Position-dependent mass quantum Hamiltonians: general approach and duality

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Abstract
We analyze a general family of position-dependent mass (PDM) quantum Hamiltonians which are not self-adjoint and include, as particular cases, some Hamiltonians obtained in phenomenological approaches to condensed matter physics. We build a general family of self-adjoint Hamiltonians which are quantum mechanically equivalent to the non-self-adjoint proposed ones. Inspired by the probability density of the problem, we construct an ansatz for the solutions of the family of self-adjoint Hamiltonians. We use this ansatz to map the solutions of the time independent Schrödinger equations generated by the non-self-adjoint Hamiltonians into the Hilbert space of the solutions of the respective dual self-adjoint Hamiltonians. This mapping depends on both the PDM and on a function of position satisfying a condition that assures the existence of a consistent continuity equation. We identify the non-self-adjoint Hamiltonians here studied with a very general family of Hamiltonians proposed in a seminal article of Harrison (1961 Phys. Rev. 123 85) to describe varying band structures in different types of metals. Therefore, we have self-adjoint Hamiltonians that correspond to the non-self-adjoint ones found in Harrison’s article.

Keywords: position dependent mass, non-self-adjoint Hamiltonians, exact solutions

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1. Introduction

The problem of electron tunneling in systems where the band structure depends on the position, like in semiconductors, began to be treated in the early 1960s [1]; later it was proposed that this variation is simulated by a position-dependent effective mass in the one-electron Hamiltonian [2], and in the Hamiltonian describing graded mixed semiconductors [3]. From this time on the position-dependent mass (PDM) Hamiltonians were studied in many articles in a wide range of areas other than electronic properties of semiconductors [4–9], like, for example, quantum wells and quantum dots [10–12], polarons [13], etc.

In most of those articles the choice of the PDM Hamiltonians was guided by the characteristic of being self-adjoint, in the sense that the mean values of the physical quantities were consistently calculated in the associated Hilbert space with the usual integration measure. With this spirit, many PDM Hamiltonians were proposed and studied [3–6, 12, 14, 15, 17]. As a consequence some physically consistent and possibly relevant Hamiltonians have been discarded because they were not self-adjoint.

In the last decades PDM Hamiltonians have also been theoretically treated in a number of articles. The interest was directed to issues like non-self-adjointness [18], solutions of the corresponding Schrödinger equations [16, 18–27], ordering ambiguity [28], coherent states [29] and application to some particular systems, like, for example the Coulomb problem [30]. More recently, the issue of the PDM Hamiltonians which were not within the standard self-adjoint class mentioned above were analyzed following a different approach [20–22]. An approach to consistently quantize a nonlinear system [31] was recently developed. In this approach it was necessary to introduce an additional independent field which is the analog of the complex conjugate field for standard linear quantum systems.

In this paper we study a family of linear PDM Hamiltonians and show that the problem of self-adjointness is completely solved under certain conditions. We depart from the approach of two independent fields and define a connection between the two fields through a mapping that depends on the position dependent mass $m(x)$ and of a function $g(x)$. In order to have appropriately well-defined probability and current densities that satisfy a continuity equation, $g(x)$ must obey a condition that depends on the form of the Hamiltonian. We show that our general non-self-adjoint Hamiltonians can be identified with the very general family of Hamiltonians proposed by Harrison [1] to calculate wave functions in regions of varying band structure in superconductors, simple metals and semimetals. Inspired in the form of the probability density, we propose then an ansatz that takes the solutions $\Psi(x)$ of the time independent Schrödinger equations for the original non-self-adjoint Hamiltonian into new wave functions $\Omega(x)$. The wave functions $\Omega(x)$ are the solutions of the dual Hamiltonians which are self-adjoint with the usual inner product and quantum mechanically equivalent to the original non-self-adjoint ones. We also define an inner product for the solutions $\Psi(x)$ with a generalized measure that is a function of $m(x)$ and $g(x)$. We study three different examples of the proposed family of PDM Hamiltonians. All of them belong to the Harrison’s family of Hamiltonians [1]. For these cases we obtain the respective dual self-adjoint Hamiltonians. In one of them the kinetic part of the dual PDM Hamiltonian belongs to the von Roos general kinetic operator class [6], but the same does not happen in the other two cases.

