The Effect of Different Ordering Ambiguityon the Wave Functions Corresponding to a Velocity-Dependent Potential

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Abstract

The problem of ordering ambiguity in constructing the Hamiltonian for a positiondependenteffective massis investigated. This has been achieved by studying the continuityof the wave function and its derivative for a constant mass moving in a velocitydependentpotential. The results suggest one possible ordering for which physicallyacceptable solutions can be obtained. We also studied the effect of different orderingson perturbation theory developed for velocity- dependent potentials. Furthermore, theconvergence properties of the bound-state perturbation series, developed in an earlierwork for velocity-dependent potentials, has been investigated. Old and recent worksin the literature have successfully used the velocity - dependent potential to model the*pion - nucleus* and *nucleon - nucleus* interactions. In the latter case, the variations ofthe optical potential parameters with the incident nucleon energy were reduced.

Keywords: Velocity-Dependent Potential, Position-Dependent Effective Mass, Ordering Ambiguity.

1. Introduction

Physical systems with a position-dependent effective mass (PDEM) have attractedthe attention of many works. For examples; the Schrödinger equation fora PDEM has been used in describing the dynamics of electrons in semiconductor heterostructures such as, compositionally graded crystals (Michael and Walter, 1993), quantum dots (Serra and Lipparini, 1997) and liquid crystals (Barranco at el., 1997). In nuclear physics, such an equation is relevant in modelingthe nucleon-nucleon interaction (Razavy et al., 1962). Choosing the correct form of the Hamiltonianoperator for a position-dependent effective mass has been a long standing problemin quantum mechanics. There is an ordering ambiguity which stems from thenon-commutativity between the spatially variable mass and the momentum operator. Von Roos suggested the following most general kinetic energy term that describes aPDEM (Von, 1981):

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

where the ambiguity parameters obey the constraint$\delta + \beta + \gamma = -1$ and$m = m(r)$is a spatially variable mass. No derivation exists that defines a unique and universalset of values for the ambiguity parameters. However, several choices that have beenfound useful in describing the motion of electrons in compositionally graded crystalsinclude BenDaniel and Duke (BenDaniel and Duke, 1966)($\delta = 0, \beta = -1$), Bastard (Bastard, 1981)($\delta = -1\,, \beta = 0$) andLi and Kohn (Li and Kohn, 1993)($\delta = 0, \beta = -1/2$). The corresponding kinetic energy operators,respectively, are

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$$T = -\frac{\hbar^2}{2}\left[\nabla\frac{1}{m}\nabla\right], \quad (2)$$

$$T = -\frac{\hbar^2}{4}\left[\frac{1}{m}\nabla^2 + \nabla^2\frac{1}{m}\right], \quad (3)$$

$$T = -\frac{\hbar^2}{4}\left[\nabla\frac{1}{\sqrt{m}}\nabla\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{m}}\nabla\frac{1}{\sqrt{m}}\nabla\right], \quad (4)$$

Many old and recent works have been carried out in order to limit the possible choicesof the ambiguity parameters. For examples; Morrow and Brownstein (Morrow and Brownstein, 1984) addressedthe problem of abrupt heterojunctions between two crystals, and showed that$\delta = \gamma$;otherwise the wave function vanishes at the heterojunction, which is clearly an unphysicalresult. Similarly, Thomsen et al. also concluded that $\delta = \gamma$; otherwisethe ground state energy diverges in the abrupt limit (Thoomsen, 1989). Obviously, this conditionexcludes the forms of the operators in Eqs.(3) and (4). Furthermore, by studyingthe connection rules at the heterostructure boundary, and assuming the $\delta = \gamma$constraint, Zhu and Kroemer (Zhu and Kroemer, 1983) suggested that $\beta = 0$, while Morrow (Morrow, 1987) concludedthat $\beta \approx 0$. In contrast, other works (Von and Mavromatis, 1985; Galbraith and Duggan, 1988; L'evy, 1995) suggested that $\beta = -1$. However,upon studying the matching conditions of the wave function and its derivativein three dimensions across an abrupt heterojunction between two crystals, Morrowchanged his earlier conclusion $\beta \approx 0$ to $\beta = -1$(Morrow, 1987). In a more recent work Dutraand Almeida discussed the problem of exact solvability and ordering ambiguityin quantum mechanics (Dutra and Almeida, 2000). By considering specific examples they showed thatthe orderings $(\delta = -1, \beta = 0)$ and $(\delta = 0, \beta = -1)$ lead to physically unacceptablecomplex energies. Therefore, they suggested that such orderings could possibly bediscarded.

