Effective mass Schrödinger equation with Thomas-Fermi potential

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Abstract. The exactly-solvable position-dependent mass Schrödinger equation (PDMSE) for the Thomas-Fermi potential is presented. The PDMSE is transformed into a standard Schrödinger equation (SSE) with constant mass by means of a point canonical transformation scheme. By proposing an exponential type potential of the SSE it is possible to determine a PDMSE with the Thomas-Fermi potential. The resulting PDMSE is carried to the Sturm-Liouville form and the corresponding theory is developed for the particular resulting problem in order to obtain closed solutions in terms of Bessel functions of the first kind. Beyond the case considered in this work, the approach is general and can be useful in the study of electronic properties of non-uniform materials in which the carrier effective mass depends on the position as well as in the search of new solvable potentials suitable for quantum systems.

Keywords and Phrases: Position-dependent mass, Point canonical transformation, Thomas-Fermi potential, Schrödinger equation.

1. Introduction.
The quantum problem of position-dependent mass comes from the effective mass approximation [1] used for studying the motion of carrier electrons in nanostructured systems. The one-dimensional position-dependent mass Schrödinger equation (PDMSE) occurs in the quantum treatment of the electronic properties of semiconductors, liquid crystals, quantum dots and non uniform materials in which the carrier effective mass depends on the position [2]-[5]. The exactly solvable PDMSE has attracted considerable theoretical attention as demonstrated by already published methods on the subject such as the kinetic energy operator [6], Lie algebras [7],[8], supersymmetry [9] and path integration [10] approaches. Besides, the point canonical transformation method (PCTM) is an approach providing exact eigenvalues and eigenfunctions [11],[12] and can also be used to solve the PDMSE [13],[14]. In section II we describe the fundamentals of PCTM used to transform the PDMSE in variable \( x \) into a standard Schrödinger equation (SSE), in a new variable \( u \), where the mass no longer depends on the position. The potential associated to the PDMSE and the potential involved in the SSE are connected through a Riccati-type relationship which includes a superpotential intrinsically determined by the mass distribution. To attain the purpose of this work, in section III, we assume that the superpotential is constant and consequently it is recognized an exactly-solvable PDMSE with the Thomas-Fermi potential for a specific mass function. This important potential has been studied previously under position-dependent mass conditions [15],[16]. In this work, orthogonal...
eigenfunctions and normalization constants are calculated in closed form by developing the particular details involved in the Sturm-Liouville theory for the corresponding SSE. It is proved that the eigenstates are those of definite parity with eigenvalues expressed through the order of the Bessel functions of the first kind. Straightforwardly, the proposal can be used with another former potential in the search of those PDMSE that could be useful in quantum applications where, for example, the chemical composition is a point to consider.

2. Position-dependent mass Schrödinger equation.

The PDMSE for known $\psi_n(x)$ in the Levy-Leblond representation is given by [17]

$$\frac{\hbar^2}{2m(x)} \psi''_n(x) - \left( \frac{\hbar^2}{2m(x)} \right)' \psi'_n(x) + (E_n - V(x)) \psi_n(x) = 0,$$

(1)

where $E_n$ is the energy spectra, $m(x)$ is the position-dependent mass function and $V(x)$ is the potential function. With the aim to transform the equation above into a Schrödinger equation for constant mass, it is proposed the point canonical transformation

$$x = F(u) = g^{-1}(u),$$

(2)

such that

$$u = g(x) = \int_x^\infty \sqrt{M(t)} dt,$$

(3)

$(M(x) = m(x)/m_0$ being the dimensionless form of the mass function and $m_0$ the mass of the carrier particle) and the similarity transformation

$$\psi_n(x) = \varphi(g(x)) \sqrt{g'(x)}.$$

(4)

With this elements, the PDMSE given in Eq.(1) is transformed into the SSE given by

$$-\frac{\hbar^2}{2m_0} \varphi''_n(u) + U(u) \varphi_n(u) = E_n \varphi_n(u),$$

(5)

where the potentials are related by the Riccati-type equation

$$U(u) = V(F(u)) + \frac{\hbar^2}{2m_0} \left( W^2(u) + \frac{dW(u)}{du} \right),$$

(6)

with

$$W(u) = -\frac{1}{4} \frac{d}{du} \ln (M(F(u)),$$

(7)

which determines the position-dependent mass distribution in the form

$$M(x) = \exp \left( -4 \int_{g(x)}^{g(t)} W(t) dt \right).$$

(8)

Previous Eq. (6) shows that $W(x)$ is an essential function because it plays the role of a link between the PDMSE and the SSE. We can use $W(x)$ as in the case of the Witten superpotential [18], that is, to generate solvable cases for the PDMSE. In this case the scheme depends on the proposed solvable potential for the SSE [14]. The proposal of constant values for the function $W(x)$ has allowed to select an appropriate mass distribution Eq. (8) as well as an exactly-solvable exponential-type potential for the SSE in order to solve analytically the PDMSE for the Thomas-Fermi potential, as it will be seen in the next section. Eventually, the same procedure can be extended for other potential models.
3. PDMSE for the Thomas-Fermi Potential.