This paper is organized as follows. In section 2 we present a family of Hamiltonians with a real general potential $V(x)$ depending on a function $f(m, m')$, $m(x)$ a position dependent mass and $m'(x)$ its derivative, and on a constant parameter $\alpha$. We obtain the Schrödinger equations generated by these Hamiltonians departing from a Lagrangian density which depends on two

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4 See, for example, equation (1) in [3].
different fields $\Psi(x,t)$ and $\Phi(x)$ and on their time and spatial derivatives. We define a transformation between these two fields that allows us to work with only one, say $\Psi(x,t)$, of them and to have a probability and a current density that satisfy a continuity equation. We build the quantum mechanically equivalent dual self-adjoint Hamiltonians on the Hilbert space of the solutions $\Omega(x)$ of the time independent Schrödinger equations generated by them. We define the inner products for both $\Psi(x,t)$ and $\Omega(x)$. In section 3 we analyze three different examples of the family of Hamiltonians presented, by choosing particular values for the constant parameter and for the function $f(m, m')$ and find the particular function $g(x)$. In all of them we present the particular values of the parameters that identify them with Harrison’s Hamiltonians. The three examples chosen are interesting: the first one recovers a model for abrupt heterojunction between two semiconductors studied in [5]; the other two are typical, in the sense that they introduce scales. In these two cases the kinetic part of the dual Hamiltonian does not reduce to the von Roos general kinetic operator. Finally, in section 4 we present our conclusions.

2. A family of general PDM Hamiltonians

In this section we present a family of position-dependent-mass Hamiltonians which depend on a real function $f(m(x), m'(x))$, $m(x)$ a general position dependent mass and $m'(x)$ its derivative, with a general real potential $V(x)$, given by

$$H = -\frac{\hbar^2}{2m(x)}\partial_x^2 + \frac{\hbar^2}{2}f(m(x), m'(x))\partial_x + V(x),$$

(1)

where $\alpha \in \mathbb{R}$ is a dimensionless constant. $m(x)$ is an analytical positive function for any value of $x$. These Hamiltonians lead to Schrödinger equations which are not, as will be seen, self-adjoint in the usual Hilbert space of their eigenfunctions. In what follows we show the conditions for (1) to be self-adjoint.

2.1. Deriving the Schrödinger equations from a classical Lagrangian density

When we solve the Schrödinger equation for a non-self-adjoint Hamiltonian with respect to the usual inner product we have to take into account also the adjoint equation [22]. Therefore our solution includes, in principle, two different fields, $\Psi(x,t)$ and $\Phi(x,t)$, and their conjugates. Note that $\Phi(x,t)$ is not the complex conjugate of $\Psi(x,t)$. Therefore we develop here an approach where we depart from a Lagrangian density $\mathcal{L}$ (as it was done in [23]), which depends on these fields, and on their time and spatial derivatives, that is

$$\mathcal{L} = \frac{i\hbar}{2} \Phi(x,t) \partial_t \Psi(x,t) - \frac{\hbar^2}{4m(x)} \partial_x \Psi(x,t) \partial_x \Phi(x,t)$$

$$+ \frac{\hbar^2}{4} \frac{m'(x)}{m(x)} \Phi(x,t) \partial_x \Psi(x,t) - \frac{\hbar^2}{4} f(m, m') \Phi(x,t) \partial_x \Psi(x,t)$$

$$- \frac{i\hbar}{2} \Phi^*(x,t) \partial_t \Psi^*(x,t) + \frac{\hbar^2}{4m(x)} \partial_x \Phi^*(x,t) \partial_x \Psi^*(x,t)$$

$$+ \frac{\hbar^2}{4} \frac{m'(x)}{m(x)} \Phi^*(x,t) \partial_x \Psi^*(x,t) - \frac{\hbar^2}{4} f(m, m') \Phi^*(x,t) \partial_x \Psi^*(x,t)$$

$$- \frac{1}{2} V(x) \Phi^*(x,t) \Psi^*(x,t) - \frac{1}{2} V(x) \Phi(x,t) \Psi(x,t),$$

