Eur. Phys. J. A **28**, 253–257 (2006)
DOI 10.1140/epja/i2006-10047-3

THE EUROPEAN PHYSICAL JOURNAL A

# Effect of ordering ambiguity in constructing the Schrödinger equation on perturbation theory

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Received: 22 February 2006 /
Published online: 9 June 2006 – 
Communicated by V. Vento

**Abstract.** This work explores the application of perturbation formalism, developed for isotropic velocity-dependent potentials, to three-dimensional Schrödinger equations obtained using different orderings of the Hamiltonian. It is found that the formalism is applicable to Schrödinger equations corresponding to three possible ordering ambiguities. The validity of the derived expressions is verified by considering examples admitting exact solutions. The perturbative results agree quite well with the exactly obtained ones.

**PACS.** 03.65.Ge Solutions of wave equations: bound states – 31.15.Md Perturbation theory

## 1 Introduction

In a recent work we considered the time-independent Schrödinger equation for a constant mass moving in a velocity-dependent potential [1]. Treating the velocity-dependent potential as a small perturbation, we developed formulae for the changes in the bound-state energy and wave function of a quantum state. Unlike the standard perturbation theory, the results show that determination of the changes in the energy and wave function of a state only requires knowledge of the unperturbed ground-state wave function in addition to the perturbing potential.

The Schrödinger equation for a constant mass experiencing a velocity-dependent potential has the same form as one of the equations that have been proposed to describe a particle endowed with a position-dependent effective mass $m(r)$. The multiplicity of possible Schrödinger equations stems from an ambiguity in constructing the kinetic energy term. This in turn is a direct consequence of the non-commutativity of the spatially variable mass with the momentum operator.

The most general kinetic energy term used to describe a position-dependent mass is that proposed by von Roos [2],

$$T_{VR} = -\frac{\hbar^2}{4}\left[m^{\delta}(\vec{r})\,\nabla\, m^{\beta}(\vec{r})\,\nabla\, m^{\gamma}(\vec{r}) + m^{\gamma}(\vec{r})\,\nabla\, m^{\beta}(\vec{r})\,\nabla\, m^{\delta}(\vec{r})\right], \quad (1)$$

where the ambiguity parameters obey the constraint $\delta + \beta + \gamma = -1$. This ambiguity is relevant to many physical systems that have attracted much research activity. For examples; impurities in crystals [3–5], dependence of nuclear forces on the relative velocity of the two nucleons [6, 7]. More recent works include the study of semiconductor heterostructures [8,9].

Work has been done in order to single out a unique set of values for the ambiguity parameters. For example in [10] the case of a one-dimensional, position-dependent effective mass $m(x)$ was considered. It was suggested that there is a privileged ordering namely $\delta = 0, \beta = -1$, which was achieved by demanding the continuity of the term $[m(x)]^{-1}\partial\psi/\partial x$ at the point of discontinuity of $m(x)$. However, another work [11] also addressed the problem of abrupt heterojunctions and concluded that, for the generalized kinetic energy operator given in eq. (1), the quantities which are continuous are

$$m(x)^{\delta}\psi(x) \qquad \text{and} \qquad m(x)^{(\delta+\beta)}\frac{\partial\psi}{\partial x}\,, \quad (2)$$

with the constraint $2\delta + \beta = -1$. Further, the formalism of supersymmetric quantum mechanics and the notion of shape invariant potentials were extended to the Schrödinger equation for an effective position-dependent mass [12]. The authors considered an equation constructed using the set of parameters $\delta = 0, \beta = -1$. However, a more recent work [13] extended the supersymmetric formalism in such away that the ambiguity parameters were all taken into account. The authors started from the generalized kinetic energy term in eq. (1).

Clearly, there is no one single set of values that is universally agreed for the ambiguity parameters. Nonetheless, some of the choices that have been found useful for describing the motion of electrons in composition-

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ally graded crystals include those of BenDaniel and Duke (BDD) [14] ($\delta = 0, \beta = -1$), Zhu and Kroemer (ZK) [15] ($\delta = -\frac{1}{2}, \beta = 0$), Bastard [16] ($\delta = -1, \beta = 0$) and the redistributed model [17] ($\delta = 0, \beta = -\frac{1}{2}$).

