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Perturbation theory for isotropic velocity-dependent potentials: Bound-states case

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Abstract. Starting from the time-independent Schrödinger equation we develop formulae for the changes in the bound-state energies in the presence of an isotropic, velocity-dependent perturbing potential. The corresponding changes in the wave functions are also obtained. Unlike the case of the standard perturbation theory, determination of the changes in the energy and the wave function of a state only requires knowledge of the unperturbed ground-state wave function in addition to the perturbing potential. Evaluations of the energy changes and the corresponding wave functions are given for two examples in the s-wave case.

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

1 Introduction

Approximation methods are vitally important tools in the theory of quantum mechanics. This is so as there are relatively few interesting physical problems that are exactly solvable. Although numerical solutions can be obtained to high accuracy, having an analytical formula gives more physical insight into the problem at hand. The standard perturbation theory estimates the changes in the bound-state energies and the corresponding wave functions when small perturbations in the local potential are introduced. In doing so, the theory makes use of the orthogonality of different wave functions. A well-known feature of the theory is that the second-order energy correction involves sums over the spectrum of wave functions of the corresponding unperturbed problem [1].

In this work the Schrödinger equation with a velocity-dependent potential will be considered. Our aim is to develop formulae for the changes in the bound-state energies and the corresponding wave functions due to the presence of an isotropic, velocity-dependent perturbing potential. It will be shown that the changes are determined to any order and neither the unperturbed energy spectrum nor the excited-state wave functions are needed. Only knowledge of the unperturbed ground-state wave function, as well as the purturbing potential, are required. This is in contrast with the standard perturbation theory, where the second-order perturbation correction involves sums over intermediate states.

An Isotropic velocity-dependent potential may be expressed in the form

$$\nabla \cdot [f(r)\nabla\psi(\vec{r})] = f(r)\nabla^2\psi(\vec{r}) + \nabla f(r) \cdot \nabla\psi(\vec{r}), \quad (1)$$

where $\psi(\vec{r})$ is a three-dimensional wave function and $f(r)$ is an isotropic function of the radial variable r. The first term on the right is essentially a kinetic energy term and hence the name velocity-dependent potential, which combines with the kinetic energy term in the Schrödinger equation. Such a potential was derived by Kisslinger [2] and correctly predicted the predominantly p-wave nature of the pion-nucleon scattering. The isotropic function $f(r)$ may be taken to represent the nuclear density. Consequently, the second term in eq. (1) is sensitive to the diffuse edge in nuclei which is most important in light ones.

In the presence of the above velocity-dependent potential the s-wave, time-independent Schrödinger equation for a particle of mass m and energy E moving in a given isotropic local potential $U(r)$ may be written as

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

In terms of the reduced wave function $u(r) = rR(r)$, where $R(r)$ is the radial wave function, the time-independent, s-wave radial Schrödinger equation including the velocity-dependent term takes the form

$$(1-f(r))u''(r) - \left[u'(r) - \frac{u(r)}{r}\right] f'(r) = [U(r) - E]\, u(r), \quad (3)$$

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where E and $U(r)$ are measured in units of $\hbar^2/2m$. The derivative with respect to the radial variable r is indicated by a prime.

In the absence of a velocity-dependent term, Bender developed a form of perturbation theory when a local perturbing potential is introduced. The changes in the energy and wave function of a state are obtained without requiring knowledge of the full spectrum of wave functions of the unperturbed problem [3]. He normalized the wave functions such that they vanish at an arbitrary radius a. However, we choose a different normalization such that each wave function correction is orthogonal to the unperturbed ground-state wave function. As will be seen, this simplifies the derived expressions for the changes in the energies.

It is worth noting that the Schrödinger equation with a non-constant term by the second-order derivative has been the interest of important recent works. Such an equation has been proposed to describe particles with a position-dependent effective mass [4]. Furthermore, since the mass is position dependent it does not commute with the momentum operator, which leads to an ordering ambiguity of the operators involved in the Schrödinger equation. This results in different ways of constructing the Schrödinger equations for particles endowed with position-dependent effective mass. Different ordering possibilities have been investigated in detail in [5].

In an earlier work [6] we derived formulae for the energy and wave function changes starting from the probability density equation in the presence of a velocity-dependent term. The corrections were given up to second order only and no general form was possible to deduce. However, the expressions derived here are simpler, easier to evaluate and given to all orders.

