Exact solutions of effective-mass Schrödinger equations

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Abstract

We outline a general method for obtaining exact solutions of Schrödinger equations with a position dependent effective mass and compare the results with those obtained within the frame of supersymmetric quantum theory. We observe that the distinct effective mass Hamiltonians proposed in the literature in fact describe exactly equivalent systems having identical spectra and wave functions as far as exact solvability is concerned. This observation clarifies the Hamiltonian dependence of the band-offset ratio for quantum wells.

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1 Introduction

An interesting question arises when one tries to formulate the correct Hamiltonian for a particle with spatially dependent mass in an arbitrary potential well. This problem often arises 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 nanostructures. Since the mass and the momentum operators no longer commute, the correct ordering of these operators within the kinetic energy operator cannot be trivially assigned. This problem of ordering ambiguity is a long standing one in quantum mechanics, see for instance the excellent critical review by Shewell [1]. The study of quantum systems with

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position dependent effective masses has been the subject of much activity in recent years. Apart from being an interesting topic itself such equations have found wide applications in the search of not only electronic properties of semiconductors [2] but also quantum dots [3], quantum liquids [4], $^3$He clusters [5], and metal clusters [6].

Although the treatment of effective-mass Schrödinger equations with non-constant mass is difficult, some exactly solvable models for such systems have been recently introduced [7-11]. However, from the physics point of view, none of these works seem completely convincing. For example, Dekar and his co-workers [7] solved exactly the one-dimensional Schrödinger equation, derived from the general form of the effective-mass Hamiltonian without any restriction in the ordering parameters, for a system with smooth potential and mass step. The effective mass Hamiltonian and the connection rules for a system with abrupt heterojunction were deduced from the study of the limiting case when the smooth step potential and mass tend to an abrupt potential and mass step, which suggest that the appropriate form of the effective-mass Hamiltonian for an abrupt heterojunction is the form proposed by [12]. However, this modelling of the position dependent potential and mass by a discontinuous profile is not physically acceptable, because in the real world neither the potential nor the effective mass can change abruptly across the heterojunction. In a different perspective, Dutra and Almeida [8] discussed the relationship between exact solvability of the effective-mass Schrödinger equations and the ordering ambiguity. They introduced a simple technique to transform mass dependent Schrödinger equations to the conventional Schrödinger equation with a constant mass to obtain in a closed form of the full spectrum and wavefunctions of the original system. As an illustrative example they considered a physically plausible case (an exponentially changing mass and potential) and obtained the corresponding exact solutions by mapping the system onto the well known harmonic oscillator with centripetal barrier. It was nicely clarified that in this case the energy levels are redefined in such a way that the ordering ambiguity disappear. However their model has a drawback, which works only for a restricted choice of mass and potential functions to be able to serve exact solutions. Although the works in Refs. [9, 10] within the frame of supersymmetric quantum theory, together with a more recent work [11] used a Lie algebra, provide a powerful treatment for the systems of interest, all the formulations introduced in these models are only valid for the BenDaniel and Duke Hamiltonian [12] as they followed the work of Levy-Leblond [13].

Notwithstanding, taking into account the spatial variation of semiconductor type, some effective Hamiltonians have been proposed with a coordinate-dependent mass for the carrier [12,14-18], and many authors have been trying to determine the correct Hamiltonian phenomenologically, for a review see [17]. Although, there has been growing consensus in favor of the BenDaniel-Duke Hamiltonian, see the related references in [17], the form of the effective-mass Hamiltonian has been still a controversial subject due to the location dependence
of the effective mass and the question of the exact form of the kinetic energy operator is still an open problem. In the light of all these, the present work addresses a more general and compact framework introducing two different models to solve exactly for a physical system involving a position dependent mass with the consideration of all physically acceptable Hamiltonians proposed in the literature. We will make clear that though the effective Hamiltonians appear in a different form, they describe in fact exactly equivalent systems having identical spectra and wavefunctions as far as exact solvability is concerned. Although the literature covered similar problems, to our knowledge an investigation such as the one we have discussed in this paper was missing.

The paper is organized as follows. Using the spirit of the works [19] we introduce, in the next section, a generalized exact treatment procedure for effective-mass Hamiltonians and use the works in [9, 10] to extend their scenario and involve all possible Hamiltonians. Section 3 involves applications of the models developed for two different but physically meaningful mass considerations. Discussion and analysis of the results obtained are given in section 4. Finally, some conclusions are drawn in section 5.