Previous considerations have carried us to consider the mass distribution

$$M(x) = \frac{1}{(\alpha \, |x| + 1)^2},$$

(9)

that gives respectively the transformation \(g(x)\) and its corresponding inverse function \(F(u)\), see Eqs.(3,4), in the form

$$g(x) = \frac{1}{\alpha} \ln(\alpha \, |x| + 1), \quad x \in (-\infty, \infty), \quad u \in (0, \infty).$$

(10)

$$F(u) = \pm \frac{e^{\alpha u} - 1}{\alpha}, \quad u \in (0, \infty).$$

(11)

In consequence, \(W(u) = \alpha/2\), with \(\alpha\) constant. Also, from the Eq.(6), the potentials are related by

$$V(F(u)) = U(u) - U_0,$$

(12)

with \(U_0 = \frac{\hbar^2 \alpha^2}{8m_0}\). Let us propose as solvable potential for the SSE Eq.(5) the exponential-type potential given by

$$U(u) = -V_0 e^{-\beta u} + U_0,$$

(13)

for which the potential of the PDMSE is

$$V(x) = -V_0 (\alpha \, |x| + 1)^{-\beta/\alpha},$$

(14)

and which corresponds, in the special case of \(\beta = 4\alpha\), to the Thomas-Fermi potential [15]

$$V(x) = -\frac{V_0}{(\alpha \, |x| + 1)^4}.$$ 

(15)

To find the solution of this potential we solve the SSE Eq.(5) with the exponential potential given in Eq.(13), which is

$$-\frac{\hbar^2}{2m_0} \varphi''_\rho(u) - V_0 e^{-4\alpha u} \varphi'_\rho(u) = \epsilon_\rho \varphi_\rho(u),$$

(16)

with \(\epsilon_\rho = E_\rho - U_0\). Solutions of Eq.(16) are given in terms of the Bessel functions of the first kind as

$$\varphi_\rho(u) = N_\rho \, J_\rho(ae^{-2\alpha u}),$$

(17)

with \(a = \sqrt{\frac{m_0 V_0}{2\hbar^2 \alpha^2}}\), \(\epsilon_\rho = -16U_0 \rho^2\), \(N_\rho\) the normalization constant and \(\rho\) the order of the Bessel functions that will be determined under condition to have an orthogonal system of eigensolutions. Let us consider the new variable

$$t = e^{-2\alpha u} = \frac{1}{(\alpha \, |x| + 1)^2},$$

(18)

defined in the interval \(t \in (0, 1)\), and the eigenfunctions expressed through this variable

$$y(t) = \varphi_\rho(u(t)),$$

(19)
in such a way that Eq. (16) is reduced to the Sturm-Liouville form

\[(t \ y'(t))' + \left( a^2 t - \frac{\rho_j^2}{t} \right) y(t) = 0. \]  

(20)

So, by considering \(\rho_j\) and \(\rho_k\) two distinct eigenvalues with respective eigensolutions \(y_j(t)\) and \(y_k(t)\), such that

\[(t \ y'_j(t))' + \left( a^2 t - \frac{\rho_j^2}{t} \right) y_j(t) = 0, \]  

(21)

\[(t \ y'_k(t))' + \left( a^2 t - \frac{\rho_k^2}{t} \right) y_k(t) = 0, \]  

(22)

and performing the usual combination of Sturm-Liouville theory, that is, the product of first equation by \(y_k(t)\) minus the product of the second equation by \(y_j(t)\), then arranging derivatives, we obtain

\[ [t (y'_k(t) y_j(t) - y_k(t) y'_j(t))]' + y_k(t) y_j(t) \frac{\rho_j^2 - \rho_k^2}{t} = 0, \]  

(23)

from which we can evaluate the integral over the range of variable \(t\) of the product \(y_k(t) y_j(t)\), that is

\[ (\rho_k^2 - \rho_j^2) \int_0^1 y_k(t) y_j(t) \frac{dt}{t} = y_k(1) y_j(1) - y_k(1) y'_j(1). \]  

(24)

This equation allows to recognize conditions for the orthogonality of the eigenfunctions \(\psi_{\rho_j}(x)\), \(\psi_{\rho_j}(x)\) because of the identity

\[ \int_{-\infty}^{\infty} \psi_{\rho_j}(x) \psi_{\rho_j}(x) \ dx = \int_{-\infty}^{\infty} \varphi_{\rho_j}(u) \varphi_{\rho_j}(u) \ du = \frac{1}{2\alpha} \int_0^1 y_j(t) y_k(t) \frac{dt}{t}. \]  

(25)