2 Perturbation theory

We shall treat the velocity-dependent potential as a perturbing potential. Consequently, when $f(r) = 0$ eq. (3) reduces to

$$u_0''(r) = [U(r) - E_0]u_0(r), \tag{4}$$

where the unperturbed ground-state energy E_0 and wave function $u_0(r)$ are assumed to be known. Now consider the expansions

$$u(r) = u_0(r) + \lambda u_1(r) + \lambda^2 u_2(r) + \ldots, \tag{5}$$

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \ldots, \tag{6}$$

and set

$$f(r) = \lambda\rho(r), \tag{7}$$

where λ is a real expansion coefficient such that $0 \leq \lambda \leq 1$. When $\lambda = 0$ then the perturbation is switched off.

Substituting eqs. (5) to (7) in (3) and equating the coefficients of λ^0 results in the unperturbed Scrödinger equation given in eq. (4). For $n \geq 1$ equating the coefficients of λ^n leads to the general expression

$$u_n''u_0 - u_0''u_n - u_0\frac{\mathrm{d}}{\mathrm{d}r}(\rho u_{n-1}') + \frac{\rho'}{r}u_0u_{n-1} = -\sum_{k=1}^{n} E_k u_0 u_{n-k}, \tag{8}$$

where we have substituted for $U(r) - E_0$ using the unperturbed equation given in (4) and multiplied by u_0. Further, we have suppressed the dependence on the radial variable r for clarity.

2.1 First-order energy correction

To get the first-order energy correction we equate the coefficients of λ by setting $n = 1$ in (8):

$$u_1''u_0 - u_0''u_1 - u_0\frac{\mathrm{d}}{\mathrm{d}r}(\rho u_0') + \frac{\rho'}{r}u_0^2 = -E_1u_0^2. \tag{9}$$

The last equation may be rearranged as

$$\frac{\mathrm{d}}{\mathrm{d}r}(u_1'u_0 - u_0'u_1) - u_0\frac{\mathrm{d}}{\mathrm{d}r}(\rho u_0') + \frac{\rho'}{r}u_0^2 = -E_1u_0^2. \tag{10}$$

The unperturbed wave function u_0 represents a bound state hence it vanishes both at the origin and at infinity. In addition, it must be normalized to unity, that is

$$\int_0^\infty u_0^2 \ \mathrm{d}r = 1. \tag{11}$$

Further, since $u(r)$ on the left-hand side of eq. (5) represents a bound state, then each wave function correction on the right must also vanish at $r = 0$ and at infinity. Integrating eq. (10) from zero to infinity leads to the first-order energy correction, namely

$$E_1 = -\int_0^\infty u_0' \ \rho \ u_0' \ \mathrm{d}r - \int_0^\infty \frac{\rho'}{r} \ u_0^2 \ \mathrm{d}r \ . \tag{12}$$

It is worth noting that the energy correction E_1 depends not only on the form of ρ but also on its derivative with respect to the radial variable r. This, for example, highlights the importance of the diffuse edge in nuclei. As r approaches zero we have $u_0 \sim r$ in the s-wave case. Consequently, for the integrals in the last equation to be convergent, then in the vicinity of the origin, $\rho(r)$ must behave like r^p where $p \geq 0$. More details on the behaviour of $\rho(r)$ are found in [7,8].

2.2 First-order correction for the wave function

To obtain the first-order correction for the wave function we start with eq. (10) and integrate form the origin to r, which leads to

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{u_1}{u_0}\right) = \frac{1}{u_0^2}\int_0^r \left\{u_0\frac{\mathrm{d}}{\mathrm{d}r'}(\rho u_0') - \frac{\rho'}{r'}u_0^2 - E_1u_0^2\right\}\mathrm{d}r', \tag{13}$$

where we have used the fact that both u_0 and u_1 vanish at the origin. Integrating once again with respect to r we get

$$u_1 = u_0\int_0^r \frac{\mathrm{d}r'}{u_0^2}\int_0^{r'} \left\{u_0\frac{\mathrm{d}}{\mathrm{d}r''}(\rho u_0') - \frac{\rho'}{r''}u_0^2 - E_1u_0^2\right\}\mathrm{d}r'' + C_1u_0 \tag{14}$$

with C_1 being an integration constant. We shall construct the wave function corrections such that each is orthogonal to the unperturbed ground-state wave function u_0. Hence, we impose the condition

