On the position-dependent mass Schrödinger equation for Mie-type potentials

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Abstract. The exactly solvable Position Dependent Mass Schrödinger Equation (PDMSE) for Mie-type potentials is presented. To that, by means of a point canonical transformation the exactly solvable constant mass Schrödinger equation is transformed into a PDMSE. The mapping between both Schrödinger equations lets obtain the energy spectra and wave functions for the potential under study. This happens for any selection of the O von Roos ambiguity parameters involved in the kinetic energy operator. The exactly solvable multiparameter exponential-type potential for the constant mass Schrödinger equation constitutes the reference problem allowing to solve the PDMSE for Mie potentials and mass functions of the form given by $m(x) = \frac{ske^{-x}}{(x^2 + 1)}$. Thereby, as a useful application of our proposal, the particular Lennard-Jones potential is presented as an example of Mie potential by considering the mass distribution $m(x) = \frac{ske^x}{(x^2 + 1)}$\textsuperscript{2}. The proposed method is general and can be straightforwardly applied to the solution of the PDMSE for other potential models and/or with different position-dependent mass distributions.

1. Introduction

Historically, the Position Dependent Mass Schrödinger Equation (PDMSE) comes as a proposition to solve many-body problems in solid state and condensed matter physics [1]. To mention some of them, in the study of the dynamics of electrons in semiconductor heterostructures [2-3], graded crystals [4], quantum liquids [5], crystal-growth techniques [6], quantum wells and quantum dots [7], Helium clusters [8] and so on. To that purpose, different approaches has been used to find analytical solutions of the PDMSE as, among others, the Green’s function [9], the Heun equations [10], Lie algebras [11], factorization method and supersymmetry [12], and the point canonical transformation method [13]. Also, in the case of particular ambiguity ordering parameters in the kinetic energy operator of the PDMSE Hamiltonian, stand out the BenDaniel and Duke [14], Gora-Williams [6], Zhu-Kroemer [15] and Li-Kuhn [16] proposals. In addition, the general ambiguity ordering has been treated by means of the Nikiforov-Uvarov method [17]. So, on one hand the study of physical systems endowed with a position-dependent mass remains a fundamental issue of quantum mechanics and on the other hand the Mie potential [18] is a model of molecular interaction, very useful in the study of diatomic molecules because it comprises a repulsive part at short distances and an attractive part for large distances allowing to describe the softness/hardness of the repulsive interactions as well as the range of

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attractions. Consequently, the Mie potential and one of its particular cases, the Lennard-Jones potential [19], are the most celebrated interaction potential models used to get thermodynamic properties [20], phase diagrams of fluids [21], molecular dynamics calculations [22] and so on. However, as far as we know, the Mie potential has not been considered in the frame of the PDMSE reason why their study constitutes the objective of this work. For that, in order to find the exactly solvable PDMSE for Mie-type potentials with an specific position dependent mass distribution \( m(x) \), in this contribution we present an algorithm based on the point canonical transformation method [23] applied to the PDMSE together with the procedure used to find the exactly solvable Schrodinger equation for a class of multiparameter exponential-type potential [24] with the aim to get the eigensolutions of the Mie potential models. In this way, the next section outlines the algebraic relation between the PDMSE and the Constant Mass Schrödinger Equation (CMSE). Section 3 is devoted to show the use of the multiparameter exponential-type potential method in order to solve the required Mie potential. The application of our proposal for the position dependent mass distribution \( m(x) = \left( skx^{n-1}/(x^n + 1) \right)^2 \) is given in section 4. Finally, section 5 is devoted to the concluding remarks where we emphasize the importance of the position dependent mass for Mie-type potentials.

2. The point canonical transformation applied to PDMSE.

The O von Roos's Hamiltonian [11] given by

\[
\hat{H}_a = \frac{i}{\hbar} \left[ \hat{\eta}^{-}\hat{\eta}^{+} \hat{\eta}^{\beta} \hat{\eta}^{\beta} \hat{\eta}^{\gamma} + \hat{\eta}^{\beta} \hat{\eta}^{\beta} \hat{\eta}^{\gamma} \right] + V(x) \tag{1}
\]

where \( \hat{m} = 2m_0m(x) \) 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 ambiguity ordering parameters \( \alpha, \beta, \gamma \) satisfy the constraint \( \alpha + \beta + \gamma = -1 \). Using natural units \( \hbar = 2m_0 = 1 \), and following the presentation of BenDaniel-Duke [14], the general form of the position-dependent mass Schrödinger equation (PDMSE) \( \hat{H}_a \psi(x) = E \psi(x) \), is written as

\[
-\frac{d}{dx} \left( \frac{1}{m(x)} \frac{d}{dx} \psi(x) \right) + V_{\text{eff}}(x) \psi(x) = E \psi(x),
\tag{2}
\]

where \( V_{\text{eff}}(x) = V(x) + U(x) \) and

\[
U(x) = (\alpha \gamma + \alpha + \gamma) \frac{m^2(x)}{m^3(x)} - \frac{1}{2} (\alpha + \gamma) \frac{m''(x)}{m^2(x)} \tag{3}
\]

