Explicit solutions for N-dimensional Schrödinger equations with position-dependent mass

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Abstract

With the consideration of spherical symmetry for the potential and mass function, one-dimensional solutions of non-relativistic Schrödinger equations with spatially varying effective mass are successfully extended to arbitrary dimensions within the frame of recently developed elegant non-perturbative technique, where the BenDaniel-Duke effective Hamiltonian in one-dimension is assumed like the unperturbed piece, leading to well-known solutions, whereas the modification term due to possible use of other effective Hamiltonians in one-dimension and, together with, the corrections coming from the treatments in higher dimensions are considered as an additional term like the perturbation. Application of the model and its generalization for the completeness are discussed.

Keywords: Schrödinger equation, Position-dependent mass, N−dimension
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1 Introduction

Gaining confidence from the successful applications [1] of the recently developed simple model [2] in different fields of physics, we have investigated [3] the relation between the solutions of physically acceptable effective mass Hamiltonians proposed in the literature for the treatment of one dimensional problems. Using the spirit of the prescription suggested in [3], we aim here to tackle the more difficult problem of generating exact solutions for position-dependent mass Schrödinger equations (PDMSE) in N−dimension, as the most of the related works in the literature have been devoted to one-dimensional systems except the ones in [4].

The concept of PDMSE is known to play an important role in different branch of physics. This formalism has been extensively used in nuclei, quantum liquids, $^3He$ and metal clusters. Another area wherein the such concepts provide very
useful tool is the study of electronic properties of many condensed-matter systems, such as semiconductors and quantum dots. In particular, recent progress in crystal-growth techniques for producing non-uniform semiconductor specimens, wherein the carrier effective mass depends on position, has considerably enhanced the interest in the theoretical description of semiconductor heterostructures. It has also recently been signalled in the rapidly growing field of PT-symmetric or more generally pseudo-Hermitian quantum mechanics. For an excellent recent review, leading to the related references, the reader is referred to [4].

In Section 2, the systematic treatment of $N$-dimensional PDMSE is presented and closed expressions corresponding to the full wave function and energy spectrum for exactly solvable potentials are given. Section 3 contains the application of the model while the generalization of the formalism is discussed in Section 4. Concluding remarks are given in the last section.

2 Theoretical Consideration

Tracking down solvable potentials in PDMSE has always aroused interest. Apart from being useful in understanding of many physical phenomena, the importance of searching for them also stems from the fact that they very often provide a good starting point for undertaking perturbative calculations of more complex systems.

As is well known (see, e.g., [3, 5]), the general form of radial PDMSE with Hermitian Hamiltonians in one-dimension gives rise to

$$-rac{d}{dz} \left[ \frac{1}{M(z)} \frac{d\Phi(z)}{dz} \right] + V^{eff}(z)\Phi(z) = \lambda \Phi(z),$$

(1)

where the effective potential

$$V^{eff}(z) = V_0(z) + U_{\alpha\gamma}(z) = V_0(z) - \frac{(\alpha + \gamma)}{2} \frac{M''}{M^2} + (\alpha\gamma + \alpha + \gamma) \frac{M'^2}{M^3},$$

(2)

depends on the mass term and ambiguity parameters. Here a prime denotes derivative with respect to the variable, $M(z)$ is the dimensionless form of the mass function $m(z) = m_0 M(z)$ and we have set $\hbar = 2m_0 = 1$. The effective potential is the sum of the real potential profile $V_0(z)$ 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. Some of them are the ones proposed by [6] BenDaniel-Duke ($\alpha = \gamma = 0$), Bastard ($\alpha = -1$), Zhu-Kroemer ($\alpha = \gamma = -1/2$) and Li-Kuhn ($\gamma = -1/2, \alpha = 0$).