(2)

where $*$ denotes the standard complex conjugate.
Using the usual Euler–Lagrange equations for the fields \( \Phi(x, t), \Psi(x, t) \) and their conjugates, we straightforwardly get the following Schrödinger equations:

\[
\begin{align*}
\imath \hbar \partial_t \Psi(x, t) &= -\frac{\hbar^2}{2m(x)} \partial_x^2 \Psi(x, t) + \frac{\hbar^2}{2} \alpha f(m, m') \partial_x \Psi(x, t) + V(x) \Psi(x, t), \\
-\imath \hbar \partial_t \Psi^*(x, t) &= -\frac{\hbar^2}{2m(x)} \partial_x^2 \Psi^*(x, t) + \frac{\hbar^2}{2} \alpha f(m, m') \partial_x \Psi^*(x, t) + V(x) \Psi^*(x, t),
\end{align*}
\]

Note that when the mass is a constant, (3) and (4) are the same as, respectively, (6) and (5).

\[\text{2.2. The continuity equation}\]

We define the function \( \rho(x) \) as

\[
\rho(x, t) = \frac{1}{2m_0} (\Psi(x, t) \Psi^*(x, t) + \Phi^*(x, t) \Phi(x, t)),
\]

where \( m_0 \) is a mass dimensional constant. We are considering here only systems for which the integral of \( \rho(x) \) over the whole space is finite. Besides, in order to be a probability density, \( \rho(x) \) has to be non-negative. This can be assured if \( \Phi(x, t) = H(x) \Psi^*(x, t) \), with \( H(x) > 0 \).

For the sake of convenience, we choose \( H(x) = g(x)m(x) \), and

\[
\Phi(x, t) = g(x)m(x) \Psi^*(x, t),
\]

where \( m(x) \) is obviously positive and we impose \( g(x) > 0 \). Then, (7) becomes

\[
\rho(x, t) = \frac{1}{m_0} (g(x)m(x) \Psi(x, t) \Psi^*(x, t)).
\]

It is straightforward to show that (9) obeys the continuity equation

\[
\partial_t \rho(x, t) + \partial_j j(x, t) = 0,
\]

where, using Schrödinger equations (3) and (4), we find the current density to be

\[
j(x, t) = \frac{\hbar}{2im_0} g(x) \{ (\partial_x \Psi(x, t)) \Psi^*(x, t) - \Psi(x, t) (\partial_x \Psi^*(x, t)) \}.
\]

This result is not valid for any function \( g(x) \), but only for those obeying the condition

\[
\frac{dg(x)}{dx} = -\alpha f(m, m') m(x) g(x),
\]

which is a consequence of the continuity equation (10). Also, it is very simple to show that (12) makes equations (3) and (6) reduce to each other (respectively, (4) and (5)). This means that the class of fields \( \Psi(x, t) \) and \( \Phi(x, t) \) related through (8) and submitted to condition (12) are not two independent fields. Condition (12) also means that given a particular Hamiltonian of the family (1), once we know \( \alpha \) and \( f(m, m') \), we have the function \( g(x) \) and the probability and current densities that obey the continuity equation.
In [1], Harrison proposed a family of Hamiltonians to describe regions of varying band structure in semiconductors, semimetals and transition metals. By comparing his current density, equation (2) in [1],

$$j(x, t) = \frac{\hbar}{2im_0} \gamma \left[ (\partial_x \beta \phi(x, t)) \beta \phi^*(x, t) - \beta \phi(x, t)(\partial_x \beta \phi^*(x, t)) \right],$$

(13)

with our definition of current density, equation (13), and identifying $\beta \phi = \psi$, we have that

$$\frac{\gamma}{\beta} = g(x).$$

(14)

Besides, comparing his wave equation (4) in [1], which is the limiting case of continuous variations of the band structure, and where $\beta, \gamma$ and $k_x$ are functions of position

$$\beta \partial_x \left[ \frac{\gamma}{\beta} \partial_x [\beta \phi(x)] \right] + \gamma k_x^2 \beta \phi(x) = 0,$$

(15)

with the time independent Schrödinger equation for the Hamiltonian (1), $H\psi(x) = E\psi(x)$, with $V(x) - E = \gamma k_x^2$, and taking (14) into account, we find

$$\beta = -\frac{\hbar^2}{2g(x)m(x)}$$

(16)

and recover condition (12), that is, $g'(x) = -\alpha f(m, m')m(x)g(x)$.