2 Theoretical considerations

The single-band effective-mass approach to a quantum-well problem requires that the envelope function $\psi$ satisfy the effective-mass equation

$$\hat{H}\psi = E\psi$$

where $E$ is the energy eigenvalue and $\hat{H}$ is the Hamiltonian operator consisting of kinetic energy operator ($\hat{T}$) and the potential energy operator ($\hat{V}$),

$$\hat{H} = \hat{T}(\hat{z}) + \hat{V}(\hat{z})$$

Due to the compositional variation in a quantum well as a function of location, the kinetic energy and the potential energy are expressed as position-dependent operators in Eq. (2). The kinetic energy operator can be considered to be composed of four elements: $1/\sqrt{m(z)}$, $1/\sqrt{m(z)}$, $\hat{p}$, and $\hat{p}$, where $\hat{z}$ and $\hat{p}$ are position and momentum operators, respectively. Because $1/\sqrt{m(z)}$ and $\hat{p}$ are not commutable, there are different possible permutations to represent the kinetic energy operator [12,14-18]. All of these single-band effective-mass Hamiltonians are special cases of a general form of the Hamiltonian introduced by von Roos [20],

$$H_{vR} = \frac{1}{4} \left[ m^{\alpha}(\hat{z})\hat{p}m^{\beta}(\hat{z})\hat{p}m^{\gamma}(\hat{z}) + m^{\gamma}(\hat{z})\hat{p}m^{\alpha}(\hat{z})\hat{p}m^{\beta}(\hat{z}) \right] + V(\hat{z}) ,$$

where $\alpha + \beta + \gamma = -1$. 

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By the correspondence in wave mechanics $\hat{p} \rightarrow -i\hbar d/dz$ and $\hat{z} \rightarrow z$, the effective mass equation, Eq. (1), together with any possible Hamiltonian proposed in the literature as the special cases of Eq. (3) can be written in a differential form,

$$
\frac{-\hbar^2}{2} \frac{d}{dz} \left[ \frac{1}{m(z)} \frac{d\psi(z)}{dz} \right] + V^{\text{eff}}(z)\psi(z) = E\psi(z),
$$

(4)

where $V^{\text{eff}}(z)$ is termed the effective potential energy whose algebraic form depends on the Hamiltonian employed (see Table 1),

$$
V^{\text{eff}}(z) = V(z) + U_{\alpha\gamma}(z)
$$

$$
= V(z) - \frac{\hbar^2}{4m^3(z)} \left[ (\alpha + \gamma) m(z)m''(z) - 2(\alpha\gamma + \alpha + \gamma) m'^2(z) \right],
$$

(5)

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

In the following section we introduce two different theoretical models to solve Eq. (4) exactly, which lead us to define analytically solvable potentials for the systems undertaken.

### 2.1 Coordinate transformation method

In a recent work, Roy and Roy [19] have presented a coordinate transformation method to solve analytically an effective-mass Hamiltonian corresponding to the one proposed by BenDaniel-Duke [12]. We extend and generalize their model by tackling the problem with a fundamental point of view, i.e., without using a particular form of the effective potential in (5) and arrive at a conceptually consistent result for exactly solvable systems with location dependent masses. Our generalization is based on the work of De et all [19] in which they gave explicit point canonical transformations and interrelated many shape-invariant exactly solvable potentials within the frame of the usual Schrödinger equation with a constant mass. We show that their simple approach, which consists of mapping through canonical transformations of coordinates, can also be used to interrelate two distinct systems having constant and position-dependent masses.

