Bound state perturbation theory for the one-space and one-time dimension Klein–Gordon equation

C. K. Au
Department of Physics and Astronomy, University of South Carolina, Columbia, South Carolina 29208

Y. Aharonov
Department of Physics and Astronomy, University of South Carolina, Columbia, South Carolina 29208 and Department of Physics, University of Tel Aviv, Tel Aviv, Israel

(Received 8 December 1980; accepted for publication 27 February 1981)

We present a perturbation theory for an arbitrary bound state in the one-space and one-time dimension Klein–Gordon equation in the presence of a scalar potential and a vector (fourth component only) potential by reducing it to a Ricatti equation with the method of logarithmic perturbation expansions. All corrections to the energies and wavefunctions, including corrections to the positions of the nodes in excited states, are expressed in quadratures in a hierarchical scheme, without the use of either the Green's function or the sum over intermediate states.

PACS numbers: 03.65.Ge

I. INTRODUCTION

Recently, in a series of papers,[1–3] we have presented perturbation theories for an arbitrary bound state in static potentials for the Schrödinger equation and the Dirac equation. In central field problems[3] and in problems reducible to one dimension in the case of the Schrödinger equation,[1,2] we have shown that all corrections to the energies and wavefunctions, including corrections to the positions of the nodes in excited states, can be expressed in quadratures in a hierarchical scheme, without the use of either the Green's function or the sum over intermediate states. This is achieved through the reduction of the differential equations involved to a Ricatti equation, followed by a perturbation expansion. In the case of the Schrödinger equation,[1,4,5] this is equivalent to performing a perturbation expansion on the logarithmic derivative of the wavefunction instead of on the wavefunction itself. In the case of the Dirac equation,[3,6] this is equivalent to carrying out a perturbation expansion on the ratio between the radial parts of the small and large components of the Dirac spinor. We emphasize that in the case of excited states where the wavefunctions possess nodes,[1,3,4] the zeros must be factored out first. We have also shown that the first-order perturbation iteration method (FOPIM), first introduced by Hirschfelder,[7] can be incorporated into this perturbation approach to yield accelerated convergence, if convergence exists.[3,8] In nonrelativistic problems that are not reducible to one dimension, we show that, for the ground state, the method of logarithmic perturbation leads to a hierarchy of equations that determines the corrections to the energy and wave function for each order. In this hierarchy, the equation for the ith-order correction is isomorphic to the equation for the first-order correction. Moreover, these equations have the same form as Gauss' law in classical electrodynamics.[2] As an application, we have shown that this method can be used to obtain the corrections to the energy and the logarithm of the wavefunction of the ground state of a hydrogen atom in a multipole field or a linear combination of static multipole fields to any order in perturbation theory.[9]

In this paper, we would like to extend similar techniques to the one-space and one-time dimension Klein–Gordon equation. We shall assume that it is possible to solve this equation with a certain scalar potential and a fourth component vector potential. The problem of a charged spinless boson in a central field is reducible to this form. We then consider the change in the energy and in the wavefunction as a perturbation is introduced to the fourth component vector potential or to the scalar potential. This will be developed in Secs. II and III. In Sec IV, we conclude by mentioning some possible applications of the presently developed techniques.

II. PERTURBATION IN THE FOURTH COMPONENT VECTOR POTENTIAL

The single-particle one-space and one-time dimension Klein–Gordon equation in the presence of a fourth component vector potential V and a scalar potential S can be written as[10,11] in natural units $\hbar = c = 1$:

$$[E - V(x)]^2\psi(x) = \left[-\frac{d^2}{dx^2} + m^2 + 2mS(x)\right]\psi(x). \tag{2.1}$$