2.3. Building the dual self-adjoint Hamiltonian

Suggested by the form of the probability and current densities, (9) and (13), let us define a new wave function

$$\Omega(x, t) = \sqrt{g(x)m(x)} \Psi(x, t)$$

(17)

and, using equation (12), rewrite equation (3) for this new wave function:

$$i\hbar \partial_t \Omega(x, t) = -\frac{\hbar^2}{2m(x)} \partial_x^2 \Omega(x, t) + \frac{\hbar^2}{2} \frac{m'(x)}{m(x)} \partial_x \Omega(x, t)$$

$$-\frac{\hbar^2}{4m(x)} \left[ -\frac{1}{2} \alpha^2 f(m, m')^2 m(x)^2 - \alpha f(m, m')m'(x) - \frac{3}{2} \frac{m'(x)}{m(x)} \right] \Omega(x, t) + V \Omega(x, t).$$

(18)

It is straightforward to show that the following Hamiltonian, defined from the above Schrödinger equation

$$H = -\frac{\hbar^2}{2m(x)} \partial_x^2 + \frac{\hbar^2}{2} \frac{m'(x)}{m(x)} \partial_x - \frac{\hbar^2}{4m(x)} \left[ -\frac{1}{2} \alpha^2 f(m, m')^2 m(x)^2$$

$$-\alpha f(m, m')m'(x) - \frac{3}{2} \frac{m'(x)}{m(x)} \right] \alpha f'(m, m')m(x) + \frac{m''(x)}{m(x)} + V(x)$$

(19)

is self-adjoint on the Hilbert space of the solutions $\Omega(x, t)$ of equation (18) with the usual inner product for two given solutions $\Omega_1$ and $\Omega_2$.  

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\[ \langle \Omega_1(x, t), \Omega_2(x, t) \rangle \equiv \int dx \, \Omega_1^*(x, t) \Omega_2(x, t). \]  

Relation (17) can be seen as a mapping from the solutions of Schrödinger equations (3) and (4) into the solutions of time independent equation (18) and its Hermitian conjugate. Thus, motivated by (9), given two solutions of equation (3), namely \( \Psi_1 \) and \( \Psi_2 \), we can now define their inner product as

\[ \langle \Psi_1(x, t), \Psi_2(x, t) \rangle_{gm} \equiv \int dx \, g(x)m(x)\Psi_1^*(x, t)\Psi_2(x, t). \]  

Having the inner product above and a consistent definition of the probability density \( \rho(x, t) \) (9) we can calculate mean values for the system described by Hamiltonian (1). Therefore, we have a method to deal with the non-self-adjoint Hamiltonian (1). This result is valid for any analytical positive functions \( m(x) \), for the functions \( g(x) \) obeying condition (12) and for any real potential \( V(x) \). A similar result for a particular form of \( m(x) \), \( g(x) = 1 \) and \( V(x) \) was proved in theorem 1 of [20].

It is easy to see that the energy spectra computed from Hamiltonians (1) and (19) are the same; in the same way as it happens to the Hamiltonians, that is, the dual self-adjoint is a quantum mechanically equivalent.

This is a general result, in the sense that it is valid for all the non-self-adjoint Hamiltonians (1) depending on a real function \( f(m, m') \), with \( \alpha \) a real constant and any real potential \( V(x) \), provided the two fields \( \Psi(x, t) \) and \( \Phi(x, t) \) are related by (25) and \( g(x) \) obeys condition (12). Besides, this is a general method to find the dual self-adjoint Hamiltonians for systems described by non-self-adjoint Hamiltonians who belong to the family of Hamiltonians (1), under the conditions just mentioned. The non-self-adjointness was the reason for discarding PDM Hamiltonians which appeared in phenomenological approaches to semiconductors (see, for instance, [3, 17]).

In 2.2 we showed that our Hamiltonian (1) is identified to the family of Hamiltonians proposed by Harrison in [1]. It is important to note that with the method here presented we can find the dual self-adjoint Hamiltonian to any non-self-adjoint contained in Harrison’s family. That is, given specific forms of the functions \( \beta, \gamma \) and \( m(x) \), we can find the corresponding parameters \( \alpha \) and the functions \( f(m, m') \) and \( g(x) \) satisfying condition (12) and therefore the quantum mechanically equivalent self-adjoint Hamiltonian (19).