As the aim is to solve Eq. (4) in a closed form to obtain the corresponding full energy spectrum and wavefunctions exactly for a solvable potential, one needs to transform Eq. (4) into a workable frame. Proceeding with a transformation of both the independent and dependent variables of the form

$$
z = f(\tilde{z}) \quad , \quad \psi(z) = \nu(\tilde{z})\tilde{\psi}(\tilde{z}) \quad , \quad m(z) = m[f(\tilde{z})] = \tilde{m}(\tilde{z}),
$$

(6)
we transform Eq. (4) to

\[-\frac{\hbar^2}{2m} \left\{ \frac{d^2 \tilde{\psi}}{d\tilde{z}^2} + \left( \frac{2\nu'}{\nu} - \frac{f''}{f'} \tilde{m}' \right) \frac{d\tilde{\psi}}{d\tilde{z}} - \left[ \left( \frac{\nu'}{\nu} \right) \left( \frac{\tilde{m}'}{m} + \frac{f''}{f'} \right) - \frac{\nu''}{\nu} \right] \tilde{\psi} \right\} \]

\[+ f'^2 \left\{ V_{\text{eff}}[f(\tilde{z})] - E \right\} \tilde{\psi} = 0 , \quad (7)\]

in which the prime denotes differentiation with respect to $\tilde{z}$. One can now easily reduce Eq. (7) to the Schrödinger equation with constant mass, which requires

\[\nu(\tilde{z}) = C \sqrt{f'(\tilde{z})\tilde{m}(\tilde{z})} , \quad f'(\tilde{z}) = \sqrt{\frac{m_0}{\tilde{m}(\tilde{z})}} , \quad (8)\]

where $m_0$ stands for a constant effective mass, and $C$ is a constant of integration. Eq. (7) in this case reads

\[-\frac{\hbar^2}{2m_0} \frac{d^2 \tilde{\psi}}{d\tilde{z}^2} + \left\{ \frac{\hbar^2}{2m_0} \left( \frac{5}{16} \frac{\tilde{m}''(z)}{\tilde{m}(z)} - \frac{1}{4} \frac{\tilde{m}''(z)}{\tilde{m}(z)} \right) + V_{\text{eff}}[f(\tilde{z})] \right\} \tilde{\psi}(\tilde{z}) = E \tilde{\psi}(\tilde{z}) . \quad (9)\]

It is important to note that Eqs. (4) and (9) have identical spectra. With the wavefunctions $\psi(z)$ being square integrable, i.e., $\langle \psi(z) | \psi(z) \rangle = 1$ , setting the integral constant $C = 1/\sqrt{m_0}$ in Eqs. (6) and (8) and having in mind that $m(\tilde{z}) > 0$ we find that $\langle \tilde{\psi}(\tilde{z}) | \psi(\tilde{z}) \rangle = 1$ as well, i.e., the functions $\tilde{\psi}(\tilde{z})$ are also square integrable.

For further simplification, we recall the mathematical definition used in arriving at Eq. (8), $f'^2(\tilde{z}) [\tilde{m}(\tilde{z})/m_0] = 1$, and remind that it may be inverted and written as

\[\tilde{z} = \frac{1}{\sqrt{m_0}} \int_0^z \sqrt{m(z)} \, dz = f^{-1}(z) \quad , \quad (10)\]

which defines (though in implicit form) the mapping function $f(\tilde{z})$ and consequently enables finding $\tilde{m}(\tilde{z})$ , together with the effective potential $V_{\text{eff}}[f(\tilde{z})]$. Bearing in mind that

\[\tilde{m}' = \frac{d\tilde{m}(\tilde{z})}{d\tilde{z}} = \frac{dz}{d\tilde{z}} \frac{d}{dz} [\tilde{m}(\tilde{z})] = f'(z)\tilde{m}'(z) = \frac{m_0}{m(\tilde{z})} \frac{dm(z)}{dz} , \quad (11)\]

Eq. (9) can also be reduced to the form,

\[-\frac{\hbar^2}{2m_0} \frac{d^2 \tilde{\psi}(\tilde{z})}{d\tilde{z}^2} + \left\{ \left( \frac{\hbar^2}{32m^3(\tilde{z})} \left[ 7m^2(z) - 4m(z)m''(z) \right] \right) + V_{\text{eff}}(z) \right\}_{z=\tilde{z}} \tilde{\psi}(\tilde{z}) = E \tilde{\psi}(\tilde{z}) \quad , \quad (12)\]

It is worth to note that the change of variable in (10) may not always be invertible or not easily be invertible. But this does not really pose a problem as far as solvability of Eq. (4) is concerned. This is because the new coordinate $\tilde{z}$ as a
function of the old coordinate $z$ is explicitly known from (10) and if we choose $V^{\text{eff}}$ such that
\begin{equation}
V^{\text{eff}}(z) = V_{ES}(\tilde{z}) - V_m(\tilde{z}),
\end{equation}
where $V_{ES}$ is an exactly solvable potential and $V_m$ is the mass-dependent part of the full potential,
\begin{equation}
V_m = \frac{\hbar^2}{32m^3(z)} \left[ 7m^2(z) - 4m(z)m''(z) \right]_{z=\tilde{z}},
\end{equation}
obviously one then finds exactly the spectrum of the system in (4). The corresponding wavefunctions can be obtained using Eq. (6).