In sect. 3 we shall explore the application of the perturbation formalism developed in [1] to different constructions of the Schrödinger equation obtained using different orderings. However, we shall start by giving a brief outline of the perturbation formalism.

## 2 Brief summary of the perturbation formalism

In [1] we considered an isotropic velocity-dependent potential of the form [18],

$$\nabla \cdot f(r)\nabla = f(r)\nabla^2 + \nabla f(r) \cdot \nabla, \tag{3}$$

where $f(r)$ is an isotropic function of the radial variable $r$. In the presence of the above velocity-dependent potential the $s$-wave, time-independent Schrödinger equation for a particle of constant mass $m_0$ and energy $E$ moving in some isotropic local potential $U(r)$ may be expressed as

$$\left[\frac{-\hbar^2}{2m_0}\{(1-f(r))\nabla^2 - \nabla f(r)\cdot\nabla\} + U(r)\right]\psi(\vec{r}) = E\psi(\vec{r}). \tag{4}$$

Using the reduced wave function $u(r) = rR(r)$ the above equation takes the form

$$(1-f(r))u''(r) - \left[u'(r) - \frac{u(r)}{r}\right]f'(r) = [U(r) - E]\,u(r), \tag{5}$$

where the prime denotes a derivative with respect to $r$ and we have expressed $E$ and $U(r)$ in units of $\hbar^2/2m_0$. Following Bender in his perturbative approach for local potentials [19], we considered the expansions

$$u(r) = u_0(r) + \lambda u_1(r) + \lambda^2 u_2(r) + \ldots, \tag{6}$$

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \ldots, \tag{7}$$

and set

$$f(r) = \lambda\rho(r), \tag{8}$$

with $\lambda$ being a real expansion coefficient such that $0 \leq \lambda \leq 1$. Switching off the perturbation corresponds to setting $\lambda = 0$. Further, the unperturbed ground-state wave function $u_0(r)$ and the corresponding energy $E_0$ are assumed known. In addition, $u_0(r)$ is normalized to unity.

Substituting eqs. (6) to (8) in (5) and equating coefficients of $\lambda^n$, for $n \geq 1$, leads to the general expression

$$u_n''u_0 - u_0''u_n - u_0\frac{\mathrm{d}}{\mathrm{d}r}(\rho u_{n-1}') + \frac{\rho'}{r}u_0u_{n-1} = -\sum_{k=1}^{n}E_k u_0 u_{n-k}. \tag{9}$$

Since we are dealing with bound states then $u_n(0) = u_n(\infty) = 0$ for all $n$. Integrating (9) over all $r$ results in the following energy and wave function corrections:

$$E_n = -\int_0^\infty u_0'\,\rho\,u_{n-1}'\,\mathrm{d}r - \int_0^\infty \frac{\rho'}{r}\,u_0\,u_{n-1}\,\mathrm{d}r, \tag{10}$$

$$u_n = u_0\int_0^r \frac{\mathrm{d}r'}{u_0^2}\int_0^{r'}\left\{u_0\frac{\mathrm{d}}{\mathrm{d}r''}\left(\rho u_{n-1}'\right) - \frac{\rho'}{r''}u_0u_{n-1} - \sum_{k=1}^{n}E_k u_0 u_{n-k}\right\}\mathrm{d}r'' + C_n u_0. \tag{11}$$

We determined the integration constants $C_n$ by demanding that each wave function correction $u_n$ be orthogonal to the ground-state wave function $u_0$. Hence multiplying the last equation by $u_0$ and integrating over all $r$ results in

$$C_n = \int_0^\infty u_0^2\,\mathrm{d}r\int_0^r\frac{\mathrm{d}r'}{u_0^2}\int_0^{r'}\left\{-u_0\frac{\mathrm{d}}{\mathrm{d}r''}\left(\rho u_{n-1}'\right) + \frac{\rho'}{r''}u_0u_{n-1} + \sum_{k=1}^{n}E_k u_0u_{n-k}\right\}\mathrm{d}r''. \tag{12}$$

It is worth noting that the energy corrections not only depend on the form of $\rho(r)$ but also on its derivative with respect to $r$. Further, the values of the energy corrections are decoupled as a direct consequence of constructing $u_n$ to be orthogonal to $u_0$.

