Supersymmetric approach to exactly solvable systems with position-dependent effective masses

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November 20, 2002

Abstract

We discuss the relationship between exact solvability of the Schrödinger equation with a position-dependent mass and the ordering ambiguity in the Hamiltonian operator within the frame of supersymmetric quantum mechanics. The one-dimensional Schrödinger equation, derived from the general form of the effective mass Hamiltonian, is solved exactly for a system with exponentially changing mass in the presence of a potential with similar behaviour, and the corresponding supersymmetric partner Hamiltonians are related to the effective-mass Hamiltonians proposed in the literature.

PACS Numbers: 03.65Ca, 03.65Fd, 03.65Ge

1 Introduction

The study of quantum systems with position-dependent effective masses has been the subject of much activity in recent years. The Schrödinger equation with nonconstant mass provides an interesting and useful model for the description of many physical problems. The most extensive use of such an equation is in the physics of semiconductor nanostructures. This field has arisen due to the impressive development of sophisticated technologies of semiconductor growth, like molecular beam epitaxy, which made it possible to grow ultrathin semiconductor structures, with very prominent quantum effects [1]. The motion of electrons in them may often be described by the envelope function effective-mass Schrödinger equation, where the material composition- (i.e., the position-) dependent effective mass of electrons replaces the constant particle mass in the conventional Schrödinger equation. The most popular of these structures is the semiconductor quantum well, and the Schrödinger equation here is effectively one-dimensional. Another instance where such an equation is employed, this time three-dimensional and with spherical symmetry, is in the pseudopotential-theory-based density functional calculations in solids: to reduce the computational load, model pseudopotentials with position-dependent electron mass which replace nonlocal pseudopotentials have been considered [2].

Since the momentum and the mass operators no longer commute in case of spatially varying mass, a question concerning the correct form of the kinetic energy operator of the generalized Hamiltonian has arisen. This problem of ordering ambiguity is a long standing one in quantum mechanics, see for instance the excellent critical review by Shewell [3]. There are many examples
of physically important systems, for which such ambiguity is quite relevant. For instance we can cite the problem of impurities in crystals [4, 5, 6], the dependence of nuclear forces on the relative velocity of the two nucleons [7, 8], the minimal coupling problem in systems of charged particles interacting with magnetic fields [9], and more recently the study of semiconductor heterostructures [1, 10, 11].

Notwithstanding, taking into account the spatial variation of the semiconductor type, some effective Hamiltonians are proposed with a spatially dependent mass for the carrier [12-17], and many authors have been trying to determine the correct Hamiltonian phenomenologically. In this article we try to circumvent the problem of ambiguity by presenting a scheme to obtain unambiguously the Schrödinger equation with spatially varying particle mass, which makes clear the link between possible choices of the kinetic energy operator for quantum systems with position-dependent effective mass, within the frame of supersymmetric quantum mechanics [18]. The strategy here is to tackle the problem with a fundamental point of view, i.e., without using a particular form of the effective potential. Within this framework and using the supersymmetric formalism we will show that one can arrive at a conceptually consistent result for exactly solvable systems.

The application of supersymmetry ideas to nonrelativistic quantum mechanics has provided a deeper understanding of analytically solvable Hamiltonians, as well as a set of powerful approximate schemes for dealing with problems admitting no exact solutions. The concept of shape invariance [19] has played a fundamental role in these developments. The aims of the present work are to consider the application of the supersymmetric approach to quantum systems with position-dependent mass and to extend the concept of shape invariant potentials to the nonconstant mass scenario to see clearly the relation between the effective-mass potentials existing in the literature and supersymmetric partner potentials.

The paper is organized as follows. In section 2 we provide a brief review of the Schrödinger equation for systems with position-dependent effective mass. Section 3 deals with the exact solvability of a system involving a particle with a spatially dependent mass in an arbitrary potential well. The application of supersymmetric approach to this system, together with the use of shape invariance concept to deduce the correct operator ordering for the Hamiltonian, are also studied in this section. Finally, some conclusions are drawn in section 4.