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 behavior description of some physical systems is usually very complicated, but in some cases such systems can be modelled by means of a quite simple Hamiltonian which leads to standard problems of quantum mechanics, as the one presented in this section. As the spectral properties of the constant-mass Schrödinger equation of solvable potentials are well known in the literature, one can readily obtain a corresponding potential for the effective-mass Schrödinger equation with identical spectra. 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.

In the next section, we discuss an alternative treatment for the problem under consideration and illustrative examples will be given in section 3.

### 2.2 Supersymmetric approach

In the light of the recent works [9, 10], we introduce a superpotential $W(z)$ and the associated pair of operators $A$ and $A^+$ defined by
\begin{equation}
A\psi(z) = \frac{\hbar}{\sqrt{2m(z)}} \frac{d\psi(z)}{dz} + W(z)\psi(z), \quad A^+\psi(z) = -\frac{d}{dz} \left[ \frac{\hbar\psi(z)}{\sqrt{2m(z)}} \right] + W(z)\psi(z)
\end{equation}

Notice that, due to the location dependence of the mass, $d/dz$ and $\hbar/\sqrt{2m(z)}$ do not commute anymore. Within the frame of supersymmetric quantum mechanics [21], the partner Hamiltonians read
\begin{align}
H_1 &= A^+A = -\frac{\hbar^2}{2m(z)} d^2 + \left( \frac{\hbar^2}{2m(z)} \right)' \frac{d}{dz} + \left[ W^2(z) - \left( \frac{\hbar W(z)}{\sqrt{2m(z)}} \right)'' \right],
\end{align}
\begin{align}
H_2 &= AA^+ = H_1 + \frac{2\hbar W'(z)}{\sqrt{2m(z)}} - \frac{\hbar}{\sqrt{2m(z)}} \left( \frac{\hbar}{\sqrt{2m(z)}} \right)''.
\end{align}
We see that the two partner Hamiltonians describe particles with the same effective mass-spatial dependence but in different potentials. As the usual exactly solvable potentials, as well as many recently discovered ones, are given in the form of the first partner potential in (16), we will work through the applications in the next section with the consideration that the effective potential in (5) should satisfy the condition,

\[ V_{\text{eff}}(z) = V_1 = W^2(z) - \left( \frac{\hbar W(z)}{\sqrt{2m(z)}} \right)'. \] (17)

The second partner potential is used for obtaining the corresponding energy spectrum. Considering the shape invariance concept [21], the supersymmetric partner potentials in (16) obey the integrability condition

\[ V_2(z, a_1) = V_1(z, a_2) + R(a_1), \quad a_2 = f(a_1). \] (18)

The above relation means that the partner potentials \( V_1 \) and \( V_2 \) have the same form, but are characterized by different values of the parameter sets. The energy eigenvalues, \( E_n = \sum_{i=1}^{n} R(a_i) \), and eigenfunctions of shape invariant potentials can be obtained in algebraic fashion. For more details the reader is referred to [9, 10, 21].

3 Applications

A square quantum well subject no external field is usually modeled by a step profile which discontinues at the heterojunctions. The commonly used interface conditions at the heterojunctions are: (i) the continuity of the envelope function and its first derivative, or (ii) the continuity of the envelope function and its first derivative divided by the effective mass. Within each flat region of the square quantum well, the mass is a constant, and the effective potentials, Eq. (5), are identical because the derivatives of the mass with respect to the position vanish. Thus envelope functions within each flat region are independent of the Hamiltonian used for the analysis. If the same interface conditions at the discontinute points between two adjacent regions are essentially imposed for the distinct effective Hamiltonians, the eigensolutions will be exactly identical. As a result, the effective-mass Hamiltonians in (5) are expected to produce the same transition energy, namely, the band-offset ratio will be independent of the Hamiltonian if the heterojunction is modeled by a step function with essentially imposed interface conditions. This point will be discussed in the next section within the frame of our results.