$$\int_0^\infty u_0\, u_n\, \mathrm{d}r = \delta_{0,n}\,. \tag{15}$$

In the next section, it will be seen that this condition will simplify the expressions for the higher-order energy corrections. To find the constant C_1 we multiply eq. (14) by u_0 and then integrate from zero to infinity. According to eq. (15), the integral on the left-hand side vanishes leaving us with an expression for C_1 given by

$$C_1 = \int_0^\infty u_0^2 \mathrm{d}r \int_0^r \frac{\mathrm{d}r'}{u_0^2} \int_0^{r'} \Big\{ -u_0 \frac{\mathrm{d}}{\mathrm{d}r''}\left(\rho u_0'\right) + \frac{\rho'}{r''} u_0^2 + E_1 u_0^2 \Big\} \mathrm{d}r''\,. \tag{16}$$

Of course one may choose to solve the differential equation (9) directly to obtain u_1.

2.3 Second- and higher-order energy corrections

In order to determine the second-order energy correction we start by equating the coefficients of λ^2, which according to eq. (8) may be expressed as follows:

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(u_2' u_0 - u_0' u_2\right) - u_0 \frac{\mathrm{d}}{\mathrm{d}r}\left(\rho u_1'\right) + \frac{\rho'}{r} u_0 u_1 = -E_1 u_0 u_1 - E_2 u_0^2. \tag{17}$$

Both u_0 and u_2 vanish at the origin and at infinity. Consequently, integrating from zero to infinity and using the condition given in eq. (15) leads to the second-order energy correction, which reads

$$E_2 = -\int_0^\infty u_0'\, \rho\, u_1'\, \mathrm{d}r - \int_0^\infty \frac{\rho'}{r}\, u_0 u_1\, \mathrm{d}r\,. \tag{18}$$

It is worth noting that the normalization condition in eq. (15) made the term containing E_1 in eq. (17) vanish, thus decoupling different energy corrections and simplifying their expression. This will happen for all higher-order corrections.

Working with the coefficient of λ^3 and proceeding in the same manner as above we arrive at the following expression for the third energy correction:

$$E_3 = -\int_0^\infty u_0'\, \rho\, u_2'\, \mathrm{d}r - \int_0^\infty \frac{\rho'}{r}\, u_0 u_2\, \mathrm{d}r\,. \tag{19}$$

By inspecting the first three energy corrections it is easy to deduce that a general expression for the n-th order energy correction is given by

$$E_n = -\int_0^\infty u_0'\, \rho\, u_{n-1}'\, \mathrm{d}r - \int_0^\infty \frac{\rho'}{r}\, u_0\, u_{n-1}\, \mathrm{d}r\,. \tag{20}$$

2.4 Second- and higher-order corrections for the wave function

To determine the second-order correction for the wave function we start by integrating eq. (17) from zero to r which leads to

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{u_2}{u_0}\right) = \frac{1}{u_0^2}\int_0^r \Big\{ u_0 \frac{\mathrm{d}}{\mathrm{d}r'}\left(\rho u_1'\right) - \frac{\rho'}{r'} u_0 u_1 - E_1 u_0 u_1 - E_2 u_0^2 \Big\} \mathrm{d}r'. \tag{21}$$

To arrive at the last result we used the fact that u_0 and u_2 vanish at $r = 0$. Performing an indefinite integration with respect to r results in

$$u_2 = u_0 \int_0^r \frac{\mathrm{d}r'}{u_0^2} \int_0^{r'} \Big\{ u_0 \frac{\mathrm{d}}{\mathrm{d}r''}\left(\rho u_1'\right) - \frac{\rho'}{r''} u_0 u_1 - E_1 u_0 u_1 - E_2 u_0^2 \Big\} \mathrm{d}r'' + C_2 u_0, \tag{22}$$

where C_2 is an integration constant that may be determined by using the normalization condition in eq. (15). Hence multiplying the above equation by u_0 and integrating over all r results in the following expression for the constant C_2:

$$C_2 = \int_0^\infty u_0^2\, \mathrm{d}r \int_0^r \frac{\mathrm{d}r'}{u_0^2} \int_0^{r'} \Big\{ -u_0 \frac{\mathrm{d}}{\mathrm{d}r''}\left(\rho u_1'\right) + \frac{\rho'}{r''} u_0 u_1 + \sum_{k=1}^{2} E_k u_0 u_{n-k} \Big\} \mathrm{d}r''. \tag{23}$$

An expression for the third-order correction for the wave function can be easily obtained starting from the coefficient of λ^3 and proceeding in the same manner as above. By inspection a general expression for the n-th order correction is

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

where

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

It is also possible to obtain the wave function correction u_n by directly solving the differential equation obtained by equating the coefficients of λ^n.