2 Generalized Schrödinger equation

We start this section by defining a quite general Hermitian effective Hamiltonian for the case of a spatially varying mass which will be denoted by $m = m(x)$ throughout the present work. In general, the Hamiltonian proposed by von Roos [20] is used,

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

but to accomodate the possibility of including the case of the Weyl ordering [21] in a more evident way, we will use an effective Hamiltonian with four terms given by [22]

$$H = \frac{1}{4(a+1)} \left\{ a \left[ m^{-1} p^2 + p^2 m^{-1} \right] + m^\alpha p m^\beta p m^\gamma + m^\gamma p m^\beta p m^\alpha \right\} .$$  

In both cases, Eqs. (1) and (2), there is a constraint over the parameters such that $\alpha + \beta + \gamma = -1$. 

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The one-dimensional time-independent Schrödinger equation reads

\[-\left(\frac{\hbar^2}{2m}\right) \frac{d^2 \psi}{dx^2} + \frac{\hbar^2}{2} \left(\frac{m'}{m^2}\right) \frac{d \psi}{dx} + [U_{\alpha\gamma a} + V] \psi = E \psi,\]

where $U_{\alpha\gamma a}$ involving all the ambiguity is

\[U_{\alpha\gamma a}(x) = -\frac{\hbar^2}{4m^3(a+1)} \left[(\alpha + \gamma - a) m \ m'' + 2(a - \alpha \gamma - \alpha - \gamma) m'^2\right],\]

in which the first and second derivatives of $m(x)$ with respect to $x$ are denoted by $m'$ and $m''$. It is clear that the effective potential is the sum of the real potential profile $V(x)$ and the modification $U_{\alpha\gamma a}$ emerged from the location dependence of the effective mass. A different Hamiltonian leads to a different modification term, see Table 1.

It is curious to note that all the ambiguity is in the $U_{\alpha\gamma a}$ term, and that it can be eliminated by imposing some convenient constraints over the ambiguity parameters, namely

\[\alpha + \gamma - a = 0, \quad a - \alpha \gamma - \alpha - \gamma = 0,\]

which have two equivalent solutions, (i) $\alpha = 0$ and $a = \gamma$, or (ii) $a = \alpha$ and $\gamma = 0$. In this case the effective Schrödinger equation will not depend on the ambiguity parameters, but will contain a first order derivative term. In the next section, we will be interested in getting exact solutions of the resulting equation for a particular potential, and trying to get some information about the proposed orderings appearing in the literature.

3 An exactly solvable system

The interest in exactly solvable problems in quantum physics has increased sharply in the last few years. This is concerned, of course, with the fact that the description of the behaviour of nonconservative physical systems is usually very complicated, but in some cases such systems can be modelled by means of quite a simple Hamiltonian, which leads to standard problems of quantum mechanics.

Starting with the Schrödinger equation in Eq. (3) and making a new definition for the wave function

\[\psi(x) = m^{1/2} \varphi(x),\]

one gets a differential equation in a more familiar form

\[-\frac{\hbar^2}{2m} \frac{d^2 \varphi}{dx^2} + (U_{eff} - E) \varphi = 0,\]

with a new effective potential defined through

\[U_{eff}(x) = V(x) + U_{\alpha\gamma a}(x) + \frac{\hbar^2}{4m} \left[\frac{3}{2} \left(\frac{m'}{m}\right)^2 - \frac{m''}{m}\right].\]

To demonstrate the simplicity of the present method, we consider here a particular case, which has been recently studied \[22\], where one have exact solution for the above equation. That is a particle with exponentially decaying or increasing mass in the presence of a potential with similar behaviour,

\[m(x) = m_0 e^{cx}, \quad V(x) = V_0 e^{cx},\]
where $m_0$ is a constant mass. This problem is often encountered in the calculation of confined energy states for carriers in semiconductor quantum well structures under the envelope-function and the effective-mass approximations where the effective mass of a carrier is spatially dependent on the graded composition of the semiconductor alloys used in the barrier and the well region of the microstructures.

