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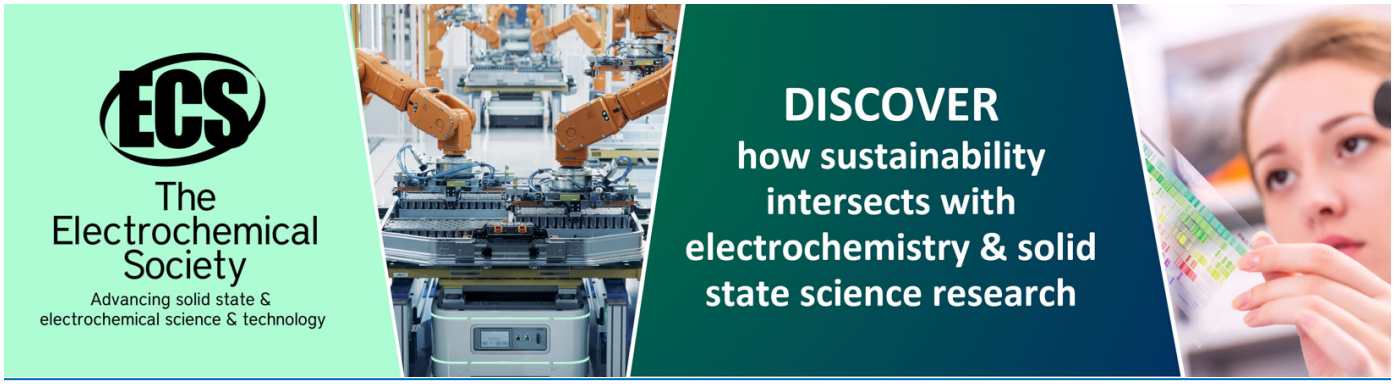

Position-Dependent Mass Schrödinger Equation for the Morse Potential

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Abstract. The position dependent mass Schrödinger equation (PDMSE) has a wide range of quantum applications such as the study of semiconductors, quantum wells, quantum dots and impurities in crystals, among many others. On the other hand, the Morse potential is one of the most important potential models used to study the electronic properties of diatomic molecules. In this work, the solution of the effective mass one-dimensional Schrödinger equation for the Morse potential is presented. This is done by means of the canonical transformation method in algebraic form. The PDMSE is solved for any model of the proposed kinetic energy operators as for example the BenDaniel-Duke, Gora-Williams, Zhu-Kroemer or Li-Kuhn. Also, in order to solve the PDMSE with Morse potential, we consider a superpotential leading to a special form of the exactly solvable Schrödinger equation of constant mass for a class of multiparameter exponential-type potential along with a proper mass distribution. The proposed approach is general and can be applied in the search of new potentials suitable on science of materials by looking into the viable choices of the mass function.

1. Introduction

The Morse potential [1] has been an adequate model for the potential energy function of diatomic molecules, which is the reason for its relevance in chemistry and molecular physics. Although there have been proposed several alternative models of potential functions in order to improve experimental data [2]-[8], Morse potential has maintained its relevance until nowadays [9]. In addition, alternative mentioned potentials are equivalent between them [10], a fact that contributes to maintaining the importance of the Morse potential. On the other hand, the position-dependent mass Schrödinger equation (PDMSE) has been of recent interest for its applications in fields such as condensed matter theory [11]-[15], hetero-structures [16]-[19], nuclear clusters [20]-[21], density functional theory [22]-[26] and related problems. At this regard, different proposals of the kinetic energy operator in the PDMSE Hamiltonian [27] have been considered as useful operators for applications, as for example BenDaniel and Duke [28], Gora-Williams [29], Zhu-Kroemer [30], Li-Kuhn [31], and so on.

In this work we present exact solutions of the Morse potential for the PDMSE and analyze the influence of the position-dependent mass (PDM) in the energy spectra. To solve the PDMSE is used

the point canonical transformation scheme [32], which algebraic presentation is known [33]-[34]. In this context it is revealed the potential function of a constant mass Schrödinger equation (CMSE) involved in the resolution. Our exposition considers obtain solutions for any kinetic energy operator of the PDMSE. The general ordering ambiguity has also been treated by means of the Nikiforov-Urvanov method [35]. To perform our task, we use the exact solution of the multiparameter exponential-type potential in the constant mass Schrödinger equation [36]. In this way, the next section outlines the algebraic relation between the PDMSE and the CMSE. Section 3 is devoted to show the use of the multiparameter exponential-type potential in order to solve the required Morse potential. Finally, we study the influence of the position-dependent mass on the energy spectra, which means comparing the CMSE energy spectrum and the PDMSE energy spectrum for the same Morse potential.

