Quantum Operator Approach Applied to the Position-Dependent Mass Schrödinger Equation

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Abstract. In this work, the quantum operator approach is applied to both, the position-dependent mass Schrödinger equation (PDMSE) and the Schrodinger equation with constant mass (CMSE). This fact enable us to find the factorization operators that relates both Hamiltonians by means of a kinetic energy operator that comes from the proposal of Morrow and Brownstein. With this approach is possible to find the exactly-solvable PDMSE, for any value of the parameters α and γ in the von Roos's Hamiltonian. For that, our proposal can be considered as a unified treatment of the PDMSE because it contains as particular cases, the kinetic energy operators of various authors such as BenDaniel-Duke, Gora-Williams, Zhu-Kroemer and Li-Kuhn among others. To show the usefulness of our result, we show the solvable PDMSE that comes from the harmonic oscillator potential model for the CMSE. The proposal is general and can easily be extended to other potential models and mass distributions which will be given in the extended paper.

Keywords and Phrases: Schrödinger equation, Position-dependent mass, Solvable potentials, Factorization operators.

1. Introduction.

The position-dependent mass Schrödinger equation (PDMSE) has been of recent interest for its applications in fields such as condensed matter theory [1],[2], heterostructures [3],[4], nuclear clusters [5],[6] and DFT related problems [7],[8]. At this regard, different proposals of the kinetic energy operator have been given as for example, the BenDaniel and Duke [9], the Gora-Williams [10], the Zhu-Kroemer [11], Li-Kuhn [12], and so on. However, each proposal has been worked individually by means of standard approaches. For that, in this work we propose a unified treatment of the PDMSE which includes as particular cases, already published results. To this aim, the quantum operator method is applied to the PDMSE and the constant mass Schrodinger equation (CMSE) with the purpose to relate factorization of both problems. This correspondence allows to construct a unified treatment to generate solvable PDMSE starting from known solutions of CMSE, as it will be seen next.

2. Quantum Operator Method to the PDMSE.

Let us consider the position-dependent mass kinetic energy operator [13]

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

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where $m = m(x) = M(x)/2m_0$ is the non-dimensional mass operator, m_0 is the mass of the involved particle, $p = -i\hbar\, d/dx$ is the linear momentum operator and $\alpha+\beta+\gamma = -1$. We have selected the natural unit system with $\hbar = 2m_0 = 1$. In order to display a simple and symmetrical factorization of the PDMSE we will follow the proposal of Morrow and Brownstein [14] who have argued that position-dependent mass Hamiltonians of physical interest must comply with the condition $\alpha = \gamma$; then, previous operator has the form $T_{(\alpha,\gamma)} = \left(m^{\alpha}\, p\, m^{\beta/2}\right)\left(m^{\beta/2}\, p\, m^{\alpha}\right)$. By choosing $\beta/2 = \alpha = -1/4$ we will have operators A_0, $A_0^{\dagger}$ in terms of a single power of the mass operator. This selection corresponds to the kinetic energy operator $T = T_{(-1/4,-1/4)}$ factorized in the form $T = A_0^{\dagger}\, A_0$, with

$$A_0^{\dagger} = -\eta \frac{d}{dx}\eta, \qquad\qquad A_0 = \eta \frac{d}{dx}\eta, \tag{2}$$

where

$$\eta = (2m)^{-1/4}\,. \tag{3}$$

Consequently, in this case the PDMSE is written as

$$H\,\psi(x) = (T + V(x))\;\psi(x) = E\,\psi(x) \tag{4}$$

where the Hamiltonian H is factorized as $H = A^{\dagger}\, A$ by means of

$$A = \eta\, \frac{d}{dx}\,\eta + W(x), \qquad\qquad A^{\dagger} = -\eta\, \frac{d}{dx}\,\eta + W(x), \tag{5}$$

on condition that

$$V(x) = W(x)^2 - \eta^2\, \frac{d}{dx}\, W(x) \tag{6}$$

where $W(x)$ is a superpotential.

Next, by defining A as the annihilation operator such that $A\,\psi_0 = 0$, which is

$$\eta\, A\,\psi_0 = \eta^2\, \frac{d}{dx}\;(\eta\,\psi_0) + W(x)\,(\eta\,\psi_0) = 0, \tag{7}$$

where ψ_0 represents the ground-state wavefunction, it is possible to find the suitable variable change needed to conect the PDMSE with the CMSE in an new variable u. In fact, similarly to equation (7) the operator a applied to the ground-state wavefunction of the CMSE Hamiltonian reads

$$a\,\phi_0 = \frac{d}{du}\,\phi_0 + w(u)\,\phi_0 = 0, \tag{8}$$

where $w(u)$ is the corresponding superpotential, ϕ_0 is their ground-sate wavefunction and a is the annihilation operator. This one and the $a^{\dagger}$ creation operator are