Multiplying each term in Eq. (7) by $m(x)$ and dividing by $m_0$, one arrives at an usual Schrödinger equation for the system of interest,

$$-\frac{\hbar^2}{2m_0} \frac{d^2\varphi}{dx^2} + \left( V_0 e^{2cx} - E e^{cx} \right) \varphi = \varepsilon \varphi,$$

(10)

where

$$\varepsilon = \frac{\hbar^2}{m_0} (q - c^2/8), \quad q = \frac{c^2}{4(a+1)} (a - 2a\gamma - \alpha - \gamma).$$

(11)

Note that Eq. (10) corresponds to a Schrödinger equation for a particle with constant mass under the influence of the Morse potential [23]. It is thus clear that if one knows the spectral properties of the constant-mass Schrödinger equation of any potential, one then can readily obtain a corresponding potential for the effective-mass Schrödinger equation with identical spectral properties. Proceeding with the well known energy spectrum of the Morse potential,

$$-\frac{\hbar^2 c^2}{2m_0} \left[ \sqrt{2m_0 V_0} \right]^2 - \left( n + \frac{1}{2} \right)^2 = \frac{\hbar^2}{m_0} \left( q - \frac{c^2}{8} \right),$$

(12)

from which we find the energy spectrum of the effective potential appearing in Eq. (7), that is

$$E_n = \hbar c \sqrt{\frac{V_0}{2m_0}} \left[ 2n + 1 + \nu(\alpha, \gamma, a) \right].$$

(13)

where the ordering term $\nu(\alpha, \gamma, a)$ is

$$\nu(\alpha, \gamma, a) = \sqrt{1 - \frac{2}{a+1}} (a - 2a\gamma - \alpha - \gamma).$$

(14)

One can now study the effect of using some of the orderings appearing in the literature. Considering Table 1, it is not difficult to see that the ambiguous term $\nu$ is zero for the effective Hamiltonians in Refs. [15, 16, 21], although they have different orderings, while $\nu = 1$ for the BenDaniel-Duke Hamiltonian [12]. For both cases ($\nu = 0, 1$), the corresponding Hamiltonians have exactly the same spectra except for the fact that the Hamiltonians in Refs. [15, 16, 21] have one bound state more than the BenDaniel-Duke Hamiltonian. Thus, they can be treated as the supersymmetric partner Hamiltonians [18] which is the subject of the next section. Furthermore, one ends with a complex energy for the orderings proposed in the literature [13, 14], which could be possibly discarded due to the physically unacceptable energies. This makes clear that unacceptable physics consequences may occur unless specific choices are made in the Hamilton operator ordering for a system undertaken.

As we are dealing with a confined particle system, one may wish also to confirm Eq. (13) by mapping the Morse potential onto harmonic oscillator system, which seems more realible than the Morse oscillator for the system of interest. For this purpose, we invoke the change in the variable as well as in the wave function,

$$x = \ln y^{2/c}, \quad \varphi(x) = \sqrt{2/c} y^{-1/2} F(y).$$

(15)
This reduces Eq. (10) to an equivalent Schrödinger equation

\[
-\frac{\hbar^2}{2m_0} \frac{d^2 F}{dy^2} + \left[ \frac{4V_0}{c^2} y^2 - \left( \frac{\hbar^2 c^2 + 32m_0\varepsilon}{8m_0c^2y^2} \right) \right] F = \frac{4E}{c^2} F ,
\]

(16)
in a more familiar form involving a harmonic oscillator potential with centripetal barrier. In contrast to Eq. (10), which contains a variable parameter \(\varepsilon\) representing the Morse oscillator energy, we have a constant term on the right-hand side of Eq. (16), and the energy term \((\varepsilon)\) is contained in the effective potential parameter. Thus Eq. (16) may be looked upon as the radial Schrödinger equation with a fixed energy but with a variational angular momentum quantum number. From which one can easily arrive at Eq. (13), which clarifies that both treatments (Morse and harmonic oscillator mapping) are equivalent to each other.

In the following section, we will focus our attention on how to apply the supersymmetric quantum mechanical formalism to the system under consideration in order to clear out the hidden relation between the effective Hamiltonians proposed in the literature for the spatially dependent mass.

### 3.1 supersymmetric approach

The problem of generating isospectral potentials in quantum mechanics has been considered for more than 50 years, but recently the research efforts on this topic have been considerably intensified. A new field, supersymmetric quantum mechanics (SUSYQM), devoted to this class of problems has emerged, which deals with pairs of Hamiltonians that have the same energy spectra, but different eigenstates. A number of such pairs of Hamiltonians share an integrability condition called shape invariance [19]. Although not all exactly solvable problems are shape invariant [24], shape invariance, especially in its algebraic formulation, is a powerful technique to study exactly integrable systems which have always been at the centre of attention in physics and mathematics.