Clearly, various techniques have been adopted to investigate the problem andresulted in dfferent sets of possible parameters leaving the problem of ordering ambiguityfar from being resolved. One of our aims in this work is to study the problemof ordering ambiguity by considering a closely related system, which is the motionof a constant-mass particle in a velocity-dependent potential. For such a system,we shall show in section [2] that the boundary conditions on the derivatives of theradial and reduced wave functions are consistent only when the Hamiltonian is constructed

using the ordering $\beta = -1$. In reference (Jaghoub, 2006)Jaghoub discussed the effectof ordering ambiguity on the perturbation theory, for isotropic velocity-dependentpotentials, that is developed in (Jaghoub, 2006). It was concluded that the perturbation formalismis applicable to Schrödinger equations corresponding to the orderings leading toEqs.(2) to (4). In contrast, the results of this work show that the derived perturbationformalism corresponding to the orderings $(\delta = -1, \beta = 0)$ and $(\delta = 0, \beta = -1/2)$produces accurate results only when the potentials used lead to vanishing wave functionsat the boundary. It is also shown that the ordering $(\delta = 0, \beta = -1)$leads toperturbation formalism whose results agree well with the exact values, regardless ofthe value of the wave functions at the potential boundary. Finally, in reference (Jaghoub, 2006)Jaghoub developed a perturbation series for the bound-state energy corrections uponthe introduction of a small isotropic velocity-dependent perturbing potential. In thiswork, we shall investigate the convergence properties of this series in section [4].

2. Boundary ConditionsAcrossan Abrupt Junction

According to the von Roos operator given in Eq.(1), themost general Schrödingerequation for a spatially variable mass$m = m(r)$ assumes the form,

$$-\frac{\hbar^2}{2m}\left\{\nabla^2 - \frac{m'}{m}\frac{d}{dr} + (\delta+\gamma)\left[\frac{1}{r}\frac{m'}{m} + \frac{m''}{2m} - \frac{m'^2}{m^2}\right] - \delta\gamma\frac{m'^2}{m^2}\right\}\psi(\vec{r}) + V(r)\psi(\vec{r}) = E\psi(\vec{r}), \quad (5)$$

where the prime means derivation with respect to the radial variable $r, \psi(\vec{r})$ is athree-dimensional wave

function and $V(r)$ is an isotropic local potential. In terms ofthe reduced wave function, $u(r) == rR(r)$, the above equation becomes:

$$-\frac{\hbar^2}{2m}\left\{\frac{d^2}{dr^2}-\frac{m'}{m}\left[\frac{d}{dr}-\frac{1}{r}\right]+(\delta+\gamma)\left[\frac{1}{r}\frac{m'}{m}+\frac{m''}{2m}-\frac{m'^2}{m^2}\right]-\delta\gamma\frac{m'^2}{m^2}\right\}u(r)+V(r)u(r)=Eu(r), \quad (6)$$

where, for simplicity, we have considered the $l=0$ case. In what follows we shallfirst transform the above equation into a Schrödinger equation for a particle experiencinga velocity-dependent potential that is taken to have an abrupt edge. Thecontinuity of the wave function derivative across the potential boundary will then bestudied corresponding to each of the three orderings that lead to Eqs.(2), (3) and (4).Such a velocity - dependent potential has recently been successfully used to describethe nucleon - nucleus scattering process from light and heavy nuclei (Jaghoub, 2011; Jaghoub,2012; Zureikat and Jaghoub, 2013; Ghabar and Jaghoub, 2015). Theuse of this potential resulted in best fit optical potential parameters which showedreduced variation with the energy of the incident nucleon.

2.1. The First Ordering: $(\delta=0,\beta=-1)$

We shall start by transforming the last equation into an equation for a constantmass m_0 experiencing an isotropic velocity-dependent potential. This can beachieved by using the substitution;

$$\frac{1}{m}=\frac{1-\rho(r)}{m_0}, \quad (7)$$

where$\rho(r)$ is an isotropic function of the radial variable r. Evaluating, $(\delta=0,\beta=-1)$in Eq.(6) leads to

$$\big(1-\rho(r)\big)u''(r)-\left[u'(r)-\frac{u(r)}{r}\right]\rho'(r)=\frac{2m_0}{\hbar^2}[V(r)-E]\,u(r). \quad (8)$$