A general kinetic-energy operator for a PDM \( m(x) \) system was introduced by von Roos [6]. In one-dimension this operator is written

\[ T = - \frac{\hbar^2}{4} [ (m(x)^a \partial_x m(x)^a \partial_x m(x)^c + m(x)^a \partial_x m(x)^a \partial_x m(x)^c] \]  

and the arbitrary constants \( a, b \) and \( c \) obey the constraint \( a + b + c = -1 \). Taking this constraint into account this operator can be written

\[ T = - \frac{\hbar^2}{2m(x)} \partial_x^2 + \frac{\hbar^2}{2m(x)^2} m'(x) \partial_x \]

\[ + \frac{\hbar^2}{4m(x)} \left[ -2(1 + a + a^2 + b + ab) \left( \frac{m'(x)}{m(x)} \right)^2 + (1 + b) \frac{m''(x)}{m(x)} \right] \]  

The comparative analysis of von Roos kinetic operator, equation (23), and the kinetic part of our Hamiltonian given by equation (19) will be performed in the examples below.
3. Three examples

We have so far shown that it is possible to construct a well-defined continuity equation for the general PDM Hamiltonian (1).

In this subsection we analyze three different classes of Lagrangian (2) specified by different choices of \( f(m, m') \) and \( \alpha \), namely:

- **Case (a):** \( \alpha = 0 \)
- **Case (b):** \( \alpha = \frac{1}{c_2 m_0}, f(m, m') = \frac{m'}{m(x)}, [\alpha] = M^{-1} \)
- **Case (c):** \( \alpha = 2\alpha_0 c_2, f(m, m') = \frac{1}{m(x)}, \alpha_0 \) a constant, \([\alpha_0] = L^{-1}. \)

Both constants \( c_1 \) and \( c_2 \) are dimensionless. These three cases are typical in the sense that the constant \( \alpha \) has no scale or scales as mass or length.

3.1. Case (a):

In case (a) the non-self-adjoint Hamiltonian (1) becomes

\[
H = -\frac{\hbar^2}{2m(x)} \frac{\partial^2}{\partial x^2} + V(x) \tag{24}
\]

From condition (12), as \( \alpha = 0 \), we have \( g'(x) = 0 \) and \( g \) is a constant; we take it equal to 1. Therefore, according to (8),

\[
\Phi(x, t) = m(x)\Psi^*(x, t). \tag{25}
\]

The functions \( \Psi(x, t) \) (respectively, \( \Phi(x, t) \)) are the solutions of the Schrödinger equations (3) (respectively, (5)) for the Hamiltonian (24).

In the limit \( m(x) = \) constant, we recover the usual expressions for both the probability and current densities.

The dual self-adjoint Hamiltonian (19) corresponding to Hamiltonian (24) is then

\[
H_d = -\frac{\hbar^2}{2m(x)} \frac{\partial^2}{\partial x^2} + \frac{\hbar^2}{2m(x)^2} m'(x) \frac{\partial}{\partial x} + \frac{\hbar^2}{4m(x)} \left[ -\frac{3}{2} \left( \frac{m'(x)}{m(x)} \right)^2 + \frac{m''(x)}{m(x)} \right] + V(x). \tag{26}
\]

Comparing (23) with the kinetic part of (26), we see that they are the same for \( a = c = -1/2 \) and \( b = 0 \).

From (17) we have in this case

\[
\Omega(x, t) = \sqrt{m(x)} \Psi(x, t), \tag{27}
\]

where \( \Omega(x, t) \) is the solution of the Schrödinger equations (18) in case (a).

Hamiltonian (24) was proposed in [5] as a model for the abrupt junction between two different semiconductors and rendered self-adjoint by an empirical approach which is a particular case of the method presented here.

As we have showed in the general case, in 2.2, the Hamiltonians of the family (1) are equivalent to those proposed by Harrison in [1]. In this particular case, the \( \beta \) and \( \gamma \) functions of Harrison’s Hamiltonian (15) are \( \beta = \gamma = \frac{\hbar^2}{2m(x)} \) and \( V(x) - E = -\frac{\hbar^2}{2m(x)} \).