However, the discontinuity of the square quantum-well model implies an infinite external electric field at the heterojunctions, and this is not physically
possible. In reality, the potential changes over a few monolayers for a perfect microscopic interface. In this section, the square quantum well is modeled by more realistic smoothed profiles, which leads to different effective potential descriptions. This modified realistic potential profiles remove the discontinuity of the sharp square quantum well. Considering the realistic quantum well applications in the works [17, 22], we test our models introduced in section 2 employing the two different but physically meaningful effective mass variations discussed in the following.

3.1 For \( m(z) = m_0 \exp(\lambda z) \)

To demonstrate the simplicity of the models used we consider here a particular case, as a first illustrative example, for which one have exact solutions. That is a particle with exponentially increasing or decaying, \(|\lambda| \propto 1/L\) with \(L\) being the quantum-well width, in the presence of a potential with similar behaviour that will be defined for each Hamiltonian in this section.

Starting with Eqs. (12-14), within the framework of the coordinate transformation technique and taking the harmonic oscillator potential as a solvable potential, \( V_{ES}(z) = Bz^2 \), and bearing in mind that \( \tilde{z} = (2/\lambda) \exp(\lambda z/2) \) from Eq. (10), we obtain a variety of exactly solvable effective potential descriptions appearing in the original effective mass equation, Eq. (4). These are, corresponding to distinct effective mass Hamiltonians presented by Eqs. (3) and (5),

\[
V_{eff}^{BD}(z) = V_0 \exp(\lambda z) - \frac{3\hbar^2 \lambda^2}{32m_0} \exp(-\lambda z) \quad , \quad \alpha = \gamma = 0 \quad , \quad \beta = -1 \quad , \quad (19)
\]

for the BenDaniel-Duke Hamiltonian [12],

\[
V_{eff}^{GW}(z) = V_0 \exp(\lambda z) + \frac{5\hbar^2 \lambda^2}{32m_0} \exp(-\lambda z) \quad , \quad \beta = \gamma = 0 \quad , \quad \alpha = -1 \quad , \quad (20)
\]

for the Gora and Williams (or the Bastard) Hamiltonian [14, 15], and

\[
V_{eff}^{ZK}(z) = V_0 \exp(\lambda z) + \frac{\hbar^2 \lambda^2}{32m_0} \exp(-\lambda z) \quad , \quad \alpha = \gamma = -\frac{1}{2} \quad , \quad \beta = 0 \quad , \quad (21)
\]

for the Zhu and Kroemer Hamiltonian [16]. We also obtain exactly the same result as in (21) for the Li-Kuhn Hamiltonian [17] \((\beta = \gamma = -1/2 \ , \alpha = 0)\). In the above equations, \( V_0 = 4B/\lambda^2 = \hbar^2 \lambda^2/32m_0 \). From Eqs. (4) and (12), it is clear that though the appearance and behaviour of the potentials in (19)-(21) are dissimilar, they have identical spectra, \( E_n = (n + 1/2)\hbar\omega \), where \( \omega = \sqrt{2B/m_0} \). This result supports the similar discussion presented in the section 3 of a recently published paper [11]. Moreover, from Eqs. (6) and (8), these Hamiltonians have the same wavefunctions, \( \psi_n(z) = N_n [\exp(\lambda z)]^{1/4} \tilde{\psi}_n(\tilde{z}) \) where
\( \psi_n(\tilde{z}) = \left\{ \frac{1}{2m^2} \sqrt{\pi} \right\}^{1/2} H_n \left( \sqrt{\eta} \tilde{z} \right) \exp \left( -\frac{n^2 \tilde{z}^2}{2} \right) \) with \( \eta = \sqrt{2Bm_0}/\hbar \). As a result, the distinct effective Hamiltonians considered here are not only isospectral but also describe identically equivalent systems as far as exact solvability is concerned. This significant result is also confirmed below with use of the supersymmetric approach described in section 3 as an alternative treatment.