The above formalism was applied to two simple examples admitting exact solutions. As will be seen in sect. 3.1, the perturbative solutions agree quite well with the exactly obtained ones. Although we considered the $s$-wave case, the above expressions are valid for all values of the orbital angular quantum number $l$ when the appropriate ground-state wave functions are used. The centrifugal barrier term can be included in $U(r)$ which does not appear explicitly in the derived results.

## 3 Effect of different orderings on the perturbative approach

From now on $m \equiv m(r)$ denotes a position-dependent effective mass, while $m_0$ denotes a constant mass as stated earlier. According to eq. (1) the most general, time-independent, three-dimensional Schrödinger equation for a position-dependent effective mass is

$$-\frac{\hbar^2}{2m}\left\{\nabla^2 - \frac{m'}{m}\frac{\mathrm{d}}{\mathrm{d}r} + (\delta+\gamma)\left[\frac{1}{r}\frac{m'}{m} + \frac{m''}{2m} - \frac{m'^2}{m^2}\right] - \delta\,\gamma\,\frac{m'^2}{m^2}\right\}\psi(\vec{r}) + U(r)\psi(\vec{r}) = E\psi(\vec{r}), \tag{13}$$

where we have used the condition $\delta + \beta + \gamma = -1$. In terms of the reduced wave function $u(r) = rR(r)$, the above equation may be presented in the form

$$-\frac{\hbar^2}{2m}\left\{\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{m'}{m}\left[\frac{\mathrm{d}}{\mathrm{d}r} - \frac{1}{r}\right] + (\delta+\gamma)\left[\frac{1}{r}\frac{m'}{m} + \frac{m''}{2m} - \frac{m'^2}{m^2}\right] - \delta\,\gamma\,\frac{m'^2}{m^2}\right\}u(r) + U_l(r)u(r) = Eu(r), \tag{14}$$

where $U_l(r) = U(r) + l(l+1)\hbar^2/2mr^2$ includes the centrifugal barrier term.

In what follows we shall explore the application of the perturbation formalism to Schrödinger equations constructed using different orderings. For simplicity, the $s$-wave case will be considered. Further, throughout the calculations $U(r)$ and $E$ are measured in units of $\hbar^2/2m_0$.

### 3.1 $\delta = 0, \beta = -1$

Using this set of the ambiguity parameters and making the substitution

$$\frac{1}{m} = \frac{1-f(r)}{m_0}, \tag{15}$$

eq. (14) takes the form

$$(1-f(r))u''(r) - \left[u'(r) - \frac{u(r)}{r}\right] f'(r) = [U(r) - E]\, u(r), \tag{16}$$

which coincides with the Schrödinger equation (5) that describes a constant mass moving in a velocity-dependent potential. As outlined in sect. 2, this equation was used to derive the perturbation formulae for the energy and wave function corrections given in (10) and (11). To test the validity of the derived expressions, two examples admitting exact solutions were considered [1]. In either case, the local potential $U(r)$ was assumed to have the simple form of an infinite spherical well of radius 1. The first example took $\rho(r)$ to be constant inside the infinite well. This resulted in a first-order perturbative solution that coincided with the exact one. In the second example, however, we considered a harmonic-like isotropic term $\rho(r) = \rho_0 r^2$. Inside the spherical local well the corresponding exact wave function is

$$u(r) =_2 F_1(a, b, c, \rho_0 r^2), \tag{17}$$

which is a hypergeometric function. Upon evaluating for $a$,$b$ and $c$, we obtain

$$u(r) = D\, r \left[1 - \frac{1}{6}E\, r^2 + \frac{1}{120\rho_0}E(E-10\rho_0)\, r^4 - \frac{1}{5040\rho_0^2}E(E-10\rho_0)(E-28\rho_0)\, r^6 + \ldots\right]. \tag{18}$$