3 Examples

In order to test the perturbation formulae derived in the last section we shall consider a particle moving freely in a box of radius $a = 1$. The unperturbed Shrödinger equation for this particle is

$$u_0''(r) = -k^2 u_0(r)\,, \tag{26}$$

where $u_0(r)$ is the unperturbed ground-state wave function inside the well given by

$$u_0(r) = \sqrt{2}\sin(kr), \tag{27}$$

and E_0 is the corresponding ground-state energy:

$$E_0 = k^2 = \pi^2\,. \tag{28}$$

We shall now consider two types of velocity-dependent perturbing potentials $\rho(r)$ such that the energy eigenvalues can be determined exactly and by the perturbation formulae. The results will then be compared.

3.1 Constant perturbing potential

In this example we define the velocity-dependent potential as follows:

$$\begin{aligned} \rho(r) &= \rho_0, \qquad & r < a \\ &= 0, \qquad & r > a\,, \end{aligned} \tag{29}$$

where ρ_0 is a constant. In this case the Shrödinger equation in (3) reduces to

$$(1 - \rho_0) u''(r) = -K^2 u(r), \tag{30}$$

where

$$E = K^2. \tag{31}$$

It can be easily shown that the exact energy eigenvalue, E, is given as

$$E = (1 - \rho_0)\, E_0 = E_0 - \rho_0\, E_0, \tag{32}$$

which corresponds to an exact eigenfunction $u(r) = u_0(r) = \sqrt{2}\sin(kr)$. Now we calculate the first-order energy correction E_1 using eq. (12) with $\rho(r) = \rho_0$. This leads to

$$E_1 = -\rho_0\, E_0\,. \tag{33}$$

Using the expression for the first-order wave function correction given in eq. (14) shows that $u_1 = 0$. Consequently, we have

$$E_n = 0, \qquad n \geq 2 \tag{34}$$

and

$$u_n = 0, \qquad n \geq 1 \tag{35}$$

and hence according to eqs. (5) and (6) the perturbation theory results are

$$u(r) = u_0(r) = \sqrt{2}\sin(kr) \tag{36}$$

and

$$E = E_0 - \rho_0\, E_0. \tag{37}$$

Clearly, the results of the developed perturbation expressions are identical with the exactly obtained ones.

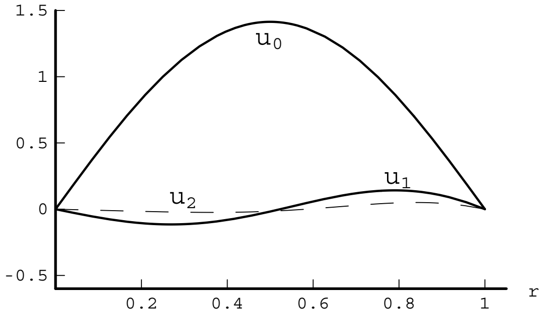

Fig. 1. The unperturbed ground-state wave function u_0, the first-order wave function correction u_1, and the second-order wave function correction u_2. The wave function corrections vanish at the origin and at $r = a = 1$ as expected, where a is the radius of the spherical well.

3.2 Variable perturbing potential

Here we shall consider a harmonic-oscillator–type perturbing potential defined as

$$\begin{aligned} \rho(r) &= \rho_0 r^2, \qquad & r < a \\ &= 0, \qquad & r > a\,. \end{aligned} \tag{38}$$

Inside the spherical well the exact solution is

$$u_0(r) = {}_2F_1(a, b, c, \rho_0 r^2), \tag{39}$$

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

$$\begin{aligned} u_0(r) = Dr \Bigg[1 - \frac{1}{6} E\, r^2 + \frac{1}{60\rho_0} E(E - 10\rho_0)\, r^4 \\ - \frac{1}{840\rho_0^2} E(E - 10\rho_0)(E - 28\rho_0)\, r^6 + \cdots \Bigg], \end{aligned} \tag{40}$$

where D is a constant that can be determined using the appropriate boundary condition. The above is a solution with an infinite number of terms unless we terminate the series by setting one of the factors to zero. We chose $E = 10\rho_0$, which leads to a wave function defined as