$$a = \frac{d}{du} + w(u), \qquad\qquad a^{\dagger} = -\frac{d}{du} + w(u), \tag{9}$$

which factorize the CMSE hamiltonian h in the form $h = a^{\dagger}\, a$ when relation between potential $v(u)$ and superpotential $w(u)$ is

$$v(u) = w^2(u) + \frac{d}{du}w(u). \tag{10}$$

The comparison of equation (7) and equation (8) compels to the change of variable

$$\frac{d}{du} = \eta^2\, \frac{d}{dx}, \qquad\qquad u(x) = \int^x \eta^{-2}(x)\, dx, \tag{11}$$

Journal of Physics: Conference Series **490** (2014) 012201 doi:10.1088/1742-6596/490/1/012201

to the similarity transformation connecting both wavefunctions

$$\psi_0(x) = \eta^{-1}(x)\phi_0(u(x)), \tag{12}$$

to the relation between operators $\eta\, A = a\, \eta$ and to the relation between the superpotentials

$$w(u(x)) = W(x). \tag{13}$$

To complete the algebra, it can be verified by means of the equations (5, 9-12) that $\eta\, A^\dagger = a^\dagger \eta$. Consequently, one is able to define the operator algebra

$$a^\dagger = \eta\; A^\dagger \eta^{-1}, \qquad\qquad a = \eta\; A\, \eta^{-1}, \tag{14}$$

allowing to change the CMSE operators a and $a^\dagger$ into the PDMSE operators A and $A^\dagger$ and to change variable u into variable x, or viceversa. That is, for the CMSE and PDMSE hamiltonians

$$h = a^\dagger\, a = \eta\; A^\dagger\;\; A\, \eta^{-1} = \eta\;\, H\eta^{-1}, \qquad\qquad H = \eta^{-1}\;\, h\eta. \tag{15}$$

So, let us consider the CMSE

$$h\phi_n = \epsilon_n \phi_n, \tag{16}$$

where ϵ_n is the corresponding energy spectra and ϕ_n the eigenfunctions. Similarly to equation (12), the use of

$$\phi_n = \eta\;\psi_n, \qquad\qquad \psi_n = \eta^{-1}\phi_n, \tag{17}$$

and equations (15,16) lead to

$$H\,\psi_n = E_n\,\psi_n, \tag{18}$$

indicating that $\epsilon_n = E_n$. Finally, from equations (6,10,11,13) it is obtained the relation between the PDMSE and CMSE potentials

$$V(x) = v(u(x)), \qquad\qquad v(u) = V(x(u)). \tag{19}$$

where $x(u)$ is the inverse function of $u(x)$.

3. Resolution of the PDMSE for the von Roos' Hamiltonians.

In this section we identify solvable potentials for any other PDMSE Hamiltonians. For that purpose, let us consider the Hamiltonian $H_{(\alpha,\gamma)}$ with kinetic energy operator given in equation (1) and potential $V_{(\alpha,\gamma)}$

$$H_{(\alpha,\gamma)}\psi\,(x) = \left(T_{(\alpha,\gamma)} + V_{(\alpha,\gamma)}\right)\;\psi\,(x) = E\,\psi\,(x)\,, \tag{20}$$

where as usual E and $\psi\,(x)$ are the eigenvalues and eigenfunctions respectively. To reduce the above equation to equation (18), is assumed that kinetic energy operators differ in a function of the position $U_{(\alpha,\gamma)} = T_{(\alpha,\gamma)} - T$, it becomes

$$U_{(\alpha,\gamma)} = (4\alpha+1)\,(4\gamma+1)\,\eta^2\eta'^2 + \left(\alpha+\gamma+\frac{1}{2}\right)\eta^2\left(\eta^2\right)''. \tag{21}$$

Equation (20) can be transformed in the form of equation (18) provided that

$$V(x) = V_{(\alpha,\gamma)} + U_{(\alpha,\gamma)} \tag{22}$$

which is a general result containing some outstanding particular cases such as those displayed immediately.