We assume that, for a certain V_0 and S_0, the above eigenvalue problem is solvable so that the energy eigenvalue E_0 and the corresponding wavefunction ψ_0 are known for a particular state. We shall consider the correction to the energy and wavefunction as a perturbation λV_1 is introduced to the potential V_0. In the following section, we consider the same corrections as a perturbation ηS_1 is introduced to the scalar potential S_0. For the sake of brevity, and yet without sacrificing clarity of the essense of our method, we shall limit our detailed discussions to the ground state where the wavefunction does not contain any zero and to the first excited where the wavefunction possesses one zero. The generalization to an arbitrary excited bound state with a finite number of nodes is straightforward, and the mechanism is similar to what has been reported previously.[1,3]

In the absence of any degeneracy, the wavefunction ψ can be taken as real. In order that the charge density be normalizable, we require that ψ vanishes as x approaches

 0022-2488/81/071428-05$1.00

$\pm\infty$. In the case of the ground state, ψ does not contain any zero, and so its logarithm is regular. In analogy to the nonrelativistic Schrödinger equation, we define

$$\psi(x) = \exp[-G(x)] \tag{2.2a}$$

and

$$g(x) = \frac{d}{dx}G(x). \tag{2.2b}$$

Equation (2.1) is then transformed to the Ricatti form

$$(E-V)^2 = g' - g^2 + m^2 + 2mS, \tag{2.3}$$

where a prime denotes a derivative with respect to its argument. The unperturbed Klein–Gordon equation in Ricatti form is

$$(E_0 - V_0)^2 = g_0' - g_0^2 + m^2 + 2mS_0. \tag{2.4}$$

In the presence of a perturbation to the fourth component vector potential, λV_1, Eq. (2.3) becomes

$$(E - V_0 - \lambda V_1)^2 = g' - g^2 + m^2 + 2mS_0. \tag{2.5}$$

We seek a perturbative solution to Eq. (2.5) by expanding the eigenvalue E and the logarithmic derivative of the wavefunction g in power series in λ:

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots = \Sigma \lambda^i E_i, \tag{2.6}$$

and

$$g = g_0 + \lambda g_1 + \lambda^2 g_2 + \cdots = \Sigma \lambda^i g_i. \tag{2.7}$$

We next define

$$B_0 \equiv E_0 - V_0, \tag{2.8}$$

$$B_1 \equiv E_1 - V_1, \tag{2.9}$$

$$B_i \equiv E_i \quad \text{for all } i \geqslant 2. \tag{2.10}$$

On comparing coefficients of various powers in λ, we obtain

$$B_0^2 = g_0' - g_0^2 + m^2 + 2mS_0, \tag{2.11}$$

which is the unperturbed Klein–Gordon equation for the ground state in the Ricatti form, and

$$2B_0B_1 = g_1' - 2g_0g_1, \tag{2.12}$$

$$2B_0B_k + \sum_{j=1}^{k-1}(B_jB_{k-j} + g_jg_{k-j}) = g_k' - 2g_0g_k \tag{2.13}$$

for all $k \geqslant 2$. We then observe, similar to the nonrelativistic case in the Schrödinger equation, that the square of the unperturbed wavefunction serves as an integration factor to this hierarchy of equations,

$$2B_0B_1 e^{-2G_0} = [g_1 e^{-2G_0}]', \tag{2.14}$$

and for $k \geqslant 2$

$$\left[2B_0B_k + \sum_{j=1}^{k-1}(B_jB_{k-j} + g_jg_{k-j})\right]e^{-2G_0} = [g_k e^{-2G_0}]'. \tag{2.15}$$

Equation (2.15) can be brought to a form similar to (2.14) if we define an effective k th-order perturbation potential V_k by

$$B_0V_k \equiv -\tfrac{1}{2}\sum_{j=1}^{k-1}(B_jB_{k-j} + g_jg_{k-j}). \tag{2.16}$$

Equations (2.14) and (2.15) can then be rewritten as

$$2(E_0 - V_0)(E_k - V_k)e^{-2G_0} = [g_k e^{-2g_0}]' \tag{2.17}$$

for all $k \geqslant 1$.