2. Algebraic approach to the PDMSE

Let us consider the position-dependent mass Schrödinger equation (PDMSE)

$$-\frac{d}{dx}\left(\frac{1}{2\,m(x)}\frac{d}{dx}\psi(x)\right)+\left(V(x)+U_{\alpha\gamma}(x)\right)\psi(x)=E\psi(x), \tag{1}$$

which comes from the von Roos's Hamiltonian $H_{\alpha\gamma}=T_{\alpha\gamma}+V(x)$, where the position-dependent mass kinetic energy operator $T_{\alpha\gamma}$ is [27]

$$T_{\alpha\gamma}=\frac{1}{4}\left[m^{\alpha}\,p\,m^{\beta}\,p\,m^{\gamma}+m^{\gamma}\,p\,m^{\beta}\,p\,m^{\alpha}\right], \tag{2}$$

$m=m_0\,m(x)$ is the mass operator, m_0 is the mass of the involved particle, $p=-i\hbar\,d/dx$ is the linear momentum operator and the parameters α, β, γ satisfy the constraint $\alpha+\beta+\gamma=-1$. We have selected the natural unit system with $\hbar=m_0=1$. The Eq. (1) follows after using the identity

$$T_{\alpha\gamma}=-\frac{d}{dx}\frac{1}{2m(x)}\frac{d}{dx}+U_{\alpha\gamma}(x), \tag{3}$$

with

$$U_{\alpha\gamma}(x)=\frac{1}{2}\left(\alpha\gamma+\alpha+\gamma\right)\frac{m'^{2}(x)}{m^{3}(x)}-\frac{1}{4}\left(\alpha+\gamma\right)\frac{m''(x)}{m^{2}(x)}, \tag{4}$$

and the expression $V(x)+U_{\alpha\gamma}(x)$ is usually named the effective potential $U_{\mathtt{eff}}(x)$. In [33] we proposed to use instead of Eq. (3) the one given by

$$T_{\alpha\gamma}=A_0^{+}A_0^{-}+\widehat{U}_{\alpha\gamma}(x) \tag{5}$$

where $A_0^{\pm}=\mp i\,\eta\,p\,\eta=\mp\eta\,\frac{d}{dx}\eta$, $\eta=(2m)^{-1/4}$ and

$$\widehat{U}_{\alpha\gamma}(x)=\frac{1}{2}\left(\alpha\gamma+\alpha+\gamma+\frac{7}{16}\right)\frac{m'^{2}}{m^{3}}-\frac{1}{4}\left(\alpha+\gamma+\frac{1}{2}\right)\frac{m''}{m^{2}}, \tag{6}$$

for which Eq. (1) turns to be

$$\left(A_0^{+}A_0^{-}+\widehat{U}_{\alpha\gamma}(x)+V(x)\right)\psi(x)=E\,\psi(x), \tag{7}$$

with the advantage that this form allows the factorization of the PDMSE

$$A^{+}A^{-}\psi(x)=E\,\psi(x), \tag{8}$$

with factorization operators A^{+} and A^{-} of the form

$$A^{\pm}=A_0^{\pm}+\widehat{W}(x). \tag{9}$$

By introducing the main potential

$$\widehat{V}(x)=\widehat{U}_{\alpha\gamma}(x)+V(x) \tag{10}$$

it results that function $\widehat{W}(x)$ satisfies

$$\widehat{V}(x)=\widehat{W}^2(x)-\eta^2\frac{d}{dx}\widehat{W}(x). \tag{11}$$

Then, the point canonical transformation defined by

$$\frac{d}{du}=\eta^2\frac{d}{dx}, \tag{12}$$

which means $u(x)=\int^x \eta^{-2}(x)\,dx$ and $x=x(u)$ its inverse function, and the functions of the new variable $\widehat{w}(u)=\widehat{W}(x(u))$, $\widehat{v}(u)=\widehat{V}(x(u))$ allows to get from Eq. (11)

$$\widehat{v}(u)=\widehat{w}^2(u)-\frac{d}{du}\widehat{w}(u). \tag{13}$$

This last equation is identified as the Riccati equation connecting a potential $\widehat{v}(u)$ with its superpotential $\widehat{w}(u)$ in the SUSYQM context. In fact, the factorization operators for a constant mass Schrödinger equation (CMSE) corresponding to this superpotential $a^{\pm}=\mp\frac{d}{du}+\widehat{w}(u)$ satisfy the operator identity