At this point, it should be noticed that equation (2) can have the alternative form [25]

\[
-\eta \frac{d}{dx} \eta \frac{d}{dx} \eta \psi(x) + V_{\text{eff}}^{M}(x) \psi(x) = E \psi(x),
\tag{4}
\]

where \( \eta = m^{-1/4}, V_{\text{eff}}^{M}(x) = V(x) + U^{M}(x), \) with

\[
U^{M}(x) = U(x) + \frac{7}{16} \frac{m^2(x)}{m^3(x)} - \frac{1}{4} \frac{m''(x)}{m^2(x)} \tag{5}
\]

In addition, the PDMSE of equation (4) is factorized into the form

\[
\hat{A}^{+} \hat{A}^{-} \psi(x) = E \psi(x) \tag{6}
\]

where

\[
\hat{A}^{\pm} = \mp i \eta \frac{d}{dx} \eta + W = \mp i \eta \frac{d}{dx} \eta + W \tag{7}
\]

such that a superpotential \( W(x) \) should satisfy

\[
V_{\text{eff}}^{M}(x) = W(x)^2 - \eta^2 \frac{d}{dx} W(x). \tag{8}
\]
Also, if equation (4) is expressed into the form
\[ -\eta^2 \frac{d}{dx} \eta \frac{d}{dx} [\eta \psi(x)] + V^M_{\text{eff}}(x)[\eta \psi(x)] = E[\eta \psi(x)], \tag{9} \]
the point canonical transformation defined by
\[ u = u(x) = \int^{x} \sqrt{m(t)} \, dt = \int^{x} (\eta(t))^{-2} \, dt \tag{10} \]
\[ \phi(u) = \eta(x(u)) \psi(x(u)) \tag{11} \]
transforms the PDMSE given in equation (9) into the CMSE
\[ -\frac{d^2 \phi(u)}{du^2} + [V^M_{\text{eff}} - E]\phi(u) = 0 \tag{12} \]
where \( V^M_{\text{eff}}(u) = V^M_{\text{eff}}(x(u)) \) in such a way that equation (8) is recognized as the usual relation between this CMSE potential \( V^M_{\text{eff}}(u) \) and its superpotential
\[ V^M_{\text{eff}} = W(u)^2 - \frac{dW(u)}{du}. \tag{13} \]
Consequently, the potential in CMSE and the \( V(x) \) potential in the PDMSE are related by
\[ V^M_{\text{eff}}(u) = V(x(u)) + U^M(x(u)). \tag{14} \]
Also, by means of the function
\[ Z(u) = \frac{d}{du} \ln[m(x(u))]^{-1/4} \tag{15} \]
equation (5) is rewritten as
\[ U^M = \alpha_M \gamma_M Z(u)^2 + \frac{1}{2} (\alpha_M + \gamma_M) \frac{dZ(u)}{du} \tag{16} \]
with \( \alpha_M = 4\alpha + 1, \gamma_M = 4\gamma + 1 \). Besides, it is worth noting that in the case of the BenDaniel-Duke approach \[14\] applied to the PDMSE one has \( \alpha = \gamma = 0 \), for which Equation (16) is a Riccati relationship, while in the case of \( \alpha_M = \gamma_M = 0 \), both potentials in the CMSE and PDMSE are equal, i.e. \( V^M_{\text{eff}} = V \). In short, from the above, one concludes the existence of several exactly solvable PDMSE of potential \( V^M_{\text{eff}} = V \), each one depending on the choice of the analytical form of \( m(x) \) which indicates the variable change to be used. For that, and in order to complete our proposal, next section is devoted to the treatment of the CMSE for a class of exactly solvable multiparameter exponential-type potentials.