This is the exact equation that one obtains by considering the *s-wave*Schrödingerequation for a constant mass m_0 moving in a velocity-dependent potential of theform

$$\hat{V}(r,p) = V(r)+\frac{\hbar^2}{2m_0}\nabla.\rho(r)\nabla = V(r)+\frac{\hbar^2}{2m_0}\{\rho(r)\nabla^2+\nabla\rho(r).\nabla\}. \quad (9)$$

This potential was first suggested by Kisslinger to model the pion - nucleus scatteringprocess (Kisslinger, 1955). In order to study the continuity of the wave function and itsderivative across an abrupt junction, we shall adopt the following forms for the localand velocity-dependent potentials respectively,

$$V(r)=-V_0[1-U(r-b)], \qquad \rho(r)=\rho_0[1--U(r-b)], \quad (10)$$

whereV_0 and ρ_0 are constants, while $U(r-b)$ is a step function defined as

$$U(r-b)=0, \qquad r<b \quad (11)$$

$$=1, \qquad r<b \quad (12)$$

and$b$ is the common radius of both potentials. It is worth noting that the potentialsused in physical problems are smoother than the ones stated above. However, as weshall see below, our choice of $V(r)$ and $\rho(r)$results in simple Schrödinger equationsfrom which the boundary conditions on the wave functions and their derivatives canbe readily obtained. Furthermore, as illustrated in section [3], such potentials leadto exact analytical formulas for the wave function and the corresponding energy corrections,which allows a comparison between the perturbed and exact energy values.We also point out that Razavy et al. modeled the nucleon-nucleon interaction usingthe velocity-dependent potential in Eq.(9) with the above forms for$V(r)$ and $\rho(r)$and succeeded in reproducing the *1S singlet-even* phase shifts for the two-nucleonsystem (Razavy et al., 1962). Substituting for $V(r)$ and $\rho(r)$ into Eq.(8) leads to

$$[1-\rho_0+\rho_0U(r-b)]u''(r)+\left\{k^2+\frac{2m_0V_0}{\hbar^2}[1-U(r-b)]\right\}u(r)=-\rho_0\left[v'-\frac{v}{r}\right]\delta(r-b), \quad (13)$$

where $k^2=2m_0E/\hbar^2$. As always, the wave function must be continuous across thejunction,

$$u(b^-) = u(b^+). \tag{14}$$

However, by integrating Eq.(13) from $b-\varepsilon$ to $b+\varepsilon$, where ε is vanishingly small andpositive, and then taking the limit as $\varepsilon \to 0$, the following condition must be satisfied:

$$u'(b^+) = (1-\rho_0)u'(b^-) + \rho_0 \frac{u(b)}{b}, \tag{15}$$

where$u'(b^-)$ and $u'(b^+)$ are the derivatives of the wave function at r less and greaterthan b respectively.To this end let us turn to the *s-wave*Schrödinger equation for the radial function$R(r)$ that can be obtained from Eq.(5) namely,

$$-\frac{\hbar^2}{2m}\left\{\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{m'}{m}\frac{d}{dr}+(\delta+\gamma)\left[\frac{1}{r}\frac{m'}{m}+\frac{m''}{2m}-\frac{m'^2}{m^2}\right]-\delta\gamma\frac{m'^2}{m^2}\right\}R(r)+V(r)R(r)=ER(r). \tag{16}$$

Using Eqs.(7) and (10) then evaluating for the ambiguity parameters $\delta = 0,\ \beta = -1$one ends up with:

$$[1-\rho_0+\rho_0U(r-b)]\left(R''(r)+\frac{2}{r}R'\right)+\left\{k^2+\frac{2m_0V_0}{\hbar^2}[1-U(r-b)]\right\}R(r)=-\rho_0R'\delta(r-b). \tag{17}$$

Proceeding in the same manner as we did to obtain the boundary condition in Eq.(15),one can easily show that the following continuity condition applies,

$$R'(b^+) = (1-\rho_0)R'(b^-), \tag{18}$$

where$R'(b^-)$ and $R'(b^+)$ are the derivatives of the radial wave function for r lessand greater than b respectively. Clearly, using the relation $u(r) = rR(r)$, it is easy toshow that Eq.(18) can be readily obtained from Eq.(15) and vice versa. This mightseem to be an obvious result that applies in general. However, as shown below, thisis not the case when the Schrödinger equation is constructed using the orderings($\delta = -1$, $\beta = 0$) and($\delta = 0,\ \beta = -1/2$).