Considering the works in [3, 7], the radial piece of PDMSE in arbitrary dimensions for spherically symmetric potentials and mass functions reads

$$\left\{ \frac{d^2}{dr^2} + \frac{M'}{M} \left( \frac{N-1}{2r} - \frac{d}{dr} \right) - \frac{L(L+N+2) + (N-1)(N-3)/4}{r^2} + M [E - V^{eff}(r)] \right\} \Psi(r),$$

(3)
where we assume that $\Psi(r) = F(r)G(r)$ which leads to

$$
\frac{1}{M} \left( \frac{F''}{F} + \frac{G''}{G} + \frac{2F'G'}{FG} \right) - \frac{M'}{M^2} \left( \frac{F'}{F} + \frac{G'}{G} \right) = U_{eff} - E. 
$$

The effective potential in higher dimensions ($N > 1$) now is transformed to the form

$$U_{eff}(r) = V_0(r) + U_{\alpha\gamma}(r) - \frac{M'(N-1)}{2r} + \frac{L(L + N - 2) + (N - 1)(N - 3)/4}{Mr^2},$$

in which $L$ is the angular momentum. As the one-dimensional calculations require $N = 1$ and $L = 0$, Eq. (5) reduces in this case to $U_{eff}(r) = V_{eff}(r) = V_0 + U_{\alpha\gamma}$ as in Ref. [3], which provides us a reliable testing ground.

Keeping in mind the spirit of the technique used simply in [3], we split Eq. (4) in two parts deviating from the treatments in [4]

$$W^2(r) - \left[ \frac{W(r)'}{\sqrt{M}} \right]' = V_0(r) - \varepsilon, \quad W = -\frac{F'}{\sqrt{MF}},$$

where $\varepsilon$ is the corresponding energy of the required quantum state $F_n$ ($n = 0, 1, 2, ...$) for $V_0$ which is assumed in this model as an exactly solvable mass-dependent potential, and

$$\Delta W^2(r) - \left[ \frac{\Delta W(r)'}{\sqrt{M}} \right]' + 2W(r)\Delta W(r) = \Delta V(r) - \Delta E, \quad \Delta W(r) = -\frac{G'}{\sqrt{MG}},$$

where

$$\Delta V(r) = U_{\alpha\gamma}(r) - \frac{M'(N-1)}{2r} + \frac{L(L + N - 2) + (N - 1)(N - 3)/4}{Mr^2}. \quad (8)$$

Note that the total energy appearing in (4) is $E = \varepsilon + \Delta E$ and, in one-dimension the modification term $\Delta V$ becomes $U_{\alpha\gamma}$ as in Ref. [3]. This clarifies that the corrections due to the higher dimensions arise because of the second and third term on RHS of Eq. (8).

From the present theoretical consideration, Eq. (6) has an algebraic solution leading to closed analytical expressions for the wave functions and energy eigenvalues, hence one needs to solve Eq. (7) exactly. To proceed further, with the consideration of relativistic Dirac equations having no ambiguity parameters, we confidently choose

$$\Delta W(r) = \frac{(\alpha + \gamma)}{2} \frac{M'}{M^3/2} - \frac{(N + 2L - 1)}{2\sqrt{Mr}},$$

in which the second term disappears for $N = 1$ as in [3]. Within the frame of Eq. (7), this choice leads us

$$W(r)\Delta W(r) = \frac{M'}{2rM^2} \left[ \frac{(\alpha + \gamma)(N-1)}{2} + (\alpha + \gamma + 1)L \right] - \frac{\Delta E}{2}, \quad (10)$$
that is the main result of the present Letter.

From the definition of the effective potential in Eq. (2), we also note that the use of Eqs. (7) and (8) naturally restricts the choice of some ambiguity parameters yielding different physically acceptable effective mass Hamiltonians, allowing only \( \alpha = \gamma = 0 \) (Ben-Daniel Duke Hamiltonian) and \( \alpha = \gamma = -1/2 \) (Zhu-Kroemer Hamiltonian) cases. This observation clarifies that the unperturbed part \((V_0)\) of the effective potential in (6) should corresponds to the case \( \alpha = \gamma = 0 \), having well known solutions in one dimension, while \( \alpha = \gamma = -1/2 \) is used to calculate \( U_{\alpha \gamma} \) in (8). Obviously, all the corrections coming from the higher dimensions to the energy and well-behaved wave function terms can be systematically calculated for a given \( M \) with the consideration of Eqs. (7-10) in the light of corresponding \( W \) in (6).