3. Multiparameter exponential-type potentials.
With the aim to use the method displayed above to the PDMSE with Mie type potentials, we first consider the exactly solvable CMSE for a class of multiparameter exponential-type (MET) potentials. These potentials are \[26\]
\[ V^\pm(u) = \frac{A q e^{-u/k}}{1 \pm q e^{-u/k}} + \frac{B q e^{-u/k}}{(1 \pm q e^{-u/k})^2} + \frac{C q^2 e^{-2u/k}}{(1 \pm q e^{-u/k})^2} \]

with \( k > 0, q > 0, h = 2m_0 = 1 \), having energy spectra given by
\[ E_n^\pm = -\left(\frac{1}{4k}\right)^2 \left(2n + 1 \mp h^\pm - \frac{4k^2(C \mp A)}{2n + 1 \mp h^\pm}\right)^2, \quad h^\pm = \sqrt{1 + 4k^2(C \mp B)} \]

with eigenfunctions
\[ \varphi_n^\pm(u) = (e^{-u/2k})^{b^\pm - c^\pm - n}(1 \pm q e^{-u/k})^{c^\pm/2} {}_2F_1\left(-n, b^\pm; c^\pm; 1 \pm q e^{-u/k}\right) \]

where \( {}_2F_1(a, b^\pm; c^\pm; x) \) is the hypergeometric function with \( a = -n; n = 0,1,2,3, \ldots, \) and
\[ b^\pm = \frac{2k^2(C \mp A)}{2n + 1 \mp h^\pm} + \frac{1 \mp h^\pm}{2}, \]
\[ c^\pm = 1 \mp h^\pm. \]

It should be noted that according to Peña et al [26], the condition \( (d/du) V^\pm(u) = 0 \) leads to a minimum value for \( V^\pm(u) \) with sufficient depth for the existence of bound states, namely
\[ V^\pm(u_{min}^\pm) = -\left(\frac{1}{4k}\right)^2 \frac{(A + B)^2}{(C \mp B)^2}. \]

on condition that
\[ A + B < 0 \leq C \mp B. \]

Furthermore, \( \varphi_n^\pm(u) \rightarrow 0 \) when \( u \rightarrow \infty \) implies that \( b^\pm - c^\pm - n > 0 \), for which, the number of states is
\[ 0 \leq n < \mp k \sqrt{|C \pm A|} - \frac{1 \mp h^\pm}{2}. \]

Accordingly to our proposal, the solutions of \( V^\pm(u) \) in the CMSE will be used to solve the PDMSE for the selected \( m(x) \) as indicated in the next section.

4. Applications on the PDMSE for \( m(x) = \left(\frac{skx^{s-1}}{(x^s + 1)}\right)^2 \).

The purpose now is to solve the PDMSE for the case of Mie-type potentials, which standard form is [18]
\[ V(x) = \left(\frac{n}{n - m}\right)\left(\frac{n}{m}\right)^{n-m} E \left[\left(\frac{\sigma}{x}\right)^n - \left(\frac{\sigma}{x}\right)^m\right] \]

where \( E \) is the well depth which occurs at \( x = \sigma \). We focus at the particular case when \( n = 2m \) for which, expression above simplifies to
\[ V(x) = 4E \left[\left(\frac{\sigma}{x}\right)^{2m} - \left(\frac{\sigma}{x}\right)^m\right] \]

and covers the case of the Lennard-Jones potential with explicit expression [19].
\[ V(x) = 4\varepsilon \left( \frac{a}{x}^6 - \frac{a}{x}^2 \right) \]  
(26)

As previously mentioned, the position dependent mass distribution \( m(x) = \left( s k x^{s-1} / (x^s + 1) \right)^2 \) is a versatile form that allows to adjust its parameters to match for a class of Mie potentials as described in equation (25). In this section, we use the exponential-type potentials of previous section as the effective potentials, that is, the CMSE potential in order to solve the Mie-type potential in the PDMSE. Accordingly to equation (17), it will be compulsory to analyze the above mass distribution, separately for \( V^- (u) \) and for its partner \( V^+ (u) \) potential.

4.1. The \( V^- (u) \) potential and the Mie \( V(x) \) potential.

In this case, the mass distribution

\[ m(x) = \left( s k x^{s-1} / (x^s + 1) \right)^2 \]  
(27)

is used in equation (10) to obtain \( u = k \ln(x^s + 1) + C \) where the integration constant \( C \), if assumed to be \( C = k \ln q \) allows to write the variable change as

\[ \frac{qe^{-u/k}}{1 - qe^{-u/k}} = x^{-s} \]  
(28)

for any \( q > 0 \). Without lost of generality we can take the \( V^- (u) \) in the particular case \( q = 1 \) hereafter, so that both variables \( x \) and \( u \) range in the interval \((0, \infty)\). The case \( \alpha_M = \gamma_M = 0 \) corresponds to the position dependent mass (PDM) potential, that according to equation (14) will be