2.2. The Second Ordering:$(\delta = -1, \beta = 0)$

For this set of ambiguity parameters, the corresponding s-wave Schrödingerequations for the reduced and radial wave functions respectively are:

$$[1-\rho_0+\rho_0U(r-b)]u''(r)+\left\{k^2+\frac{2m_0V_0}{\hbar^2}[1-U(r-b)]-\frac{\rho''(r)}{2}\right\}u(r)=u'(r)\delta(r-b), \tag{19}$$

and

$$[1-\rho_0+\rho_0U(r-b)]\left(R''(r)+\frac{2}{r}R'\right)+\left\{k^2+\frac{2m_0V_0}{\hbar^2}[1-U(r-b)]\right\}R(r) = \frac{\rho''(r)}{2}R(r)-\rho_0\left(\frac{R}{r}+R'(r)\right)\delta(r-b), \tag{20}$$

where we have substituted for the local and velocity-dependent parts of $\hat{V}(r,p)$ usingEq.(10). By integrating each of the above equations from $b-\varepsilon$to $b+\varepsilon$, where ε is vanishingly small andpositive, and then taking the limit as $\varepsilon \to 0$ one obtains thefollowing boundary conditions at the abrupt junction,

$$\left(1-\frac{\rho_0}{4}\right)u'(b^+) = \left(1-\frac{3\rho_0}{4}\right)u'(b^-), \tag{21}$$

and

$$\left(1-\frac{\rho_0}{4}\right)R'(b^+) = \left(1-\frac{3\rho_0}{4}\right)R'(b^-). \tag{22}$$

Substituting $u(r) = rR(r)$ in Eq.(21) leads to

$$\left(1-\frac{\rho_0}{4}\right)R'(b^+) = b\left(1-\frac{3\rho_0}{4}\right)R'(b^-)+\left(1-\frac{\rho_0}{2}\right)R(b). \tag{23}$$

Clearly, Eqs.(22) and (23) are inconsistent. Consistency can only be recovered providedR(b) = 0. That is the wave function must vanish at the boundary, which isunphysical. Therefore, the ordering $(\delta = -1,\ \beta = 0)$ seems to lead to unphysicalresults.

2.3. The Third Ordering:$(\delta = 0,\ \beta = -1/2)$

Following the same steps as in the last subsection we state the *s-wave*Schrödingerequations for the reduced and radial wave functions respectively,

$$[1-\rho_0+\rho_0 U(r-b)]u''(r)+\left\{k^2+\frac{2m_0V_0}{\hbar^2}[1-U(r-b)]\right\}u(r) = \rho_0(r)\left\{\frac{u(r)}{2r}-u'(r)\right\}\delta(r-b)+\frac{\rho''(r)}{4}u(r), \tag{24}$$

and

$$[1-\rho_0+\rho_0 U(r-b)]\left(R''(r)+\frac{2}{r}R'\right)+\left\{k^2+\frac{2m_0V_0}{\hbar^2}[1-U(r-b)]\right\}R(r) = \frac{\rho''(r)}{4}R(r)-\rho_0\left(\frac{R}{2r}+R'(r)\right)\delta(r-b), \tag{25}$$

Proceeding as in the above two cases one obtains the following boundary conditions:

$$\left(1-\frac{\rho_0}{8}\right)u'(b^+)-\left(1-\frac{7\rho_0}{8}\right)u'(b^-)=\frac{\rho_0 u(b)}{2b}, \tag{26}$$

and

$$\left(1-\frac{\rho_0}{8}\right)R'(b^+)=\left(1-\frac{7\rho_0}{8}\right)R'(b^-). \tag{27}$$

Substituting $u(r)=rR(r)$ in Eq.(26) results in

$$b\left(1-\frac{\rho_0}{8}\right)R'(b^+)=b\left(1-\frac{7\rho_0}{8}\right)R'(b^-)-\frac{\rho_0 R(b)}{4}. \tag{28}$$

Once again, the unphysical condition $R(b)=0$ must be satisfied for Eqs.(27) and(28) to be consistent.

Clearly, only the ordering $(\delta = 0,\ \beta = -1)$ leads to consistent boundary conditionsregardless of the value of the wave function at the boundary. Our conclusionis in line with other works that have suggested this ordering to be the correct one todescribe a position-dependent effective mass (Von and Mavromatis, 1985; Galbraith and Duggan, 1988; L'evy, 1995; Morrow, 1987).