As previously mentioned \(y_k(t) = N_\rho J_\rho(a \ t)\), then, according to Eq. (24) the orthogonal eigenfunctions fulfill the condition \(J_\rho(a \ t) = 0\) for \(\rho_j \neq \rho_k\), or \(J'_\rho(a \ t) = 0\) for \(\rho_j \neq \rho_k\). The first one means \(\psi_{\rho_j}(0) = 0\), which is an odd parity condition for odd parity eigenfunctions; the second one imply \(\psi'_{\rho_j}(0) = 0\), which is an even parity condition for even parity eigenfunctions. This situation ensures the orthogonality of all the eigenfunctions, that is, between those of the same parity with distinct eigenvalues \(\rho_j \neq \rho_k\) and the orthogonality of eigenfunctions of different parity because of its integral in a symmetric interval \((-\infty, \infty)\), see Eq. (25). Consequently, due that Bessel functions of first kind alternate its points where the function is zero and where its derivative is zero, this means that the odd parity eigenfunctions and the even parity eigenfunctions alternate each other. Moreover, the ground state is gotten from a function of the second condition \(J'_\rho(a \ t) = 0\) that is nonzero in the interval \(t \in (0, 1)\) except for the point \(t = 0\) (corresponding to \(|x| \rightarrow \infty\)) assuring that the ground state has no nodes. So that, the even parity eigenstates are those corresponding to eigenvalues \(\rho_0, \rho_2, \rho_4, \ldots\) and so on and the odd parity eigenstates are those of eigenvalues \(\rho_1, \rho_3, \rho_5, \ldots\) etc. In addition, we have to remark that given the fixed distance \(a\), only a finite number of Bessel functions will satisfy the limiting conditions \(J_\rho(a \ t) = 0\) or \(J'_\rho(a \ t) = 0\).

Consequently, the wavefunctions for the PDMSE with the Thomas-Fermi potential, from Eq.(4) are given by

\[ \psi_{\rho_n}(x) = \frac{N_\rho}{\sqrt{\alpha |x| + 1}} J_{\rho_n} \left( \frac{a}{(\alpha |x| + 1)^{\frac{1}{2}}} \right), \]  

(26)
**Figure 1.** PDM Thomas-Fermi potential $V(x)$, Energy $E_j$, probability densities $|\psi_j|^2$, for $j = 1, 3, 5, ... 11$, and PDM distribution $M(x)$.

with energy spectra

$$E_{\rho_n} = U_0 \left( 1 - (4\rho_n)^2 \right).$$

(27)

These features: the potential, energy levels, probability densities as well as the position-dependent mass distribution are shown in Figure 1 for the odd parity solutions.

Finally, the normalization of the eigenfunctions can be performed by evaluating the integrals coming from Eq.(24) after taking $\rho_k = \nu, \rho_j = \mu, y_k(t) = J_\nu(\alpha t)$ and $y_j(t) = J_\mu(\alpha t)$, that is

$$\int_{0}^{1} J_\nu(\alpha t) J_\mu(\alpha t) \frac{dt}{t} = \frac{J_\nu'(\alpha) J_\mu(\alpha) - J_\nu(\alpha) J_\mu'(\alpha)}{\nu^2 - \mu^2};$$

(28)

in the limit when $\nu$ tends towards $\mu$, it yields

$$\int_{0}^{1} J_\mu^2(\alpha t) \frac{dt}{t} = \lim_{\nu \rightarrow \mu} \frac{J_\nu'(\alpha) J_\mu(\alpha) - J_\nu(\alpha) J_\mu'(\alpha)}{\nu^2 - \mu^2},$$

(29)

for which evaluation we use l'Hôpital’s rule and Bessel properties [19] to obtain

$$\int_{0}^{1} J_\mu^2(\alpha t) \frac{dt}{t} = \begin{cases} 
\frac{J_{\nu+1}(\alpha)}{\nu} J_\mu(\alpha) & \text{if } J_\nu(\alpha) = 0 \\
\frac{J_{\nu}''(\alpha)}{2\nu} J_\mu(\alpha) & \text{if } J_\nu'(\alpha) = 0 
\end{cases}$$

(30)
which determine the normalization constants of Eq. (26)

\[ N_{\rho_n} = \begin{cases} 
\sqrt{\frac{4\alpha_{\rho_n}}{J_{\rho_n}(a)\frac{d}{d\rho_n}J_{\rho_n}(a)}} & n = 0, 2, 4, \ldots \\
\sqrt{\frac{4\alpha_{\rho_n}}{J_{\rho_n+1}(a)\frac{d}{d\rho_n}J_{\rho_n}(a)}} & n = 1, 3, 5, \ldots 
\end{cases} \]  

(31)

Concluding remarks

In this work, we have used again the general algorithm to find exactly solvable potentials for the effective mass Schrödinger equation of a previous work [14]. According to the proposal, the choice of the equivalent of Witten superpotential allowed obtain the position-dependent mass distribution to identify an exactly-solvable effective mass Schrödinger equation for the potential

\[ V(x) = (\alpha | x | + 1)^{-\beta/\alpha}, \]

which has as a particular case the Thomas-Fermi model when \( \beta = 4\alpha \). Although we performed calculations for this particular case, our work could be adapted for any value of \( \beta \). This feature makes a difference between our work and the one already published by Axel et al [16]. Moreover, in the present work, we considered the normalization and orthogonality of the wavefunctions following the standard procedures of the Sturm-Liouville theory. The elements exposed in this work show the powerful of the general PCTM approach in the search of solvable models that can be useful in different theoretical studies of quantum chemistry and solid state physics.

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