For a physical solution the above infinite series must be terminated by setting one of the terms to zero. Choosing $E = 10\rho_0$ results in

$$u(r) = D\, r \left(1 - \frac{5}{3}\rho_0 r^2\right). \tag{19}$$

The constant $D$ can be determined by normalizing the wave function, which must vanish at $r = 1$. This results in $\rho_0 = 3/5$, leading to an exact energy eigenvalue $E = 6.0$ in units of $\hbar^2/2m_0$. Using the expressions for the derived bound-state energy corrections given in eq. (10) we obtain

$$E_1 = -3.4739, \quad E_2 = -0.2623, \quad E_3 = -0.0791. \tag{20}$$

In the absence of the velocity-dependent potential, the ground-state energy for an infinite well is $E_0 = \pi^2$. Consequently, up to and including the third-order correction in the perturbation the energy eigenvalue is $E = 6.0543$, in good agreement with the exact value of 6.0. Clearly, the absolute value of the energy corrections gets progressively smaller. Therefore, addition of further corrections is expected to bring the approximate and exact values even closer.

### 3.2 $\delta = -1, \beta = 0$

For this set of parameters, eq. (14) with the aid of (15) turns into

$$(1-f(r))u''(r) - f'(r)u'(r) - \frac{f''(r)}{2}\, u(r) = [U(r) - E]\, u(r). \tag{21}$$

Substituting eqs. (6) to (8) in the last expression and using $f(r) = \lambda\rho(r)$ leads to the following general equation for the coefficients of $\lambda^n$:

$$\frac{\mathrm{d}}{\mathrm{d}r}(u_n' u_0 - u_0' u_n) - u_0 \frac{\mathrm{d}}{\mathrm{d}r}(\rho\, u_{n-1}') - \frac{\rho''}{2}\, u_0\, u_{n-1} + \sum_{k=1}^{n} E_k u_0\, u_{n-k} = 0, \tag{22}$$

where $n \geq 1$. By integrating the above equation over all $r$ we end up with the following expression for the bound-state energy corrections:

$$E_n = -\int_0^\infty u_0'\, \rho\, u_{n-1}'\, \mathrm{d}r + \frac{1}{2}\int_0^\infty \rho''\, u_0\, u_{n-1}\, \mathrm{d}r. \tag{23}$$

Further, integrating (22) from 0 to $r$ leads to the corresponding wave function corrections

$$u_n(r) = u_0 \int_0^r \frac{\mathrm{d}r'}{u_0^2} \int_0^{r'} \left\{ u_0 \frac{\mathrm{d}}{\mathrm{d}r''}(\rho u_{n-1}') + \frac{\rho''}{2} u_0\, u_{n-1} - \sum_{k=1}^{n} E_k u_0\, u_{n-k} \right\} \mathrm{d}r'' + C_n u_0, \tag{24}$$

where

$$C_n = \int_0^\infty u_0^2\, \mathrm{d}r \int_0^r \frac{\mathrm{d}r'}{u_0^2} \int_0^{r'} \left\{ -u_0 \frac{\mathrm{d}}{\mathrm{d}r''}\left(\rho u_{n-1}'\right) - \frac{\rho''}{2} u_0\, u_{n-1} + \sum_{k=1}^{n} E_k u_0\, u_{n-k} \right\} \mathrm{d}r''. \tag{25}$$

In order to test the validity of the above formulae we shall assume the local potential to be an infinite spherical well and $\rho(r) = \rho_0 r^2$ as before. Consequently, the exact solution of (21) takes the form

$$u(r) = D\, r \left\{1 + \frac{1}{6}(-E + 3\rho_0) r^2 + \frac{1}{120}(-E+3\rho_0)(-E+13\rho_0) r^4 + \frac{1}{5040}(-E+3\rho_0)(-E+13\rho_0)(-E+31\rho_0) r^6 + \ldots\right\}. \tag{26}$$

The choice $E = 31\rho_0$ leads to

$$u(r) = D\, r \left(1 - \frac{14}{3}\,\rho_0\, r^2 + \frac{21}{5}\,\rho_0^2\, r^4\right). \qquad (27)$$