PDM Schrödinger equations have been used to describe semiconductor heterostructures [13, 32, 33], as well as other kind of systems [10–12]. Among all the possible \( m(x) \), there is strong motivation in the literature to study the case...
which may describe the GaAs/AlGaAs system \[13, 17, 35\]. \(m_0\) is a constant with dimension of mass. We choose to study the Schrödinger equations of the cases (a)–(c), with the position dependent mass (28), and the deformed harmonic oscillator potential \(V(x)\) given by

\[
V(x) = \frac{kx^2}{2m_0} (1 + \gamma x^2)^{-1},
\]

where \(\gamma\) is a constant with dimension \(L^{-2}\) which measures the departure from the usual harmonic oscillator and \(k\) is the spring constant.

In the present case, the solutions \(\Psi_n(y)\) of the Schrödinger equation are the functions:

\[
\Psi_n(y) = c_n \exp \left( -\frac{1}{2} \sqrt{1 - 2\gamma E_{na}} \right) H_{na}(y(1 - 2\gamma E_{na})^{1/4}),
\]

where \(c_n\) is an arbitrary constant and we have defined the new variable \(y = \left( \frac{m_0 y}{k} \right)^{1/4}\) and redefined \(\gamma = \gamma \left( \frac{m_0 y}{k} \right)^{1/2}\) and \(\lambda = \frac{2E}{m_0}\), as usual, the frequency is \(\omega = \sqrt{\frac{k}{m_0}}\) and \(H_n[y]\) is the Hermite polynomial and we have the energy levels

\[
E_{na} = \frac{2n + 1}{4} \left[ 1 - \tilde{\gamma}(2n + 1) + \sqrt{4 + \tilde{\gamma}^2(2n + 1)^2} \right].
\]

\(\tilde{\gamma}(y, t)\) and \(\Omega(y, t)\) are given respectively by (25) and (27), taking into account the change of variables, with \(m(y) = 1 + \gamma y^2\). Note that when \(\gamma = 0\), we recover the energy levels of the harmonic oscillator.

In order to guarantee that the mass is positive-definite, we see in (28) that \(\gamma > 0\) for any value of \(y\). We can then easily show that the energy value is limited by \(1/2\gamma\), which is the maximum of the potential (29).

### 3.2. Case (b):

In this case Hamiltonian (1) has the form

\[
H = -\frac{\hbar^2}{2m(x)} \partial_x^2 + \frac{\hbar^2}{2c_1 m_0 m(x)} m'(x) \partial_x + V(x).
\]

Let us note that in this case the \(\alpha = \frac{1}{c_1 m_0}\) parameter has a dimension of \(M^{-1}\).

Integrating condition (12), equation (8) becomes

\[
\Phi(x, t) = e^{\frac{m(x)}{c_1 m_0} \sqrt{m(x)}} \Psi^*(x, t).
\]

The dual self-adjoint Hamiltonian (19) corresponding to Hamiltonian (32) is now

\[
H_b = -\frac{\hbar^2}{2m(x)} \partial^2_x + \frac{\hbar^2}{2m(x)^2} m'(x) \partial_x + \frac{\hbar^2}{2m(x)} \left[ \frac{3c_1^2 m_0^2}{4} - \frac{m(x)^2}{m(x)^2 - m'(x)^2} \right] + V(x).
\]

From (17) the new functions \(\Omega(x, t)\),

\[
\Omega(x, t) = e^{\frac{m(x)}{2c_1 m_0} \sqrt{m(x)}} \Psi(x, t),
\]

are the solutions of the Schrödinger equations for self-adjoint Hamiltonian (34).
In this case, the kinetic operator of Hamiltonian (34) does not reduce to the Von Roos general kinetic operator (22) for any particular values of the parameters. Indeed, it is easy to see that

\[
H_b = H_a + \frac{\hbar^2}{2} \left[ \frac{m'(x)^2}{4\epsilon_0^2m_0^2m(x)} - \frac{m''(x)}{2\epsilon_1m_0m(x)} \right],
\]

where \(H_a\) is given by equation (26). This shows that the von Roos kinetic operator is not the most general self-adjoint kinetic operator, as it has been assumed with frequency in the literature in the last decades. Equation (34) is a perfectly satisfactory PDM Hamiltonian that does not fit in the von Roos proposal.

In this particular case, the \(\beta\) and \(\gamma\) functions of Harrison’s Hamiltonian (15) are

\[
\beta = -\frac{\epsilon_0^2m_0^2}{2m(x)}, \quad \beta = -\frac{\epsilon_1^2}{2m(x)}, \quad V(x) - E = -\frac{\hbar^2}{2m(x)}k^2.
\]

In fact, this also shows that the kinetic part of Harrison’s Hamiltonian proposed in [1] is more general than the von Roos’ one.