For the supersymmetric considerations, in the light of Eq. (35) of [9] we propose a superpotential

\[
W(z) = \frac{\sqrt{2m_0} \delta}{\hbar \lambda} \exp(\lambda z/2) - \frac{\hbar \lambda}{4\sqrt{2m_0}} \exp(-\lambda z/2) ,
\]

where \( \delta = \hbar \omega \), which yields the supersymmetric partner potentials in (16) in the form

\[
V_1(z) = V_0 \exp(\lambda z) - \frac{3\hbar^2 \lambda^2}{32m_0} \exp(-\lambda z) - \frac{\delta}{2} ,
\]

\[
V_2(z) = V_0 \exp(\lambda z) - \frac{3\hbar^2 \lambda^2}{32m_0} \exp(-\lambda z) + \frac{\delta}{2} ,
\]

which is the simplest case of the shape invariance integrability condition given by (18) due to the partner potentials in (23) differing only by a uniform energy shift by \( \delta \). Note that the first partner has the same shape as in (19) corresponding to the BenDaniel-Duke effective potential. Considering the shifting term \( \delta/2 \), together with Eq. (18), one can easily find the corresponding energy spectrum, \( E_n = (n+1/2)\hbar \omega \), which overlaps with the one found through the transformation technique. For the other exactly solvable shape invariant effective potentials we use a simple expression,

\[
V^{\text{eff}}_{\text{ES}}(z) = V^{\text{eff}}_{\text{BDD}}(z) - U_{\alpha \gamma}(z) = V_1(z) - U_{\alpha \gamma}(z) ,
\]

in which \( U_{\alpha \gamma}(z) \) is the modification term in Eq. (5),

\[
U_{\alpha \gamma}^G(z) = -\frac{\hbar^2 \lambda^2}{4m_0} \exp(-\lambda z) , \quad U_{\alpha \gamma}^Z(z) = U_{\alpha \gamma}^{L-K} = -\frac{\hbar^2 \lambda^2}{8m_0} \exp(-\lambda z) .
\]

The substitution of \( V_1(z) \) in Eq. (23) into Eq. (24) leads us to arrive at Eqs. (20) and (21), which confirms the reliability of the coordinate transformation technique developed in the previous section. Once more it is clear that the potentials in (19-21) will have the same energy spectra and wavefunctions as a unique superpotential is used, (Eq. 22), for the generation of these analytically solvable potentials within the frame of supersymmetric quantum theory. For the relation between the superpotential and wavefunction in case of the supersymmetric considerations the reader is referred to [9, 10].
3.2 For \( m(z) = m_0 \left( \frac{a+q^2}{1+q^2} \right)^2 \)

This physically convenient mass variation, in which \( a \) is a positive constant and \( q(= \lambda z) \) involves the variable with a positive width parameter \( \lambda \propto 1/L \), considered here to convince the reader for that the models introduced in this paper works for all smoothly varying masses, unlike the recent models [7, 8]. There is another reason for the consideration of the work presented in this section. Among various potential shapes (quantum well profiles), there is one which has attracted some research attention recently: this is the case of Pöschl-Teller potential with a constant electron mass [23, 24]. Unfortunately, this idealized potential is not realizable in the common, graded ternary alloy based quantum wells, because of the effective mass therein necessarily varies, together with the potential. In this respect, the result shown in this section and its related discussion given in the next section would be helpful in designing realistic ternary alloy based structures with properties equivalent to those of idealized Pöschl-Teller potential.

From Eq. (10), the relation between the transformed coordinate and the old one is \( \tilde{z} = z + (1/\lambda)(a - 1) \tan^{-1} q \), and considering the Pöschl-Teller potential as one possible choice from analytically solvable potential family and working within the framework of the coordinate transformation method, one arrives at a class of exactly solvable potentials for the use in Eq. (4) belonging to different effective mass Hamiltonians,

\[
V_{\text{eff}}^{BDD}(z) = V_{PT}(\tilde{z}) + \frac{(a-1) \left[ 3q^4 + q^2(4-2a) - a \right] \hbar^2 \lambda^2}{2m_0(q^2 + a)^4},
\]

\[
V_{\text{eff}}^{Z-K}(z) = V_{PT}(\tilde{z}) - \frac{(a-1) \left[ 3q^4 + 2q^2 - a \right] \hbar^2 \lambda^2}{2m_0(q^2 + a)^4},
\]

\[
V_{\text{eff}}^{L-K}(z) = V_{PT}(\tilde{z}) - \frac{(a-1) \left[ 3q^4 + q^2(6-4a) - a \right] \hbar^2 \lambda^2}{2m_0(q^2 + a)^4},
\]