It would be interesting therefore to extend the SUSYQM to handle cases with position-dependent mass. Recently supersymmetric techniques have been applied to obtain exact solutions of Schrödinger equation with nonconstant mass [25, 26]. Using the spirit of these works, here we generalize the supersymmetric formalism for the problem considered in the previous section. All considerations are made for the one-dimensional Schrödinger equation.

Proceeding as in the case of constant mass, we introduce a superpotential \(W(x)\) and the associated pair of operators \(A\) and \(A^+\) defined by

\[
A\psi = \frac{\hbar}{\sqrt{2m}} \frac{d\psi}{dx} + W\psi \quad , \quad A^+ = -\frac{d}{dx} \left( \frac{\hbar \psi}{\sqrt{2m}} \right) + W\psi .
\]

(17)

Notice that, due to the position dependence of the mass, \(d/dx\) and \(\hbar/\sqrt{2m}\) do not commute anymore. Within the framework of SUSYQM, the first partner Hamiltonian reads

\[
H_1 = A^+A = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \left( \frac{\hbar^2}{2m} \right)' \frac{d}{dx} + \left[ W^2 - \left( \frac{\hbar W}{\sqrt{2m}} \right)' \right] ,
\]

(18)

where the prime denotes the first derivative with respect to the variable \(x\).

At this stage, we propose an ansatz for the superpotential,

\[
W(x) = \frac{\hbar c}{8m_0} \sqrt{2m} - \frac{\hbar c}{2\sqrt{2m}} ,
\]

(19)
and note that the Hamiltonian in Eq. (18) found via the supersymmetric formalism corresponds to the specific effective-mass Hamiltonians in Eq. (3) with real potential profile \( V(x) \). Explicitly, these are the Zhu and Kroemer Hamiltonian \( (a = 0, \alpha = \gamma = -1/2) \) [15], the Li and Kuhn Hamiltonian \( (a = \alpha = 0, \beta = \gamma = -1/2) \) [16], and the Weyl Hamiltonian \( (a = 1, \alpha = \gamma = 0) \) [21], in which the effective potentials (for which \( \nu(\alpha, \gamma, a) = 0 \)) may be expressed in the supersymmetric form,

\[
V_{\text{eff}}(x) = V_0 e^{cx} + U_{\alpha\gamma a}(x) = W^2 - \left( \frac{\hbar W}{2m} \right)'.
\] (20)

This justifies the operator ordering in the Hamiltonian used by many authors in the rough calculation of the confinement states in quantum well structures in the effective mass scheme, as the first partner leads to the exactly solvable Hamiltonian systems within the frame of SUSYQM.

The associated supersymmetric partner Hamiltonian, for the case \( \nu(\alpha, \gamma, a) = 1 \) which describes the BenDaniel-Duke effective mass Hamiltonian \( (a = \alpha = \gamma = 0) \) [12], is

\[
H_2 = AA^+ = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \left( \frac{\hbar^2}{2m} \right)' \frac{d}{dx} + \left[ W^2 - \left( \frac{\hbar W}{\sqrt{2m}} \right)'^2 + \frac{2\hbar W}{\sqrt{2m}} - \frac{\hbar}{\sqrt{2m}} \left( \frac{\hbar}{\sqrt{2m}} \right)'' \right]
\] (21)

We see that the two supersymmetric partner Hamiltonians \( H_1 \) and \( H_2 \) describe particles with the same effective mass-spatial dependence, but in different potentials. The second partner potential corresponding the BenDaniel-Duke effective potential does not incorporate the ambiguity term,

\[
V_{BDD}(x) = V_0 e^{cx} = W^2 - \left( \frac{\hbar W}{\sqrt{2m}} \right)'^2 + \frac{2\hbar W}{\sqrt{2m}} - \frac{\hbar}{\sqrt{2m}} \left( \frac{\hbar}{\sqrt{2m}} \right)'',
\] (22)

where the double prime denotes the second derivative with respect to \( x \).

There is a correspondence between the energy eigenvalues of the isospectral Hamiltonians \( H_1 \) and \( H_2 \), although they have different effective potentials. The energy of the \( n \)th bound state of \( H_1 \) coincides with that of the \((n - 1)\)th bound state of \( H_2 \), which is the case expressed through Eq. (13). The ground state of \( H_1 \) has no associated state of \( H_2 \). The reader is referred to Ref. [18] for a comprehensive review of the supersymmetric quantum mechanics.