### 3 Application

Recently, some researches have been devoted to the analysis of the classification of quantum systems with position-dependent mass regarding their exact solvability [3-5, and the references therein]. On a similar basis, Plastino and his co-workers [8] applied an approach within the supersymmetric quantum mechanical framework, for the case \( \alpha = \gamma = 0 \), to such systems and succeed to show that some one-dimensional systems with non-constant mass have a supersymmetric partner with the same effective mass. They were also able to solve exactly some particular cases by constructing the superpotential \([W(r)]\) from the form of the effective mass \([M(r)]\) and generalize the concept of the shape invariance for these systems.

For illustration, the superpotential expressions given by [8] for the systems having harmonic oscillator and Morse-like spectra can be easily used in Eq. (6) to serve explicit expressions for the corrections to the one-dimensional solutions obtained by considering the Ben-Daniel-Duke effective Hamiltonian in their [8] calculations. This simple investigation enables us testing our results, because all the corrections should disappear in case \( N = 1 \) and \( \alpha = \gamma = 0 \) leading to the expressions in [8]. For clarity, this section involves only the application on the harmonic oscillator system. However, the generalization of the present model yielding self-consistent calculations, reproducing \( W(r) \) term within the model for any system of interest, will be discussed in the next section.

According to Ref. [8], \( W(r) \) term in Eqs. (6) and (10) is

\[
W(r) = \frac{\omega}{2} \int r \sqrt{M(z)} dz + \frac{1}{2} \left(\frac{1}{\sqrt{M}}\right)^\prime, \quad \omega = 2\epsilon_{n=0},
\]

for the system having harmonic oscillator spectra. Hence, use of Eqs. (7) through (10) gives
\[
\Delta E = \frac{M'}{rM^2} \left[ \frac{(\alpha + \gamma)(N - 1)}{2} + L(\alpha + \gamma + 1) \right] + \frac{(N + 2L - 1)\omega}{2r\sqrt{M}} \int r \sqrt{M(z)}dz + \\
\left( \frac{1}{\sqrt{M}} \right)' \left\{ (\alpha + \gamma) \left[ \omega \int r \sqrt{M(z)}dz + \left( \frac{1}{\sqrt{M}} \right) \right] + \frac{(N + 2L - 1)}{2r\sqrt{M}} \right\},
\]

which is the explicit form of the energy corrections for a given smooth mass. Clearly, it can be seen that for a constant mass \( M \to 1 \), Eq. 12 reduces to \((n + 2L - 1)\omega/2\) for arbitrary dimensions [7] while in one dimension it goes to zero for a non-constant mass in case \( \alpha = \gamma = 0 \) [8]. Furthermore, from Eqs. (7) and (9), the modification term for the corresponding wave function is

\[
G(r) = \exp \left( -\int r \sqrt{M(z)}\Delta W(z)dz \right) = r^{(N+2L-1)/2}M^{-(\alpha+\gamma)/2}.
\]

As Eq. (6) is analytically solvable having a closed expression for \( W(r) \) given by Eq. (11) reproducing explicit expressions for \( \varepsilon \) and \( F \), the corresponding total energy and wave function can easily be calculated through \( E = \varepsilon + \Delta E \) and \( \Psi = FG \) for the system of interest with a location dependent mass. At this stage it is also note that the formalism suggested here seems superior to the usual treatment in supersymmetric quantum theory that in principle start with the ground state and builds up excited state wave functions by the use of some linear operators \( (A^\pm) \) whereas there is no such restriction in the present theory providing flexible investigations.

### 4 Discussion

Although the procedure used in the formalism seems reasonable, the use of other works as in the previous section for an appropriate \( W(r) \) term to solve Eq. (6) may be seen as a drawback of the model. To remove this seeming deficiency, we propose here a unified treatment within the model considering the recent work in [9].