We now readily see that this hierarchy of equations can be solved in quadrature. On integrating Eq. (2.17) from $-\infty$ to $+\infty$, the right-hand side vanishes according to the boundary conditions and the integration yields

$$E_k = \frac{\int_{-\infty}^{+\infty}(E_0 - V_0)V_k\psi^2(x)\,dx}{\int_{-\infty}^{+\infty}(E_0 - V_0)\psi^2(x)\,dx}. \tag{2.18}$$

If we normalize the charge of the Klein–Gordon particle to unity, then the integral in the denominator of (2.18) is equal to m, the mass of the Klein-Gordon particle in equation. In this case, the k th-order correction to the energy is given by

$$E_k = \int_{-\infty}^{+\infty}\frac{(E_0 - V_0)V_k\psi^2(x)\,dx}{m}. \tag{2.19}$$

Having obtained E_k, Eq. (2.17) can now be readily integrated to yield a solution for g_k:

$$g_k(x) = e^{2G_0(x)}\int_{-\infty}^{x} 2(E_0 - V_0)(E_k - V_k)e^{-2G_0}\,dx. \tag{2.20}$$

Since V_k is defined by E_j and g_j where $j \leqslant k-1$, it is apparent that the perturbative solution can be obtained in this hierarchical scheme.

It may appear worthwhile to show that E_1, as given by Eq. (2.19), is the same as that obtained in standard perturbation theory in terms of the two-component wave function formalism that leads to the first-order Klein-Gordon equation.[10,11] As is well known, the two-component isospinor wavefunction Ψ can be written in terms of the Klein-Gordon wavefunction ψ as

$$\Psi = \begin{pmatrix}\phi\\ \chi\end{pmatrix} = \frac{\psi}{2}\begin{pmatrix}1 + (E-V)/m\\ 1 - (E-V)/m\end{pmatrix}. \tag{2.21}$$

In terms of this isospinor, the Klein-Gordon equation can be written in Hamiltonian form

$$H\Psi = E\Psi, \tag{2.22}$$

where the operator H is identified as

$$H = (\tau_3 + i\tau_2)\left(\frac{-1}{2m}\frac{d^2}{dx^2} + S\right) + \tau_3 m + V, \tag{2.23}$$

τ_1, τ_2, τ_3 being the Pauli isospin matrices, and the scalar product is defined in general as

$$\langle \Psi \,|\, \Psi' \rangle \equiv \int \Psi^\dagger \tau_3 \Psi'. \tag{2.24}$$

Thus, the normalization that fixes the charge of the Klein-Gordon particle to be unity is equivalent to $\langle \Psi \,|\, \Psi \rangle = 1$ or

$$\int \{[1 + (E-V)/m]^2 - [1 - (E-V)/m]^2\}\psi^2/4 = 1 \tag{2.25}$$

or to

$$\int (E - V)\psi^2\,dx = m, \tag{2.26}$$

which is the condition used to replace the denominator of Eq. (2.18) by the mass of the Klein-Gordon particle in terms of the unperturbed solution. Then, as is well known, the first-order energy shift is given by

$$E_1 = \langle \Psi_0 | H_1 | \Psi_0 \rangle, \tag{2.27}$$

where Ψ_0 is the isospinor corresponding to the unperturbed solution. Here, $H_1 = V_1 \mathbb{1}$, where $\mathbb{1}$ is the unit matrix. Then Eqs. (2.27), (2.24), and (2.21) together will lead to Eq. (2.19) for $k = 1$.

Once the g_k's are obtained, they can be integrated to given the G_k's, the correction to the logarithm of the wavefunction. The integration constants here are additive constants to the logarithm of the wavefunction and are hence multiplicative constants to the wavefunction that can be fixed by normalization of the charge density.