For an exactly solvable system it is thus obvious that a proper choice of the effective mass and the corresponding superpotential would impose the elimination of the supersymmetric partner potential that involves all the ambiguity. This makes clear that which choice of the effective mass Hamiltonians proposed in the literature is physically acceptable for the system undertaken.

Finally we note that, from the relation between the superpotential and the ground state wave function of \( H_1 \),

\[
W(x) = -\frac{\hbar}{\sqrt{2m}} \frac{d\psi^{n=0}_1}{dx}/\psi^{n=0}_1,
\] (23)

it is straightforward to solve \( \psi^{n=0}_1 \), which satisfies the required boundary conditions dictated from the conservation of current through the envelope functions of heterostructures.

In sum, considering the definition of the effective potential which is the summation of a real potential \( V(x) \) and a term \( U_{\alpha\gamma a}(x) \) resulting from the mass dependence on the location, and bearing in mind that the effective potential relies on the Hamiltonian utilized, we have connected
the deviation from the real potential, due to the ordering ambiguity, to the supersymmetric partner Hamiltonians. It is found that the operator ordering in the kinetic energy operator to be the same as that endorsed by recent authors [27, and the references therein] for the calculation of confined states in semiconductor microstructures under the simplified effective-mass and envelope-function, with a correctional term $U_{\alpha\gamma\alpha}(x)$ that is proportional to the derivatives of the mass profile $m(x)$.

### 4 Concluding remarks

In this work we have first discussed the problem of solvability and ordering ambiguity in quantum mechanics, as the form of the effective mass Hamiltonian has been a controversial subject due to the location dependence of the effective mass.

It was shown through a particular example that exact solutions could be used as a kind of guide, at least, restrict the possible choices of ordering. The principal idea is to suppose that once one have found the ordering without ambiguity for a given potential or class of potentials, that ordering should be extended to remaining physical potentials.

Our work has also made clear that the Hamiltonian proposed by Li and Kuhn [16] is in fact equivalent to that coming from the Weyl ordering [21], as can be easily checked from Eqs. (4, 21, 24) the effective potentials and consequently from Eqs. (13,14) the energy spectra of both these orderings are equal. In addition, though the ordering in the Zho and Kroemer effective Hamiltonian operator [15] is different than those of Li and Khun, and that of Weyl, we have arrived at the same result in each case within the frame of both, the standard quantum theory and supersymmetric quantum mechanics. Hence, we remark that when the ambiguity term is linear in the momentum, contrary to what is usually believed, there is no ambiguity in fact. Thus, any Hermitian construction of the quantum Hamiltonian will be necessarily equivalent to that due to any other, and consequently nonambiguous. This observation supports the recent work of Dutra and Almeida [22].

On the basis of the supersymmetric ideas we have generalized the concept of shape invariance to the nonconstant scenario and shown that an appropriate choice of the potential and mass variation with the position makes clear the link between the effective potentials and the ordering ambiguity. The bound state spectra of systems with effective mass are relevant in many areas such as the study of nuclei [28] and metal clusters [29]. However, in other fields such as for instance electronic properties of semiconductors, one is interested in the properties of quantum systems with nonconstant mass endowed with continuum spectra [1,10,11]. The supersymmetric formalism developed here can also be useful tool for the treatment of such kinds of problems and it may be possible to generalize our results to such problems. Such an investigation will be deferred to a later publication.

As a final remark, an exponentially changing mass and potential have been considered in this paper, and it has been shown that the energy levels could be redefined in such a way that the ordering ambiguity disappears. However, we should note that the exact solvability does depend upon both the form of the potential and the change in mass with the position. For instance, as was discussed in [20], this cannot be done for the consideration of a quadratically growing mass in a singular potential field. However, we believe that in addition to its practical applications, the study of quantum mechanical systems with a position-dependent mass within the frame of the present technique will raise many interesting conceptual problems of a fundamental nature. In particular the method should find wide applications in the study of quasi-exactly solvable [30] and conditionally-exactly solvable [31] systems with nonconstant masses. Along this line
the works are in progress.
 References 


[23] P. M. Morse, Phys. Rev. 34, 57 (1929).


Table 1: The special cases of the effective Hamiltonian in Eq. 2.

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