$$u_0(r) = Dr\left(1 - \frac{5}{3}\rho_0 r^2\right). \tag{41}$$

The constant D can be found by normalizing the wave function, which must vanish at the origin and at $r = a = 1$. For the wave function to vanish at $r = 1$ then $\rho_0 = 3/5$, which results in an exact energy eigenvalue $E = 10\rho_0 = 6$ in units of $\hbar^2/2m$. Using the derived expressions for the energy correction given in eqs. (12), (18) and (19) we obtain in units of $\hbar^2/2m$

$$E_1 = -3.4739, \qquad E_2 = -0.2623, \qquad E_3 = -0.0791. \tag{42}$$

Clearly, the absolute values of the corrections get smaller as the order of the perturbation increases. Remembering that $E_0 = \pi^2$, then up to and including the third order in the perturbation the energy eigenvalue $E = 6.0543$ which is in good agreement with the exact value of 6. The absolute percentage difference is only 0.9%. The corresponding changes in the wave functions are plotted in fig. 1. Since the absolute values of the corrections decrease steadily, then evaluating more terms in the energy expansion series in eq. (6) is expected to reduce the slight discrepancy between the approximated and exact energy eigenvalue.

4 Results and discussions

In this work we have derived expressions for the changes in the energy eigenvalues and the corresponding wave functions due to the presence of an isotropic, velocity-dependent perturbing potential. In contrast to the standard perturbation theory, neither the unperturbed energy spectrum nor the corresponding unperturbed wave functions are required. To determine the energy and wave function corrections for a given state only the unperturbed ground-state wave function and the perturbing potential are needed. The corrections were given in general and to all orders in the perturbation. The derived expressions show that the changes in the energy eigenvalues are sensitive to both the form of the velocity-dependent part and its gradient. In the field of nuclear physics, for example, this highlights the importance of a spatially varying nuclear density, which is particularly important for light nuclei.

In addition to nuclear physics, the Schrödinger equation with a non-constant term by the second-order derivative has been used to describe a particle with a spatially varying mass [4]. The derived perturbation results may also be useful in such models. Further, the spatial dependence of the mass results in an ordering ambiguity, which in turn leads to different ways of constructing the Schrödinger equation for particles endowed with a position-dependent effective mass. It is our aim to investigate the effect of the ordering ambiguity on the above derived perturbation results in a future work.

To test our results we studied the case of a particle moving freely in a spherical box of radius 1. The energy and wave function of the particle were determined exactly and then by using perturbation theory when a velocity-dependent perturbing potential was introduced. We considered two different forms for the perturbing potential such that the resulting Shrödinger equation can be solved exactly. The first took $\rho(r)$ to be a constant. In this case we found $E_1 = -\rho_0 E_0$ and $E_n = 0$ for $n \geq 2$, which is identical with the exact solution. In the second case we considered a spatially varying potential namely $\rho(r) = \rho_0 r^2$, where ρ_0 is a constant. We evaluated the first three energy corrections in the series. Up to and including the third correction we found $E = 6.045$ in units of $\hbar^2/2m$ in good agreement with the exact result of 6.0 in units of $\hbar^2/2m$. This amounts to an absolute percentage difference of 0.9%. The absolute magnitudes of the corrections were found to be monotonically decreasing ($E_1 = -3.4739$, $E_2 = -0.2623$, $E_3 = -0.0791$) and judging by this, evaluation of higher corrections in the series is expected to remove the slight discrepancy with the exact value.

By using the appropriate change of variables, the wave equation with a non-constant term by the second-order derivative may be transformed into an ordinary Shrödinger equation, but with an energy-dependent potential. Consequently, One may consider deriving perturbation formulae starting from such a transformed equation.

We have from the start dealt with an s-wave Schrödinger equation. However, the derived expressions are equally applicable for higher waves ($l > 0$) when the appropriate wave functions are used. This is so as the centrifugal barrier term may be included within the local potential $U(r)$ that does not appear explicitly in the obtained corrections.

References

1. See, for example, L.I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968).
2. L.S. Kisslinger, Phys. Rev. **98**, 761 (1955).
3. C.M. Bender, *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1978) p. 330.
4. A.R. Plastino *et al.*, Phys. Rev. A **60**, 4318 (1999).
5. A. de Souza Dutra *et al.*, Europhys. Lett. **62**, 8 (2003).
6. M.I. Jaghoub, Eur. Phys. J. A **15**, 443 (2002).
7. M. Al Jaghoub, Eur. Phys. J. A **11**, 175 (2001).
8. M.I. Jaghoub, Eur. Phys. J. A **13**, 349 (2002).