$$a^{\pm}=\eta\,A^{\pm}\eta^{-1}, \tag{14}$$

meaning that the factorized PDMSE Eq. (8) written in the form

$$\left(\eta A^{+}\eta^{-1}\right)\left(\eta A^{-}\eta^{-1}\right)\left(\eta\,\psi(x)\right)=E\left(\eta\,\psi(x)\right), \tag{15}$$

becomes the CMSE

$$a^{+}a^{-}\,\varphi(u)=E\,\varphi(u), \tag{16}$$

with CMSE eigenfunctions $\varphi(u)$ connected with the PDMSE eigenfunctions by $\varphi(u)=\eta(x(u))\psi(x(u))$.

Previous formalism shows that we can use any solvable potential $\widehat{v}(u)$ of the CMSE to get a solvable main potential

$$\widehat{V}(x)=\widehat{v}(u(x)) \tag{17}$$

of the PDMSE Eq. (8), with solutions given by

$$\psi(x)=\eta^{-1}(x)\,\varphi(u(x)). \tag{18}$$

The ground-state energy of CMSE is set to zero (good SUSYQM) and the ground-state eigenfunction is obtained from $a^{-}\varphi_0(u)=0$, which is $\varphi_0(u)=\exp(-\int^u \widehat{w}(u)du)$, this implies the ground state of the PDMSE in the form

$$\psi_0(x)=\eta^{-1}\,e^{-\int^{u(x)}\frac{\widehat{W}(x)}{\eta^2}dx}, \tag{19}$$

although it can also be obtained from $A^{-}\psi_0(x)=0$.

The main potential Eq. (10) corresponds to the PDMSE with kinetic energy operator determined by selection of operators Eq. (8) which means $\alpha=\gamma=-1/4$. The solvable potentials for other kinetic energy operators come from Eq. (10), that is

$$V(x)=\widehat{V}(x)-\widehat{U}_{\alpha\gamma}(x), \tag{20}$$

with $\widehat{U}_{\alpha\gamma}(x)$ given in Eq. (6) or alternatively by

$$\widehat{U}_{\alpha\gamma}(x)=(4\alpha+1)(4\gamma+1)\eta^2\eta'^2+\left(\alpha+\gamma+\frac{1}{2}\right)\eta^2\left(\eta^2\right)'', \tag{21}$$

where the apostrophe indicates derivative with respect to variable x. Table I lists some solvable PDMSE for particular choices of α and γ.

$\alpha,\ \gamma$	$\widehat{U}_{\alpha\gamma}(x)$	$V(x)=\widehat{V}(x)-\widehat{U}_{\alpha\gamma}(x)$
$\alpha=\gamma=0$	0	$\widehat{V}(x)$
$\alpha=\gamma=0$	$\eta^2(\eta')^2+\frac{1}{2}\eta^2(\eta^2)''$	$V^{BDD}(x)$, BenDaniel-Duke
$\alpha=-1,\ \gamma=0$	$-3\eta^2(\eta')^2-\frac{1}{2}\eta^2(\eta^2)''$	$V^{GW}(x)$, Gora-Williams
$\alpha=\gamma=-1/2$	$\eta^2(\eta')^2-\frac{1}{2}\eta^2(\eta^2)''$	$V^{ZK}(x)$, Zhu-Kroemer
$\alpha=0,\ \gamma=-1/2$	$-\eta^2(\eta')^2$	$V^{LK}(x)$, Li-Kuhn

Table I. Parameters and solved potentials of typical Hamiltonians $H_{\alpha\gamma}$ for the PDMSE.

3. Exact solutions to the Morse potential

Now in order to solve PDMSE with Morse potential we will resort to the CMSE solutions of exponential type, given in ref. [36], and which are obtained from the superpotential

$$\widehat{w}(u)=\frac{K^2+A_0-B_0}{2K}+K\frac{e^{-u}}{1-e^{-u}}, \tag{22}$$

that allows to write the CMSE potential in the form

$$\widehat{v}(u)=\left(\frac{K^2+A_0-B_0}{2K}\right)^2+\frac{A_0e^{-u}}{1-e^{-u}}+\frac{B_0e^{-2u}}{\left(1-e^{-u}\right)^2}, \tag{23}$$