3. EffectofDifferent Orderingson Perturbation Theory

In reference (Jaghoub, 2006)Jaghoub considered the *s-wave* Schrödinger equation corresponding to the ordering $(\delta = 0,\ \beta = -1)$. Upon the introduction of a small velocity-dependentperturbing potential, we developed perturbation formulas for the changesin the energy eigenvalues and the corresponding changes in the wave functions. Forcompleteness, we shall state the derived general formulas for the energy and wavefunction corrections, which are

$$E_n=\int_0^\infty u_0\frac{d}{dr}(\rho u'_{n-1})\,dr\ -\int_0^\infty\frac{\rho'}{r}u_0u_{n-1}\ dr, \tag{29}$$

and

$$u_n=u_0\int_0^r\frac{dr'}{u_0^2}\int_0^{r'}\left\{u_0\frac{d}{dr''}(\rho u'_{n-1})-\frac{\rho'}{r''}u_0u_{n-1}-\sum_{k=1}^{n}E_k u_0u_{n-k}\right\}dr''+C_nu_0, \tag{30}$$

where the constant of integration C_n is given by

$$C_n = \int_0^\infty u_0^2 dr \int_0^r \frac{dr'}{u_0^2} \int_0^{r'} \left\{ -u_0 \frac{d}{dr''}(\rho u'_{n-1}) + \frac{\rho'}{r''} u_0 u_{n-1} + \sum_{k=1}^{n} E_k u_0 u_{n-k} \right\} dr''. \quad (31)$$

In this section we shall start by testing the applicability of the above expressionsby assuming $V(r)$ and $\rho(r)$ to have the finite square-well shapes stated in Eq.(10).As stated earlier, for such potentials the Schrödinger equation is exactly solvable,which allows the perturbed results to be compared with the exact ones. In addition,corresponding to such potentials, the above perturbation formulas produce exact analyticalexpressions for the changes in the bound-state energies and wave functions.For example, corresponding to the above potentials, the first-order energy and wavefunction corrections are

$$E_1 = \frac{1}{2b} A^2 \rho_0 [K^2 b^2 + (2 + \lambda b) sin^2(Kb)], \quad (32)$$

$$u_1(r) = \left[\frac{AE_1}{2K} + \frac{1}{2} AK\rho_0\right] r \cos(Kr) - \left[\frac{AE_1}{4K_2} + \frac{1}{4} A\rho_0 - \frac{C_1}{K}\right] \sin(Kr), \qquad r < b \quad (33)$$

and

$$u_1(r) = \left[\frac{AE_1}{2\lambda} r + \frac{A}{4\lambda^2}\right] e^{\lambda(b-r)} \sin(Kb) + D_1 e^{-\lambda r}, \qquad r > b \quad (34)$$

where

$$K = \sqrt{\frac{2m_0}{\hbar^2}(V_0 + E_0)}, \qquad \lambda = \sqrt{-\frac{2m_0}{\hbar^2} E_0}, \qquad A = \sqrt{\frac{2\lambda}{1 + \lambda b}}, \quad (35)$$

andE_0 is the unperturbed ground-state energy. Further, the constants C_1 and D_1can be determined by matching the wave functions at $r = b$ and using Eq.(31). Fortwo values of the local potential we determined the exact energies E_{ex} and the perturbedenergy corrections E_p calculated up to and including third order. The resultsare shown in Table [1] and correspond to $\beta = -1$, $\rho_0 = 0.1$ and $b = 1\ fm$. Further,throughout this work the energies and V_0 are given in units $\hbar^2/2m_0$. Clearly,the perturbed energies are in good agreement with the exact ones, especially in thesecond case where$V_0 = 4.0$is large compared to ρ_0. In addition, Figure [1] showsthe unperturbed wave function $u_0(r)$ (dashed-dotted line), the first (dashed-line) andsecond-order (solid line) wave function corrections corresponding to $V_0 = 2.8$. Itis evident that, as expected, both the energy and wave function corrections get progressivelysmaller as the perturbation order increases. Now we turn to the orderings($\delta = -1,\ \beta = 0$)and ($\delta = 0,\ \beta = -1/2$). The corresponding formulas for the energyand wave function corrections were derived in (Jaghoub, 2006). There, Jaghoub tested theapplicability of the formulas assuming the local potential to have the form of an infinitesquare well while $\rho(r)$ was taken to have the shape of a finite square well.The agreement between the exact and perturbed results was quite satisfactory. Thisleads to the conclusion that the perturbation formulas corresponding to the above twoorderings produce accurate results. However, in the present work, we tested the applicabilityof these formulas using the finite square-well forms of the potentials givenin Eq.(10). This resulted in a poor agreement between the perturbed and exact energyvalues. The disagreement may be explained as follows. As we saw in sections [2.2]and [2.3], the condition $R(b) = 0$ must be satisfied for the boundary conditions onthe derivative of the radial wave functions to be consistent. In reference (Jaghoub, 2006), wherethe local potential has the form of an infinite square-well, this condition is obviouslysatisfied. In this work, however, the potentials in Eq.(10) result in non-vanishingwave functions at the potential edge leading to inconsistent boundary conditions,which may be responsible for the poor estimation of the perturbed energy values. Incontrast to the conclusion in reference (Jaghoub, 2006), the perturbation formulas correspondingto the orderings ($\delta = -1,\ \beta = 0$) and ($\delta = 0,\ \beta = -1/2$) give accurate results onlywhen the potentials used lead to vanishing wave functions at the boundary. In reference(Jaghoub, 2006)Jaghoub started from the Schrödinger equation that is constructed using theordering ($\delta = 0,\ \beta = -1$) and developed perturbation