In this case, if we again take \(m(x) = m_0(1 + \gamma x^2)\) and \(V(x) = \frac{k^2}{2m_0}(1 + \gamma x^2)^{-1}\), we completely solve the Schrödinger equation and the energy spectrum is also found to be limited.

3.3. Case (c):

Finally, in case (c) the Hamiltonian (1) reads

\[
H = -\frac{\hbar^2}{2m(x)} \partial_x^2 + \frac{\hbar^2c_2\alpha_0}{m(x)} \partial_x + V(x);
\]

the relation between functions \(\Psi^*(x, t)\) and \(\Phi(x, t)\) is

\[
\Phi(x, t) = e^{-2c_2\alpha_0 t}m(x)\Psi^*(x, t),
\]

and the dual self-adjoint Hamiltonian has the form

\[
H_c = \frac{\hbar^2}{2m(x)} \partial_x^2 + \frac{\hbar^2}{2m(x)^2}m'(x)\partial_x - \frac{\hbar^2}{2m(x)} \left[ \frac{3}{4m(x)^2}m'(x)^2 \right. + \left. \frac{c_2^2\alpha_0^2}{4} \right] + V(x).
\]

Here, the parameter \([\alpha_0] = L^{-1}\).

Now the solutions of Schrödinger equations for Hamiltonian (39) are

\[
\Omega(x, t) = e^{-c_2\alpha_0 t}m(x)\Psi(x, t).
\]

As in case (b) Hamiltonian (39) can be written as

\[
H_c = H_a + \frac{\hbar^2c_2^2\alpha_0^2}{8m(x)},
\]

and its kinetic part does not reduce to the Von Roos general kinetic operator, being another example of a satisfactory PDM Hamiltonian that is not included in the von Roos scheme.

In this particular case, the \(\beta\) and \(\gamma\) functions of Harrison’s Hamiltonian (15) are

\[
\beta = -\frac{\epsilon_0^2c_2\alpha_0}{2m(x)}, \quad \gamma = \frac{\epsilon_0^2}{2m(x)}, \quad V(x) - E = -\frac{\hbar^2}{2m(x)}k^2.
\]

We remark that, after the introduction of the function \(\Omega(x, t)\), instead of the Lagrangian (2) we could write a Lagrangian only for the field \(\Omega(x, t)\), whose associate Hamiltonian is
self-adjoint. This procedure was done in [34]. However, with that approach we can not analyze non-self-adjoint operators.

For the choices (28) and (29), the Schrödinger equation can be completely solved as well.

4. Conclusions

The approach here used, which departs from a classical Lagrangian depending on two independent fields, allowed us to completely solve the question of self-adjointness of a class of PDM Hamiltonian systems. These Hamiltonians had been originally discarded in phenomenological approaches to semiconductors because they were not self-adjoint. We proved here that for a general class of these non-self-adjoint Hamiltonians, we can construct Hamiltonians which are quantum mechanically equivalent to the original ones and are self-adjoint in the usual Hilbert space of their Schrödinger equations solutions. This can be done if some function $g(x)$ that appears in consistent definitions of the probability and current densities, is restrained by the particular form of the non-self-adjoint Hamiltonians. By consistent we mean that the probability density is positive and that it obeys the usual continuity equation with an appropriate definition of the current density.

The general non-self-adjoint Hamiltonian proposed by us is identified with a large family of Hamiltonians constructed by Harrison in [1] to calculate wave functions in regions of varying band structure in superconductors, simple metals and semimetals. That is, given specific forms of the functions involved in Harrison’s Hamiltonians, we can find the form of our parameters and the function $g(x)$ satisfying condition (12). Therefore we obtain the quantum mechanically equivalent self-adjoint Hamiltonians, dual to the Harrison’s family.

With this method we can solve many particular cases (that is, choosing the parameter $\alpha$ and the function $f(m(x), m'(x))$ of the Hamiltonian (1) and consequently of the Harrison’s Hamiltonians. We can also expect this method to be successfully applied in Hamiltonians with non-self-adjoint potentials [36].

We believe that some Hamiltonians that were discarded because of their non-self-adjointness, like, for example, in [3], could be now treated by this method.

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