so that A_0, B_0 are the weights of the exponential functions involved and the value $K=-\left(\sqrt{1+4B_0}+1\right)/2$ is selected to acomplish the required eigenvalue $E_0=0$. There is a total of $n_{\max}+1$ eigenstates which eigenfunctions are

$$\begin{aligned}\varphi_n(u)&=N_n\left(\exp(-u)\right)^{(c-1)/2}\left(1-\exp(-u)\right)^{(-n+b-c+1)/2}\\&\quad\times{}_2F_1\left(-n,b;c;\exp(-u)\right),\\N_n&=\sqrt{\frac{(c-1)\Gamma(n+c)\Gamma(b)\Gamma(n+b)}{n!(n+b+1-c)\Gamma^2(c)\Gamma(b+1-c)}},\end{aligned} \tag{24}$$

for $n=0,1,2...n_{\max}$. The involved parameters are given by

$$\begin{aligned}c&=\frac{-2n(h+n)-2A_0}{h+2n+1}\\b&=\frac{(h+1)(h+n)-2A_0}{h+2n+1}\\h&=\sqrt{1+4B_0}\\0&<n_{\max}<\sqrt{B_0-A_0}+K\end{aligned} \tag{25}$$

and the eigenvalues are

$$E_n=\left(\frac{K^2+A_0-B_0}{2K}\right)^2-\left(\frac{(n-K)^2+A_0-B_0}{2(n-K)}\right)^2. \tag{26}$$

Let us consider the mass function

$$m(x)=\frac{1}{2}\left(\frac{a}{1+\lambda e^{-ax}}\right)^2, \tag{27}$$

associated with the η function

$$\eta=\sqrt{\frac{1+\lambda e^{-ax}}{a}}, \tag{28}$$

and the variable change

$$\lambda e^{-ax}=\frac{e^{-u}}{\left(1-e^{-u}\right)}. \tag{29}$$

Eq. (23) expressed in variable x gives the solvable potential of the main PDMSE, that is, corresponding to $\alpha=\gamma=-1/4$, which is

$$\widehat{V}(x)=\left(\frac{K^2+A_0-B_0}{2K}\right)^2+\lambda A_0 e^{-ax}+\lambda^2 B_0 e^{-2ax} \tag{30}$$

it being a Morse potential for the main PDMSE. By using Eq. (18) the eigenfunctions will be given by

$$\begin{aligned}\psi_n(x)&=\eta^{-1}\varphi_n(u(x))\\ &N_n\sqrt{\frac{a}{1+\lambda e^{-ax}}}\left(\frac{\lambda e^{-ax}}{1+\lambda e^{-ax}}\right)^{(c-1)/2}\left(\frac{1}{1+\lambda e^{-ax}}\right)^{(-n+b-c+1)/2}\\ &\times{}_2F_1\left(-n,b;c;\frac{\lambda e^{-ax}}{1+\lambda e^{-ax}}\right).\end{aligned} \tag{31}$$

A property of mass function Eq. (27) is that the corresponding solvable potential for any $T_{\alpha\gamma}$ of the PDMSE, is a generalized Morse potential, in particular, one obtains for the cases listed in Table I, the following solvable cases

$$V^{BDD}(x)=\left(\frac{K^2+A_0-B_0}{2K}\right)^2+\lambda\left(A_0-\frac{1}{2}\right)e^{-ax}+\lambda^2\left(B_0-\frac{3}{4}\right)e^{-2ax}, \tag{32}$$

$$V^{GW}(x)=\left(\frac{K^2+A_0-B_0}{2K}\right)^2+\lambda\left(A_0+\frac{1}{2}\right)e^{-ax}+\lambda^2\left(B_0+\frac{5}{4}\right)e^{-2ax}, \tag{33}$$

$$V^{ZK}(x)=\left(\frac{K^2+A_0-B_0}{2K}\right)^2+\lambda\left(A_0+\frac{1}{2}\right)e^{-ax}+\lambda^2\left(B_0+\frac{1}{4}\right)e^{-2ax}, \tag{34}$$

$$V^{LK}(x)=\left(\frac{K^2+A_0-B_0}{2K}\right)^2+\lambda A_0 e^{-ax}+\lambda^2\left(B_0+\frac{1}{4}\right)e^{-2ax}. \tag{35}$$

In Figure 1 we have drawn these potentials and also the main potential $\widehat{V}(x)$ by taking a value of