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Solvable PDMSE with BenDaniel-Duke kinetic term.
With the BenDaniel-Duke proposal $\alpha = \gamma = 0$, the kinetic energy operator becomes $T_{(0,0)} = p\left(\frac{1}{2m}\right)p$ such that the PDMSE is

$$-\frac{d}{dx}\left(\frac{1}{2m(x)}\right)\frac{d}{dx}\psi + \left(V_{(0,0)}(x) - E\right)\psi = 0. \tag{23}$$

For any solvable $v(u)$ of the CMSE, the corresponding solvable $V_{(0,0)}$ from equations (19,21,22) becomes

$$V_{(0,0)} = V(x) - \eta^2\left(\eta'\right)^2 - \frac{1}{2}\eta^2\left(\eta^2\right)''. \tag{24}$$

Solvable PDMSE with Gora-Williams kinetic term.
Similarly to the above case, now $\alpha = -1$ and $\beta = \gamma = 0$ for which, from equations (19,21)

$$V_{(-1,0)} = V(x) + 3\eta^2\eta'^2 + \frac{1}{2}\eta^2\left(\eta^2\right)'' \tag{25}$$

Solvable PDMSE with Zhu-Kroemer kinetic term.
Now, the parameters selection correspond to $\alpha = -1/2$, $\beta = 0$ and $\gamma = -1/2$ for which

$$V_{(-1/2,-1/2)} = V(x) - \eta^2\eta'^2 + \frac{1}{2}\eta^2\left(\eta^2\right)'' \tag{26}$$

Solvable PDMSE with Li-Kuhn kinetic term.
Accordingly with $\alpha = 0$ and $\beta = \gamma = -1/2$, the solvable potentials are obtained from

$$V_{(0,-1/2)} = V(x) + \eta^2\eta'^2. \tag{27}$$

The usefulness of the proposal is shown with the treatment of the PDMSE that comes from the harmonic oscillator potential model for the CMSE. That is, by considering the potential $V(u) = \kappa^2 u^2 - \kappa$ and superpotential $\omega(u) = ku$, with eigenvalues $E_n = 2n\kappa$, $n = 0, 1, 2\ldots$, and eigenfunctions given by

$$\phi_n(u) = \sqrt{\frac{\sqrt{\kappa}}{2^n n!\sqrt{\pi}}}e^{-\kappa u^2/2}H_n\left(\sqrt{\kappa}u\right). \tag{28}$$

Let us consider the mass function

$$m(x) = \frac{1}{2}\left(1 + \frac{\delta}{x^2+1}\right)^2, \tag{29}$$

which from equation (3) leads to $\eta = \left(1 + \delta/\left(x^2+1\right)\right)^{-1/2}$ and from equation (11) to the variable change $u = x + \delta\arctan x$. Consequently, the PDMSE with Hamiltonian H given in equation (18) has the solvable potential $V(x) = \kappa^2\left(x + \delta\arctan x\right)^2 - k$, with eigenfunctions

$$\begin{aligned}\psi_n(x) &= \eta^{-1}\phi_n(x + \delta\arctan x)\\ &= \sqrt{\frac{\sqrt{\kappa}}{2^n n!\sqrt{\pi}}}\left(1 + \frac{\delta}{x^2+1}\right)^{1/4} e^{\kappa(x+\delta\arctan x)^2/2}\\ &\quad\times H_n\left(\sqrt{\kappa}\left(x + \delta\arctan x\right)\right),\end{aligned} \tag{30}$$

and eigenvalues $E_n = 2nk$. The solvable potentials that match with the most common Hamiltonians $H_{(\alpha,\gamma)}$ of equation (20) have been calculated and presented in table 1.

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Table 1. The solvable potentials for some values of parameters in the kinetic energy PDMSE operator.

Author	α	γ	$V_{(\alpha,\gamma)}$
BenDaniel-Duke	0	0	$\kappa^2 (x+\delta\arctan x)^2 - \kappa - \frac{\delta(\delta+2x^2\delta-2x^2-3x^4+1)}{(x^2+\delta+1)^4}$
Zhu-Kroemer	$-1/2$	$-1/2$	$\kappa^2 (x+\delta\arctan x)^2 - \kappa - \frac{\delta(2x^2+3x^4-\delta-1)}{(x^2+\delta+1)^4}$
Gora-Williams	-1	0	$\kappa^2 (x+\delta\arctan x)^2 - \kappa + \frac{\delta(\delta+4x^2\delta-2x^2-3x^4+1)}{(x^2+\delta+1)^4}$
Li-Kuhn	0	$-1/2$	$\kappa^2 (x+\delta\arctan x)^2 - \kappa + \frac{x^2\delta^2}{(x^2+\delta+1)^4}$

Concluding Remarks

In order to solve the PDMSE from exactly solvable CMSE potentias, we have proposed a quantum operator treatment applied to PDMSE and to CMSE Hamiltonians. This can be considered as an improvement when compared with standard methods developed for the same purpose. Furthermore, our proposal is general and contains, as particular cases, the kinetic energy operators of various authors. As a useful application of our proposal, we have considered the solutions of the PDMSE by means of the CMSE with harmonic oscillator potential. However, the proposal is general and can be extended to other potential models and mass distributions as will be published elsewhere.

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