formulas for the changes in thephase shifts and the corresponding wave functions upon the introduction of a smallperturbing velocity-dependent potential. When $V(r)$ and $\rho(r)$ were assumed to havefinite square well shapes as in Eq.(10) the perturbed phase shift values compared wellwith the exact ones as can be seen in the last reference. For the other two orderings,however, an analysis similar to that for the bound states case above shows that thecorresponding perturbation formulas produce accurate results only when the wavefunctions vanish at the boundary. To avoid repeating the same type of analysis wehave not shown the detailed calculations here. Although the degree of convergenceof a perturbative approach corresponding to a given ordering should not be used as acriteria to choose or discard that ordering, it is still an indication that $\beta = -1$ mightbe applicable to a wider range of systems.

4. Convergence of the Energy Perturbation Series

The energy corrections in Eq.(29) give the terms of the energy perturbationseries, namely

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \lambda^3 E_3 + \cdots, \tag{36}$$

and the corresponding series for the wave function corrections reads

$$u(r) = u_0(r) + \lambda u_1(r) + \lambda^2 u_2(r) + \lambda^3 u_3(r) + \cdots, \tag{37}$$

where$\lambda$is a constant that defines the order of the perturbation. At this point it isworth noting that by carrying out an analysis similar to that in reference (Jaghoub, 2006), onemay show that the wave function corrections $u_n(r)$ given by Eq.(30) are finite at theorigin as well as at the zeros of the unperturbed wave function $u_0(r)$. Now let us startby expressing the n^{th}-order wave function correction as:

$$u_n(r) = \gamma_n(r) u_{n-1}(r). \tag{38}$$

First we note that the above discussion implies that the functions $\gamma_n(r)$ are finitefunctions of the radial variable r. Secondly, by repeating the pattern in Eq.(38) for$u_{n-1}(r)$, $u_{n-2}(r)$ and so on, we may express $u_n(r)$ in terms of the unperturbed wavefunction $u_0(r)$ according to

$$u_n(r) = \gamma_n(r)\gamma_{n-1}(r)\gamma_{n-2}(r) \ldots\ldots \gamma_1(r) u_0(r). \tag{39}$$

In a more compact form:

$$u_n(r) = \left[\prod_{m=1}^{n} \gamma_m(r)\right] u_0(r). \tag{40}$$

Substituting the above expression for $u_n(r)$ in Eq.(29) to obtain the energy correctionsleads to very complicated expressions. However, since we are interested in theconvergence properties of the energy series rather than the exact values of $u_n(r)$ weshall make an approximation, that overestimates each wave function correction, bysetting

$$g_m = \gamma_m(r_0), \tag{41}$$

wherer_0 is the value of r at which $\gamma_m(r)$ attains its maximum value and, hence, $g_m$is a constant. Of course, r_0 may be dierent for dierent values of m. In terms of g_m,the exaggerated wave function corrections are given by

$$u_n(r) = \left[\prod_{m=1}^{n} g_m\right] u_0(r). \tag{42}$$

In order to simplify the expression for $u_n(r)$ even further, define a constant g thatequals the maximum value of g_m, that is

$$g = (g_m)_{max}. \tag{43}$$

Evaluating g for each g_m in Eq.(42) results in

$$u_n(r) = g^n u_0(r). \tag{44}$$

Finally, using the above equation to substitute for $u_n(r)$ into Eq.(29), the n^{th}-orderenergy correction can

now be expressed as

$$E_n = g^{n-1}\int_0^\infty u_0\left[\frac{d}{dr}(\rho u_0') - \frac{\rho'}{r}u_0\right]dr = g^{n-1}E_1, \quad (45)$$

where$n \geq 1$ and we have suppressed the dependence on r for clarity of presentation.Upon setting $\lambda = 1$ in Eq.(36), the energy perturbation series may now be expressedas

$$E = E_0 + E_1(1 + g + g^2 + \cdots) = E_0 + E_1\sum_{s=0}^{\infty} g^s. \quad (46)$$