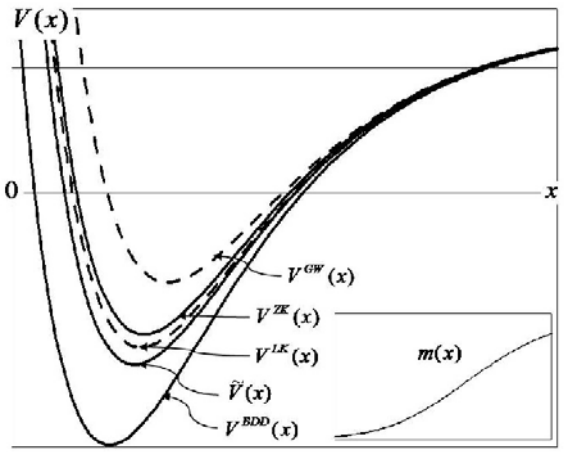

Figure 1. Solvable PDMSE Morse potentials $V(x)$ for the most important Hamiltonians listed in Table I. The graph of PDM. Mass parameter is λ= 2.5. Horizontal lines represent E_0 and E_1.

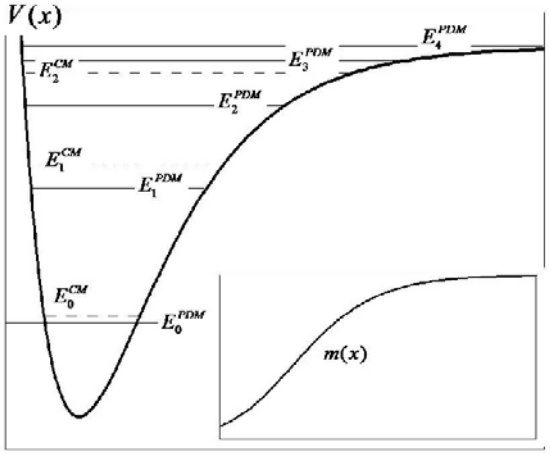

Figure 2. The PDMSE potential $\widehat{V}(x)$ given in Eq. (30) and the Morse CMSE potential of Eq. (36) are made to coincide thus we can see the changes in the eigenvalue spectra. PDM with λ = 0.5.

parameter λ which allows to elucidate a difference between the potentials up to the order of the first gap of the energies.

On the other hand, for small values of λ or $\lambda \approx 1$, the difference between the solved potentials is negligible and we can say that the reported solutions of the potential $\widehat{V}(x)$ correspond to any PDMSE with any value of α and γ. Figure 2 contains the graphs of the five reported potentials which are practically the same potential. Besides, we are able to compare the energies as given in Eq. (26) for the PDMSE, with those that come from considering the CMSE Morse potential written through its depth $D = \lambda^2 B_0 = -\lambda A_0 / 2$ in the form

$$\widehat{V}(x,\lambda) = F^2(D,\lambda) + D\left(e^{-2ax} - 2e^{-ax}\right), \tag{36}$$

where

$$F^2(D,\lambda) = \left(\frac{\left(K(D,\lambda)\right)^2 - D\left(\frac{1+2\lambda}{\lambda^2}\right)}{2K(D,\lambda)} \right)^2, \tag{37}$$

and

$$K(D,\lambda) = -\left(\sqrt{1 + \frac{4D}{\lambda^2}} + 1 \right) / 2. \tag{38}$$

We have selected a depth D in the potential of Eq. (36) that gives three eigenvalues of the constant mass case and determined the eigenenergies of the PDM case. One can see a difference between the number and value of the eigenenergies. The PDM eigenenergies are deeper and the number of eigenstates is greater as compared with those of the CMSE. We refer to the ref. [34] for similar reports on the effect of the PDM in the energy spectra.

Concluding Remarks

The point canonical transformation method to solve the PDMSE starting from exactly-solvable potentias of the CMSE is presented in an algebraic form. It consists of a unified treatment to the quantum position-dependent mass problems that contains, as particular cases, the kinetic energy operators of various authors such as BenDaniel-Duke, Gora-Williams, Zhu-Kroemer and Li-Kuhn, among others. We have considered the CMSE with multiparameter exponential-type potential to find solvable PDMSE with Morse potential. After, we have studied the influence of the position-dependent

mass on the energy spectra. Our results show that PDM distribution affects the eigenvalues, allowing a greater number of eigenstates for a potential with a specific deep. Also, it is found that in a certain range of the mass parameter, there is no difference with respect to the kinetic energy operator considered for the PDMSE. Finally, the algebraic proposal to solve the PDMSE is general and can easily be extended to other potential models and/or position-dependent mass distributions.

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