where \( V_{PT}(\tilde{z}) = -A \left[ \frac{\lambda}{\sqrt{2m_0}} \right] \sech^2 \left\{ \tilde{\lambda} \left[ z + \frac{(a-1)\tan^{-1} q}{\lambda} \right] \right\} \). Note that for \( a \to 1 \), \( m(z) \to m_0 \), all the above effective potentials reduce to the conventional Pöschl-Teller potential, \( V_{\text{eff}}(z) \to V_{PT}(z) \), due to \( \tilde{z} \to z \). From Eqs. (4), (8) and (12), the bound state energy spectra and wavefunctions corresponding to the potentials in (26) are \( E_n = - \left( A - \frac{\lambda \hbar}{\sqrt{2m_0}} \right) \) and \( \psi_n(z) = N_n \sqrt{\frac{a+q^2}{1+q^2}} \tilde{\psi}(\tilde{z}) \) with \( \tilde{\psi}(\tilde{z}) \) being the well described wavefunction [25] for the solution of the usual Schrödinger equation with a constant-mass Pöschl-Teller potential.
All these results are fully confirmed with use of the supersymmetric expressions presented in section 2 by adopting an ansatz for the superpotential,

\[
W(z) = A \tanh \left\{ \frac{\bar{\lambda}}{\lambda} \left[ z + \frac{(a-1)}{\lambda} \tanh^{-1} q \right] \right\} + \frac{(a-1)}{\lambda} q \frac{\hbar \bar{\lambda}}{\sqrt{2m_0(a+q^2)^2}}. \tag{27}
\]

4 Discussion

We discuss here the physics behind the results obtained. First, the applications given in the previous sections make clear the band-offset ratio dependence on the effective mass Hamiltonians, which is significant for quantum well applications. The conduction-band-offset ratio, which is the ratio of the conduction-band offset to the total band gap of the heterojunction, has been investigated in various quantum wells because of its fundamental importance and application. The ratio has been measured by spectroscopic and electrical methods. From Duggan’s and Kroemer’s review articles [26] about the experimental and theoretical works, it can be seen that spectroscopic techniques are preferred over electrical ones in exploring the band-offset ratio via a quantum well, and that researchers using spectroscopy usually try to match their data with the theoretical results to determine the band offset. To demonstrate simply the band-offset ratio variation due to the choice of the Hamiltonian, we will focus here on transition energies between levels in conduction and valence bands. Following the works [17, 27] and considering only single-band effective-mass equations for the electron and the hole, Eq. (4), one finds the transition energy in the form of

\[
E_T = E_e + E_h + E_G
\]

where \(E_e, E_h\) are the eigenenergies in the conduction and valence bands, respectively, and \(E_G\) is the band-gap energy. From the previous sections, it is obvious that the effective Hamiltonians undertaken will yield the same transition energies between identical transition levels due to the identical values for \(E_e\) and \(E_h\). Hence, the band-offset ratio for the BenDaniel-Duke Hamiltonian and for the others can be found by solving \(E_T^{\text{others}}(Q^{\text{others}}) = E_T^{\text{BDD}}(Q^{\text{BDD}})\), with \(Q\) being the band-offset ratio. Recall the relation between the conduction-band-offset ratio and the conduction-band-offset energy, \(V_{cb} = Q \Delta E_g\), where \(\Delta E_g\) denotes the band-gap difference between binary and ternary materials. Having in mind that the band-offset ratio of a quantum well determines the barrier height of the conduction band and valence bands, \(V_{cb}\) corresponds to the depth of the effective potentials discussed through the article. This leads to the realization of the band-offset ratio dependence on the effective-mass Hamiltonian due to the underlying differences between the strengths of the potentials obtained. As a result of this, in the interpretation of a given spectrum, the Hamiltonian employed in the analysis cannot be regarded independently of the band-offset ratio utilized, unlike the case of a simple square quantum well consideration. Therefore, an attempt to determine the band-offset ratio from experimental data by matching calculated transition energies with spectral peaks would involve large inaccuracy.
There is another interesting point behind the present results. A systematic procedure based on the inverse spectral theory and supersymmetric transformations has been recently proposed [24] for optimized design of semiconductor quantum well structures via tailoring the quantum well potential, which enables shifting bound states in a quantum well and makes the search for the best desired energy spectrum and potential shape. By varying the free parameters appearing in the procedure one can then design a convenient optimized structure. However, in these notable works the idealized constant-mass Pöschl-Teller potential, which allows one to set analytically the spacing between states, considered since a direct implementation of a more realistic position-dependent effective mass related to the position-dependent potential in their theoretical considerations is not trivial. The optimization of continuously graded structures thus require more sophisticated techniques. In this respect, we believe that the applications given in the previous section, in particular the one involved the Pöschl-Teller potential, give a lot of material for experimenting in the optimized quantum well laser design. For instance, though we have explicitly shown that the energy spectra of the realistic ternary alloy based structures with a carrier having a spatially varying mass are equivalent to those of the constant-mass Pöschl-Teller Potential, the maximization of the gain may be accomplished via changing the quantum well profile which is in turn changes the wave functions. Hence the consideration of our results within supersymmetric transformations, as an alternative to the recent procedure proposed, in particular the significant difference between the wavefunctions by \( \nu(\tilde{z}) \) shown in (6), relating the solutions of the Schrödinger equations with constant and location dependent masses, and use of the more realistic effective potentials in (26) in tailoring process instead of the standard Pöschl-Teller potential, should reproduce more reliable results in order to help for the best design of such structures. Along this line the work is in progress.