As discussed in earlier papers,[3,8] an alternative approach to the perturbation is the first-order perturbation iteration method (FOPIM). From the knowledge of E_1 and g_1, we construct the function

$$g_0^{\mathrm{I}} \equiv g_0 + \lambda g_1 \tag{2.28}$$

and

$$E_0^{\mathrm{I}} = E_0 + \lambda E_1. \tag{2.29}$$

We then seek a potential V_0^{I} that will satisfy Eq. (2.24)

$$(E_0^{\mathrm{I}} - V_0^{\mathrm{I}})^2 \equiv (g_0^{\mathrm{I}})' - (g_0^{\mathrm{I}})^2 + m^2 + 2mS. \tag{2.30}$$

This is an algebraic equation and V_0^{I} can be solved. However, because of the quadratic nature, there will be two possible solutions for V_0^{I}. The correct choice is the one that approaches V_0 as λ approaches zero. Having found this V_0^{I}, the new unperturbed potential, the perturbation can be chosen as

$$V_1^{\mathrm{I}} = V_0 + \lambda V_1 - V_0^{\mathrm{I}}. \tag{2.31}$$

It is not hard to show that from Eqs. (2.4), (2.12), (2.28), (2.29), and (2.30) that V_1^{I} is of order λ^2. We thus succeed in reducing a problem with a perturbation of order λ to the one with order λ^2. This process can be continued. The next step will reduce the perturbation to order λ^4.

We not turn to the excited states. For simplicity, we consider the first excited state where the wavefunction contains one node and give the corrections to an arbitrary order. For an arbitrary excited bound state where the wavefunction contains a finite number of, but more than one, zeros, we give the expressions for the first-order corrections. One then can use the FOPIM to generate all higher corrections.

In the case of the first excited state where the wavefunction has one node we can write

$$\psi = (x - a)e^{-G}, \tag{2.32}$$

where a is the position of the node. The Klein-Gordon equation is then transformed to the Ricatti form:

$$[g^2 - g' + (E - V)^2 - m^2 - 2mS](x - a) = 2g. \tag{2.33}$$

The unperturbed equation is

$$[g_0^2 - g_0' + (E_0 - V_0)^2 - m^2 - 2mS_0](x - a_0) = 2g_0, \tag{2.34}$$

where E_0 is the zeroth-order energy eigenvalue, and the zeroth-order eigenfunction is

$$\psi_0 = (x - a_0)e^{-G_0}, \tag{2.35}$$

where a_0 is the nodal position in the absence of any perturbation. In the presence of a perturbation λV_1, we seek the solution of E and G in power series of λ as in Eq. (2.6) and (2.7). In addition, the nodal position a is also expanded in powers of λ:

$$a = a_0 + \lambda a_1 + \lambda^2 a_2 + \cdots = \Sigma \lambda^i a_i. \tag{2.36}$$

On substituting Eqs. (2.36) and (2.6)–(2.10) in Eq. (2.33) and using (2.34), we obtain, after multiplying throughout by $(x - a_0)e^{-2G_0}$,

$$[a_1 e^{-2G_0}]' - [g_1(x - a_0)^2 e^{-2G_0}]' + 2B_0 B_1 (x - a_0)^2 e^{-2G_0} = 0, \tag{2.37}$$

and for all $i \geqslant 2$,

$$a_i [e^{-2G_0}]' - [g_i (x - a_0)^2 e^{-2G_0}]' + 2B_0 (E_i - V_i)(x - a_0)^2 e^{-2G_0} = 0, \tag{2.38}$$

where the effective ith-order perturbation potential is defined by

$$2B_0 V_i (x - a_0) \equiv \sum_{k=1}^{i-1} \{a_{i-k} [2g_0 g_k - g_k' + 2B_0 B_k + \sum_{j=1}^{k-1} (B_j B_{k-j} + g_j g_{k-j})] - [B_k B_{i-k} + g_k g_{i-k}](x - a_0)\}, \tag{2.39}$$

and the summation is understood to be zero if the upper limit of the running index is smaller than the lower limit. It is then trivial to obtain the corrections to the energy, the nodal position, and g by integrating Eqs. (2.36) and (2.37) from $-\infty$ to $+\infty$, a_0 and x in a hierarchical scheme.