Many of the special functions \( H(g) \) of mathematics represent solutions to differential equations of the form

\[
\frac{d^2H(g)}{dg^2} + Q(g)\frac{dH(g)}{dg} + R(g)H(g) = 0,
\]

where the functions \( Q(g) \) and \( R(g) \) are well defined for any particular function [10]. Since in this Letter we are interested in bound state wave functions, we should restrict ourselves to polynomial solutions of Eq. (14). Bearing in mind Eq. (14), the substitution of \( \Phi(z) = H[g(z)]f(z) \) in Eq. (1) leads to the second-order differential equation

\[
\frac{1}{M} \left( \frac{f''}{f} + \frac{H''g^2}{H} + \frac{g''H'}{H} + 2\frac{H'g'f'}{Hf} \right) - \frac{M'}{M^2} \left( \frac{f'}{f} + \frac{H'g'}{H} \right) = V_{\text{eff}} - \lambda,
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\]
in which primes denote derivatives with respect to \(g\) and \(z\) for the functions \(H(g)\), \(g(z)\) and \(f(z)\) respectively. With the confidence gained by the similarity between Eqs. (15) and (4), one can safely use the present treatment splitting Eq. (15) in two pieces

\[
W^2(z) - \left[ \frac{W(z)}{\sqrt{M}} \right]' = V_0(z) - \varepsilon, \quad W = -\frac{f'}{\sqrt{Mf}},
\]

(16)

and

\[
\Delta W^2(z) - \left[ \frac{\Delta W(z)}{\sqrt{M}} \right]' + 2W(z)\Delta W(z) = \Delta V(z) - \Delta E, \quad \Delta W = -\frac{H'g'}{\sqrt{MH}},
\]

(17)

which is similar to Eqs. (6) and (7), where \(\lambda = \varepsilon + \Delta E\) and \(V_{eff} = V_0 + \Delta V\).

After all, it can be clearly seen that Eq. (16) is the one required for obtaining an explicit expression for \(W\) term used in Eq. (6) corresponding to an exactly solvable system considered in one-dimension (\(\alpha = \gamma = 0\)). However, to proceed further, the functions \(f\) and \(g\) should be solved as \(H, Q\) and \(R\) known in principle. Now, equating like terms between the resulting expression in (15) and (14) gives

\[
Q[g(z)] = \frac{1}{g'} \left( \frac{g''}{g'} + \frac{2f'}{f} - \frac{M'}{M} \right), \quad R[g(z)] = \frac{1}{g'^2} \left[ \frac{f''}{f} - \frac{M'f'}{Mf} + M(E - V) \right],
\]

(18)

where, from the definition of \(Q\),

\[
f(z) \approx \left( \frac{M}{g'} \right)^{1/2} \exp \left[ \frac{1}{2} \int_{g(z)}^{g(z)} Q(g) \, dg \right].
\]

(19)

Consideration of Eqs. (15) through (18) suggests a novel prescription

\[
\Delta V(z) - \Delta E = -\frac{g'^2}{M} R[g(z)],
\]

(20)

which, for plausible \(M\) and \(R\) functions, provides a reliable expression for \(g(z)\). It is remarked that in the constant mass case \(M \to 1\) this procedure reduces to the well known formalism which has been thoroughly investigated [11] that, together with [9], justify our new proposal in solving PDMSE. The more detailed investigation of this treatment will be discussed elsewhere.

5 Concluding Remarks

In this Letter, a general method has been presented to address the question of corrections to the solution in one-dimension for a large class of \(N\)-dimensional and exactly solvable PDMSE. We have also described how to extend the method to the case where the necessary function \(W(r)\) in (6) generating algebraically
solvable potentials in one dimension are present, which initiates calculations in
the model leading to explicit expressions for the modifications due to both the
use of physically plausible Zhu-Kroemer effective Hamiltonian ($\alpha = \gamma = -1/2$)
and higher dimensional treatments. The main results are consistent with the
other related works in the literature, which allow a non-perturbative treatment
of these issues.

Although, for clarity we have illustrated an application of the method for an
easily accessible case of interest, it can be readily employed in various typical
situations. In view of the importance in calculating such corrections in physics,
we believe that the present model would serve as a useful toolbox to treat even
more realistic situations which now occur in experimental observations with the
advent of the quantum technology.

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