Clearly, if $g < 1$ and E_1 is finite, the above series converges to

$$E = E_0 + \frac{E_1}{1-g} \quad . \quad (47)$$

$V_0 = 2.8$	$E_0 = -0.02518$	$E_{ex} = -0.03599$	
$E_1 = -0.00870$	$E_2 = -0.00334$	$E_3 = -0.00062$	$E_p = -0.03784$
$V_0 = 4.0$	$E_0 = -0.40710$	$E_{ex} = -0.46194$	
$E_1 = -0.04765$	$E_2 = -0.01207$	$E_3 = -0.00116$	$E_p = -0.46798$

Table 1 - The exact bound-state energies in the absence (E_0) and presence (E_{ex}) of the perturbing potential.The perturbed energies E_p are determined up to and including third order in the perturbation. Allvalues correspond to $\beta - 1$, $\rho_0 = 0.1$ and $b = 1$ fm. The energies and V0 are measured in units of$\hbar^2/2m$.

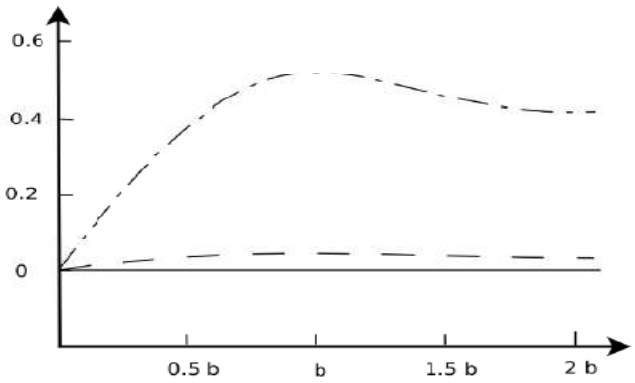

Fig. 1 – The unperturbed wave function $u_0(r)$ (dashed-dotted line), the first-order (dashed line) and second-order (solid line) wave function corrections. All correspond to $V_0 = 2.8$ in units of $\hbar^2/2m\rho_0 = 0.1$and $b = 1\ fm$. The wave function corrections are calculated due to the introduction of a small velocity-dependent perturbing potential.

Further, smaller values of g lead to faster convergence. Substituting for the energyvalues listed in Table [1] corresponding to $V_0 = 2.8$, for example, gives $g = 0.20$ inthis case. We explicitly calculated the maximum values of $\gamma_1(r)$ and $\gamma_2(r)$ and foundthem to be *0.13* and *0.03* respectively. Clearly, the maximum values of $\gamma_1(r)$ and $\gamma_2(r)$ are less than g and g^2 respectively, showing that the approximation in Eq.(44)has actually overestimated the wave function corrections as stated earlier. It is worthnoting that the small value of $g = 0.2$ has led to a good agreement between the perturbedand exact energy values after including only two energy corrections. For thesecond case, $V_0 = 4$, the value of g is *0.13*, while the maximum values of $\gamma_1(r)$ and $\gamma_2(r)$ respectively are *0.07* and *0.009*, which are smaller than g and g^2 as before. Furthermore,a good example that applies to the above formula is found in reference (Jaghoub, 2006).There, the case of a spherical box local potential of radius b was considered, while$\rho(r)$ had the form given in Eq.(10). A straight forward calculation resulted in an exactenergy $E_{ex} = E_0 - \rho_0 E_0$. However, the perturbation formulas gave, $E_1 =$

$-\rho_0 E_0, E_n = 0$for $n \geq 2$ and $u_n(r) = 0$ for $n \geq 1$. Obviously, in view of Eq.(47) this examplecorresponds to the case $g = 0$ leading to $E = E_0 + E_{1=}E_0 - \rho_0 E_0$, which coincideswith the exact value obtained in reference (Jaghoub, 2006). For $g > 1$, the energy perturbationseries diverges. However, in a case where there is only afinite number of values$g_m \geq 1$, while the rest of the g_m values are less than unity, then the series might stillconverge.