\[ V(x) = V^- (u(x)) = (A + B) x^{-s} + (B + C) x^{-2s} \]  
(29)

which matches with equation (25), i.e. the Mie potential. In the general case \( \alpha_M \neq 0 \) and \( \gamma_M \neq 0 \) of the O von Roos Hamiltonian, the equation (15) gives

\[ Z(u(x)) = \left( \frac{1}{2k} \right) (1 + (s - 1)x^{-s}) \]  
(30)

\[ \frac{dZ}{du} (u(x)) = \left( \frac{s - 1}{2k^2 s} \right) (x^{-s} + x^{-2s}) \]  
(31)

in such a way that from equation (16)

\[ U^M = D_1 + D_2 x^{-s} + D_3 x^{-2s} \]  
(32)

\[ D_1 = \frac{\alpha_M \gamma_M}{4k^2 s^2} \]  
(33)

\[ D_2 = \frac{s - 1}{4k^2 s} \left( \frac{2\alpha_M \gamma_M}{s} + \alpha_M + \gamma_M \right) \]  
(34)

\[ D_3 = \frac{s - 1}{4k^2 s} \left( \frac{s - 1}{s} \alpha_M \gamma_M + \alpha_M + \gamma_M \right) \]  
(35)
that, according with equation (14), leads to the solvable PDM potential

\[ V(x) = -D_1 + (A + B - D_2) x^{-5} + (B + C - D_3) x^{-2} \]  

which is again a Mie-type potential. The energies and wavefunctions come from equations (18) and (19) respectively. For example, in this case the energies are given by

\[ E_n^- = -D_1 - \left( \frac{1}{4k} \right)^2 \left( 2n + 1 + h^- - \frac{4k^2(C - D_3 - A + D_2)}{2n + 1 + h^-} \right)^2, \]

\[ h^- = \sqrt{1 + 4k^2(C + B - D_3)}. \]  

4.2. The \( V(u) \) potential and the \( V(x) \) Lennard-Jones potential.

The PDM distribution to be used in the Lennard-Jones (\( s = 6 \)) case is

\[ m(x) = \frac{6kx^5}{(x^6 + 1)^2} \]

for which the proposed variable change is

\[ e^{-u/k} \]

\[ 1 - e^{-u/k} = x^{-6}. \]  

Then, for \( x, u \) in the interval \((0, \infty)\) and \( \alpha_M = \gamma_M = 0 \), the PDM potential is, after equation (14), given by

\[ V(x) = V^-\left(u(x)\right) = (A + B) x^{-6} + (B + C) x^{-12} \]  

which corresponds to the Lennard-Jones potential.

In the general case \( \alpha_M \neq 0 \) and \( \gamma_M \neq 0 \) of the O von Roos Hamiltonian, one has

\[ Z(u(x)) = \frac{1}{12k^2} (1 + 5x^{-6}) \]

\[ \frac{dZ}{du}(u(x)) = \frac{5}{12k^2} (x^{-6} + x^{-12}) \]  

in such a way that from equation (16)

\[ U^M = D_1 + D_2 x^{-6} + D_3 x^{-12} \]

\[ D_1 = \frac{\alpha_M \gamma_M}{144k^2} \]

\[ D_2 = \frac{5}{24k^2} \left( \frac{1}{3} \alpha_M \gamma_M + \alpha_M + \gamma_M \right) \]

\[ D_3 = \frac{5}{24k^2} \left( \frac{1}{6} \alpha_M \gamma_M + \alpha_M + \gamma_M \right). \]
With that, according to equation (14), the solvable Lennard-Jones PDM potential is
\[ V(x) = -D_1 + (A + B - D_2)x^{-6} + (B + C - D_2)x^{-12}, \]
where as before, the energies and wavefunctions come from equations (18) and (19).

Concluding Remarks
In this work, the point canonical transformation method to solve the PDMSE starting from exactly-solvable potentials of the CMSE is presented. For the constant mass Schrödinger equation we have considered the exactly solvable Schrödinger relationship for a class of multiparameter exponential-type potential in order to find solutions of the PDMSE. As a useful application of the proposal, we have considered the PDMSE for Mie-type potentials. Explicitly, we have used the position dependent mass distribution \( m(x) = (skx^r/(x^s + 1))^2 \) for the Mie potential and \( m(x) = (6kx^5/(x^6 + 1))^2 \) for their partner Lennard-Jones model. However, the algebraic proposal to solve the PDMSE is general and can easily be extended to other potential models and/or other position-dependent mass distributions.

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