-8n^2k\,y+\beta_n^2\right)^{1/2}}\mathrm{F}\left(-\mathrm{i}n+1,2,\mathrm{i}\frac{kn}{\beta_n^2}y\right), \tag{25}$$

where

$$\beta_n=4kn\left(1+16n^2\right)^{1/2}, \tag{26}$$

and equations (9) and (20) have also been used. Here N_n is the normalization factor.

4. Discussions

This study has introduced a possible mass distribution for the Morse potential, which has an analytical bound state solution via the Laplace transformation method. We have found a closed form for the eigenvalue and eigenfunction of the corresponding one dimensional Schrödinger equation. The prominent point of this study is the considered mass distribution which depends on the quantum number n. In fact, using Eqs. (12) and (26), the mass distribution Eq. (14) yields

$$m(y)=\frac{2n^2k}{\beta_n^2}\frac{y}{-8n^2k\,y+\beta_n^2}. \tag{27}$$

This mass function is convergent and positive for

$$y<\beta_n^2/8n^2k.$$

However, the upper bound of y is given by

$$y_{\max}=k\,\mathrm{e}^{\alpha}.$$

Therefore, by considering Eq. (26), our mass function is meaningful under the condition

$$y_{\max}<\beta_n^2/8n^2k, \tag{28a}$$

or

$$\alpha<\ln[2(1+16n^2)]. \tag{28b}$$

This relation establishes a condition for the starting point of the quantum number n. The case $n\geq 0$ works only for $\alpha<0.693$. In the case of H_2 and HCl molecules with $\alpha=1.440$ and $\alpha=2.380$ respectively, conditions (28a) and (28b) require $n\geq 1$. However for I_2, with $\alpha=4.954$, we must have $n\geq 2$. In order to have a schematic representation of the considered mass function, the distribution m/m_0 is plotted in Fig. 1 for some typical molecules.

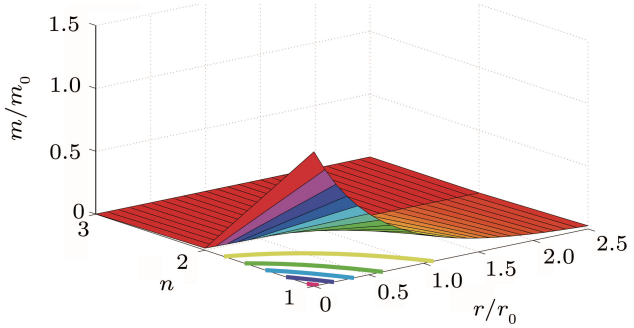


Fig. 1. (color online) Mass distribution $m(r)/m_0$ for $H_2$2 molecules versus position r/r_0 and quantum number n.

According to Fig. 1, the mass function is well concentrated around $r=r_0$.

Figure (2a) shows the energy spectra for three molecules H_2 ($D = 38292$ cm^{-1}), HCl ($D = 37244$ cm^{-1}), and I_2 ($D = 12550$ cm^{-1}). Figure(2b) presents the solutions of the eigenfunctions for H_2 molecules ($k = 34.9$) and for different quantum numbers n.

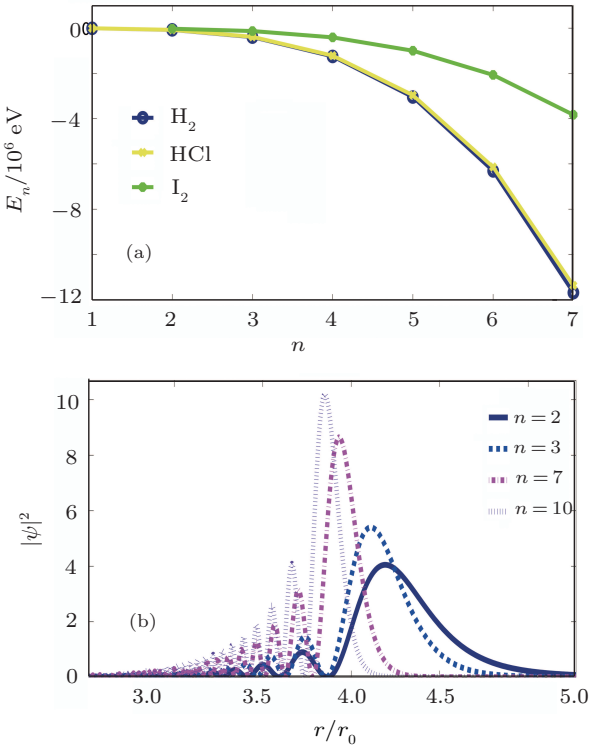


Fig. 2. (color online) The eigenvalues [Fig. (2a)] for three different kinds of molecules, and the eigenfunctions [Fig. (2b)] for H_2.

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