Conclusions

The problem of ordering ambiguity in constructing the Hamiltonian for aposition-dependent effective mass has been investigated by considering a closely related problem; that of a constant mass experiencing a velocity-dependent potential.Corresponding to each set of ambiguity parameters, we constructed the Schrödingerequation for a constant mass moving in a velocity-dependent potential with a sharpedge, and studied the continuity of the wave function and its derivative across thepotential boundary. As can be seen in subsections [2.2] and [2.3], the results suggestthat the orderings $(\delta = -1,\ \beta = 0)$ and $(\delta = 0,\ \beta = -1/2)$ lead to conflicting boundaryconditions on the derivative of the radial wave function at the sharp edge of thepotential. Consistency can only be recovered if the radial wave function vanishes atthe boundary. Only the ordering$(\delta = 0,\ \beta = -1)$ leads to consistent boundary conditionsand does not demand the vanishing of the radial wave function at the abruptjunction.

We have also investigated the effect of different orderings on the perturbativeapproach. As the results of Table [1] show, when the perturbation formulasare developed starting from the Schrödinger equation corresponding to the ordering$(\delta = 0,\ \beta = -1)$, the perturbative results compare well with the exact ones. We notethat the results given in Table [1] correspond to finite square well shapes for $V(r)$ and$\rho(r)$ as defined in Eq.(10). However, when the Schrödinger equation is constructedusing either of the other two orderings $(\delta = -1,\ \beta = 0)$and $(\delta = 0,\ \beta = -1/2)$, theagreement between the perturbed and exact energies is poor. This may be traced tothe fact that such orderings lead to conflicting boundary conditions across the abruptpotential boundary. This conclusion is supported by the results obtained in [18]where the effect of different orderings on the perturbation formalism were studied.There, the local potential to have the shape of an infinite square well is assumed.Consequently, the condition $R(b) = 0$ was automatically satisfied. As a result, theperturbative and exact results agreed well corresponding to all the different orderingsleading to the kinetic energy operators in Eqs.(2), (3) and (4). However, in view ofthe current work, the perturbation formulas corresponding to $(\delta = -1,\ \beta = 0)$ and$(\delta = 0,\ \beta = -1/2)$ produce accurate results only when the potentials used lead tovanishing wave functions at the boundary.

The above discussion also applies to the scattering case. In reference (Jaghoub, 2006) itis clear that the Schrödinger equation is constructed corresponding to the ordering$(\delta = 0,\ \beta = -1)$. Formulas for the changes in the scattering phase shifts upon theintroduction of a small perturbing velocity-dependent potential were derived. Thelocal and velocity-dependent potentials were assumed to have the square well shapesas defined in Eq.(10). As shown in (Jaghoub, 2006), the agreement between the exact and perturbedresults is quite satisfactory. Although the calculations are not shown here, wehave derived the phase shift perturbation formulae corresponding to the two otherorderings. However, as for the bound-states case above, the results showed pooragreement between the perturbed and exact phase shifts.

At this point we would note that the degree of convergence of the perturbativeapproach based on a given set of ambiguity parameters should not be used as a criteriato choose or discard a given ordering. This is supported by the work in reference(Jaghoub, 2006) where all the orderings produced accurate results. However, one cannot ruleout the possibility that the ordering $\beta = -1$ applicable to a wider range of physicalsystems than the rest of the orderings considered in this work. Although we haveconsidered the *s-wave* case, the results obtained above can also be generalized tohigher angular momenta provided the

appropriate wave functions are used. However,one should take care of the fact that the local potential includes the centrifugal barrierterm and does not have a well defined radius behind which it abruptly vanishes. Sucha case has been considered in details in reference (Jaghoub, 2006). Finally, we have investigatedthe convergence properties of the bound-states energy perturbation series given inEq.(36). By expressing $u_n(r)$ directly in terms of $u_0(r)$, as in Eq.(44), we haveshown that the series converges provided $g < 1$ and E_1 is finite. If $g > 1$ the seriesdiverges. However, if there is a finite number of terms $g_m > 1$ and the rest of the $g_m$values are less than unity, where g_m is given by Eq.(41), then the series might stillconverge. In view of the above results it seems that the ordering $(\delta = 0,\ \beta = -1)$is privileged in the sense that (a) it leads to consistent boundary conditions at thepotential boundary and (b) it seems to be applicable to a wider range of physicalsystems. Therefore, we suggest that this ordering might be the correct one to describea particle endowed with a position-dependent effective mass. This conclusion is inline with other works like, for examples, the references in (Von and Mavromatis, 1985; Galbraith and Duggan, 1988; L'evy, 1995; Morrow, 1987).

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