In the case of an arbitrary excited bound state where the wavefunction prossesses N zeros, we write the wavefunction as

$$\psi = \left[\prod_{\mu=1}^{N} (x - a_\mu)\right] e^{-G}. \tag{2.40}$$

Then the Klein-Gordon equation in Ricatti form becomes

$$[g^2 - g' + (E - V)^2 - m^2 - 2mS] \prod_{\mu} (x - a_\mu) = 2g \sum_{\nu} \prod_{\mu \neq \nu} (x - a_\mu) - \sum_{\sigma,\nu} \prod_{\mu \neq \sigma,\nu} (x - a_\mu). \tag{2.41}$$

Here, we only give the first-order corrections. The higher-order corrections can be brought to forms analogous to Eqs. (2.37) and (2.38) by keeping track of the indices. Alternatively, one can use the first-order perturbation iteration method. The first-order corrections are given by the following equation analogous to (2.36):

$$\sum_{\mu} a_{\mu 1} \left[\prod_{\nu \neq \mu} (x - a_{\nu 0})^2 e^{-2G_0}\right]' - \left[g_1 \prod_{\mu} (x - a_{\mu 0})^2 e^{-2G_0}\right]' = -2(E_1 - V_1)(E_0 - V_0) \prod_{\mu} (x - a_{\mu 0})^2 e^{-2G_0}, \tag{2.42}$$

from which the first-order energy correction E_1 can be obtained by integrating from $-\infty$ to $+\infty$, the first-order correction to the μth node $a_{\mu 1}$ can be obtained by integrating from $-\infty$ to $a_{\mu 0}$, and then g_1 can be obtained by integrating from $-\infty$ to x after E_1 and the $a_{\mu 1}$'s have been obtained. As in the case of the ground state, the additive constant to G from the integration of g is fixed by normalization of the charge density.

III. PERTURBATION IN THE SCALAR POTENTIAL

We now consider the situation where the perturbation ηS_1 is in the scalar potential S. In the case of the ground state where the wavefunction does not contain any zero, it can be written as in Eqs. (2.2a) and (2.2b), and the unperturbed equation is the same as Eq. (2.4). In the presence of the additional scalar potential ηS_1, the Klein-Gordon equation in Ricatti form becomes

$$(E - V_0)^2 = g' - g^2 + m^2 + 2mS_0 + 2m\eta S_1. \tag{3.1}$$

In analogy to Eqs. (2.6) and (2.7), we seek the solution in power series in η:

$$E = E_0 + \eta E_1 + \eta^2 E_2 + \cdots = \Sigma \eta^i E_i \tag{3.2}$$

and

$$g = g_0 + \eta g_1 + \cdots = \Sigma \eta^i g_i. \tag{3.3}$$

On comparing coefficients of various powers in η, we obtain

$$(E_0 - V_0)^2 = g_0' - g_0^2 + m^2 + 2mS_0, \tag{3.4}$$

which is the unperturbed Eq. (2.4), and

$$2E_1(E_0 - V_0) = g_1' - 2g_0 g_1 + 2mS_1, \tag{3.5}$$

$$2E_i(E_0 - V_0) + \sum_{j=1}^{i-1}(E_j E_{i-j} + g_j g_{j-j}) = g_i' - 2g_0 g_i \tag{3.6}$$

for all $i \geqslant 2$, We then readily observe, as in the previous section, that the square of the unperturbed wavefunction, e^{-2G_0}, acts as an integration factor to this hierarchy of equation:

$$2E_1(E_0 - V_0)e^{-2G_0} = [g_1 e^{-2G_0}]' + 2mS_1 e^{-2G_0}, \tag{3.7}$$

from which we obtain

$$E_1 = \int_{-\infty}^{+\infty} S_1 e^{-2G_0}\, dx, \tag{3.8}$$

on using the normalization condition (2.26), and

$$g_1 = e^{2G_0}\int_{-\infty}^{x} 2[E_1(E_0 - V_0) - mS_1]e^{-2G_0}\, dx. \tag{3.9}$$

The higher-order corrections are given by

$$2E_i(E_0 - V_0)e^{-2G_0} = [g_i e^{-2G_0}]' + 2mS_i e^{-2G_0}, \tag{3.10}$$

where we identify the ith order effective scalar perturbation potential S_i by

$$2\,mS_i \equiv -\sum_{j=1}^{i-1}(E_j E_{i-j} + g_j g_{i-j}). \tag{3.11}$$

In terms of the two-component wavefunction Ψ in Eq. (2.21), the first-order correction to the energy is given by Eq. (2.27), where $H_1 = (\tau_3 + i\tau_2)S_1$, which can be easily shown to lead to the same result as Eq. (3.8).