Moreover, Plastino and his co-workers [28] recently studied some simple one-dimensional quantum mechanical systems characterized by a piecewise flat potential and mass to illustrate the influence of a non-constant mass on the density of the bound state energy levels. With the consideration of a finite potential well they showed that the number of bound states is less than those of the constant mass situation when the effective mass inside the well is lower than that of outside \( (m_0) \), and the opposite behaviour occurs when the effective mass inside the well is larger than the mass outside. However, our applications in section 3 do not confirm their work. This contradiction may raise a further discussion on the reliability of the present results, which can be clarified as follows. In the two different variable mass definitions, \( m(z) \), for the quantum well used in the previous section, \( m(z) > m_0 \) for the case \( \lambda > 0 \) and \( a > 1 \) while \( m(z) < m_0 \) in case \( \lambda < 0 \) and \( a < 1 \). The consideration of \( m(z) > m_0 \) case leads to single potential wells, sharper than that of the standard potential corresponding to constant-mass potentials, whereas \( m(z) < m_0 \) case give rise to bistable double well potentials, like the related illustrations in [9]. In spite of the different aspects
exhibited by the effective potentials defined in section 3, we have clearly shown that they share the same energy spectra regardless of $\lambda$ and $a$ values, together with the constant-mass potentials ($\lambda = 0, a = 1$). Consequently, one expects that the density of bound states for the systems we interest should not depend on the variation of a carrier mass.

5 Concluding remarks

In this article, we have 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 particular examples that the exact solvability depends not only on the form of the potential, but also on the spatial dependence on the mass. Within the framework of the two different theoretical treatments, the effective-mass Schrödinger equation has been transformed to a constant-mass Schrödinger equation and we have clarified that the Schrödinger equations with different masses and potentials can be exactly isospectral. We have also shown that though the potential energy of the BenDaniel-Duke Hamiltonian differs from the effective potentials of other Hamiltonians proposed in the literature by a term caused by the mass dependence on location, the exact analytical solutions to the effective-mass equations do not change with the Hamiltonian. As far as we know, this feature was not perceived until now. The discussion given behind the results obtained may be of interest, e.g., in the design and optimization of semiconductor quantum wells. In addition to their practical applications, we believe that the study of quantum mechanical systems with a position-dependent mass within the framework of the present models will raise many interesting conceptual problems of fundamental nature. In particular, the methods used in this article may be extended to find applications in also the study of quasi- and conditionally-exactly solvable systems with non-constant masses.
Table 1: Single-band effective mass Hamiltonians, Eq. (3).

| Hamiltonian  | $\alpha$ | $\beta$ | $\gamma$ |
|-------------|---------|---------|----------|
| Ref. [12]   | 0       | -1      | 0        |
| Ref. [14, 15]| -1      | 0       | 0        |
| Ref. [16]   | -1/2    | 0       | -1/2     |
| Ref. [17]   | 0       | -1/2    | -1/2     |
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