For the above solution to be physically acceptable it must vanish at $r = 1$. This imposes the value

$$\rho_0 = \frac{1}{63}\left(35 - 2\sqrt{70}\right), \qquad (28)$$

leading to an exact energy of 8.9884 in units of $\hbar^2/2m_0$. Using the expressions for the derived energy corrections in (10) we obtain

$$E_1 = -0.8089, \qquad E_2 = -0.0613. \qquad (29)$$

According to (7), up to and including the second-order correction the energy eigenvalue is $E = 8.9994$ in quite good agreement with the exact value. The absolute percentage error is only 0.1%.

### 3.3 $\delta = 0, \beta = -1/2$

Proceeding in exactly the same manner as above, eq. (14) reduces to

$$(1 - f(r))u''(r) - f'(r)u'(r) + \frac{f'(r)}{2r}u(r) - \frac{f''(r)}{4}u(r) = (U(r) - E)u(r), \qquad (30)$$

and the equation for the coefficients of $\lambda^n$ for $n \geq 1$ reads

$$\frac{\mathrm{d}}{\mathrm{d}r}(u_n' u_0 - u_0' u_n) - u_0 \frac{\mathrm{d}}{\mathrm{d}r}(\rho\, u_{n-1}') + \frac{\rho'}{2r} u_0\, u_{n-1} - \frac{\rho''}{4} u_0\, u_{n-1} + \sum_{k=1}^{n} E_k\, u_0\, u_{n-k} = 0. \qquad (31)$$

Integrating the last equation form the origin to infinity leads to the energy corrections

$$E_n = -\int_0^\infty u_0'\, \rho\, u_{n-1}'\, \mathrm{d}r - \int_0^\infty \frac{\rho'}{2r} u_0\, u_{n-1}\, \mathrm{d}r + \int_0^\infty \frac{\rho''}{4} u_0\, u_{n-1}\, \mathrm{d}r. \qquad (32)$$

However, integrating from the origin to $r$ leads to the wave function corrections

$$u_n = u_0 \int_0^r \frac{\mathrm{d}r'}{u_0^2} \int_0^{r'} \left\{ u_0 \frac{\mathrm{d}}{\mathrm{d}r''}\,(\rho u_{n-1}') - \frac{\rho'}{2r''} u_0\, u_{n-1} + \frac{\rho''}{4} u_0\, u_{n-1} - \sum_{k=1}^{n} E_k\, u_0\, u_{n-k} \right\} \mathrm{d}r'' + C_n\, u_0, \qquad (33)$$

where

$$C_n = \int_0^\infty u_0^2 \mathrm{d}r \int_0^r \frac{\mathrm{d}r'}{u_0^2} \int_0^{r'} \left\{ -u_0 \frac{\mathrm{d}}{\mathrm{d}r''}\,(\rho u_{n-1}') + \frac{\rho'}{2r''} u_0\, u_{n-1} - \frac{\rho''}{4} u_0\, u_{n-1} + \sum_{k=1}^{n} E_k\, u_0\, u_{n-k} \right\} \mathrm{d}r'' \qquad (34)$$

Taking the same form of the potentials as above, the exact wave function obtained is a hypergeometric function, which may be put in the form

$$u(r) = D\, r \left\{ 1 + \frac{1}{12}(-2E + 3\rho_0) r^2 + \frac{1}{480}(-2E + 3\rho_0)(-2E + 23\rho_0) r^4 + \frac{1}{40320}(-2E+3\rho_0)(-2E+23\rho_0)(-2E+59\rho_0) r^6 + \ldots \right\}. \qquad (35)$$

To terminate the infinite series we choose $E = 59\rho_0/2$, which leads to a wave function of the same form as that in (27). By demanding that the wave function be zero at $r = 1$, the corresponding exact energy is 8.5535 in units of $\hbar^2/2m_0$. Using the results of the perturbative approach given in (10) the energy corrections acquire the following values:

$$E_1 = -1.2438, \qquad E_2 = -0.0613. \qquad (36)$$

Consequently, in units of $\hbar^2/2m_0$ the energy up to and including the second-order correction is 8.5645. The absolute percentage error is only 0.1%. Clearly, the agreement with the exact value is very satisfactory.

### 3.4 $\delta = -1/2, \beta = 0$

Using this set of parameters, and (15) the most general Schrödinger equation (14) reduces to

$$(1 - f(r))u''(r) - f'(r)u'(r) - \frac{f'(r)^2}{4(1 - f(r))}u(r) - \frac{f''(r)}{2}u(r) = (U(r) - E). \qquad (37)$$

The perturbative approach relies on expanding the wave function and the energy in terms of the expansion parameter $\lambda$, then collecting coefficients of equal powers of $\lambda$. Since $f(r) = \lambda\rho(r)$, the term $(1 - f(r))^{-1}$ in the last equation renders this process invalid. Consequently, one cannot apply the perturbative formalism in this case.

## 4 Conclusions

In a recent work, we considered the Schrödinger equation for a constant mass moving in a velocity-dependent potential. We developed expressions for the changes in the bound-state energies and the corresponding changes in the wave functions assuming the velocity-dependent potential to be a small perturbing term [1]. In this work we have explored the application of this perturbative approach to Schrödinger equations describing a particle endowed with a position-dependent effective mass. The considered Schrödinger equations correspond to different ordering ambiguities.

For the ambiguity parameters proposed by BenDaniel and Duke ($\delta = 0, \beta = -1$), the Schrödinger equation

for the spatially variable mass has the same form as the Schrödinger equation for a constant mass moving in a Kisslinger-type velocity-dependent potential given in eq. (3). This is exactly the equation we used to derive the perturbation formalism in [1]. To test the validity of the perturbation expressions, examples admitting exact solutions were considered. The local potential was taken to have the form of a spherical infinite well of radius $r = 1$. However, the isotropic term was assumed to have harmonic-like behavior, namely $\rho(r) = \rho_0 r^2$. The value $\rho_0 = 0.6$ resulted in an exact energy $E = 6.0$ in units of $\hbar^2/2m_0$. Using the expression in (10), the energy corrections were calculated to be $E_1 = -3.4739$, $E_2 = -0.2623$ and $E_3 = -0.0791$. Consequently, up to and including the third-order correction the energy eigenvalue is 6.0543 in good agreement with the exact value.

For the set $\delta = -1, \beta = 0$ proposed by Bastard, use of the same forms of the potentials as above resulted in an exact energy value of 8.9884 in units of $\hbar^2/2m_0$. The energy corrections were determined to be $E_1 = -0.8089$ and $E_2 = -0.0613$. Therefore, the energy up to and including the second-order correction is 8.9994. The absolute percentage difference is only 0.1%.

According to the redistributed model the proposed values of the ambiguity parameters are $\delta = 0, \beta = -1/2$. The exact energy corresponding to the same forms of the potentials as above is 8.5535 in units of $\hbar^2/2m_0$. While use of the perturbation expressions resulted in $E_1 = -1.2438$ and $E_2 = -0.0613$. This leads to an energy value of 8.5645 up to and including the second-order correction in good agreement with the exact value.

Finally, Zhu and Kroemer proposed the values $\delta = -1/2, \beta = 0$, which, when substituted in (14), result in an equation that has the term $(1 - \lambda\rho(r))$ in the denominator. The perturbation formalism relies on expanding the energy and the corresponding wave function in powers of $\lambda$ and then collecting the coefficients of equal powers of $\lambda$. The presence of $(1 - \lambda\rho(r))^{-1}$ makes this procedure not possible. Therefore, the perturbation formalism does not apply in this case.

In conclusion, the application of the perturbative approach to three-dimensional Schrödinger equations that describe a position-dependent effective mass has been explored. The equations were constructed using different ordering ambiguities proposed in the literature. It has been shown that the perturbative approach is applicable to Schrödinger equations corresponding to three ambiguity orderings. A fourth set of ambiguity parameters results in an equation for which the perturbation formalism does not apply.

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