We now turn to the first excited state whose wavefunction is written as in Eq. (2.32). The Klein-Gordon equation in Ricatti form is given by Eq. (2.33). We then expand the energy E and g in power series in η as in Eqs. (3.2) and (3.3). In addition, the nodal position a is also expanded in a power series of η analogous to Eq. (2.36):

$$a = a_0 + \eta a_1 + \cdots = \Sigma \eta^i a_i. \tag{3.12}$$

On executing procedures similar to the last section, we obtain the following for the first-order corrections:

$$[a_1 e^{-2G_0}]' - [g_1(x - a_0)^2 e^{-2G_0}]'$$
$$= -2[E_1(E_0 - V_0) - mS_1](x - a_0)^2 e^{-2G_0}, \tag{3.13}$$

from which the corrections E_1, a_1, and g_1 can be obtained by integrating from $-\infty$ to $+\infty$, a_0 and x. The higher-order corrections are given by

$$a_i[e^{-2G_0}]' - [g_i(x - a_0)^2 e^{-2G_0}]'$$
$$= -2[E_i(E_0 - V_0) - mS_i](x - a_0)^2 e^{-2G_0}, \tag{3.14}$$

where the effective ith-order scalar perturbation S_i is defined by

$$2mS_i(X - a_0)$$
$$\equiv \sum_{k=1}^{i-1}\Big\{a_{i-k}\Big[2g_0 g_k - g_k' + 2(E_0 - V_0)E_k + \sum_{j=1}^{k-1}(E_j E_{k-j} + g_j g_{k-j})\Big] - [E_k E_{i-k} + g_k g_{i-k}](x - a_0)\Big\}. \tag{3.15}$$

Equation (3.14) can readily be integrated to give the corrections E_i, a_i, and g_i with the same sets of integration limits. It is then obvious that Eqs. (3.13)–(3.15) can be integrated in a hierarchical scheme to yield corrections to any order in perturbation theory.

For an arbitrary excited bound state, we only give the equation for the first-order corrections:

$$\sum_{\mu} a_{\mu 1}\Big[\prod_{\nu \neq \mu}(x - a_{\nu 0})^2 e^{-2G_0}\Big]' - \Big[g_1 \prod_{\mu}(x - a_{\mu 0})^2 e^{-2G_0}\Big]'$$
$$= -2[E_1(E_0 - V_0) - mS_1]\Pi(x - a_{\mu 0})^2 e^{-2G_0}, \tag{3.16}$$

which is analogous to Eq. (2.41) and can be solved in quadrature by integration in an analogous manner.

IV. CONCLUDING REMARKS

In this paper we have presented a bound state perturbation theory for the one-space and one-time dimension Klein-Gordon equation in the presence of a scalar potential and a fourth component vector potential by reducing it to a Ricatti equation with the method of logarithmic perturbation expansions. The problem of a charged spinless boson in a central field is reducible to this form. Our results are thus applicable to the study of the perturbative corrections to the energies and wavefunctions of bound states in pionic atoms due to a screened Coulomb potential or due to a finite-sized but spherical nucleus. We have shown that it is possible to obtain all preturbative corrections in quadrature in a hierarchical scheme without the use of either the Green's function or the sum over the intermediate states, especially in the latter where negative energy states are also involved. The computation of the higher energy corrections in closed quadratures can be used to identify sum rules, as reported by us previously.[1,2]

ACKNOWLEDGMENT

This work is supported in part by the National Science Foundation under Grant Nos. PHY-79-01053 and ISP-80-11451.

[1]Y. Aharonov and C. K. Au, Phys. Rev. Lett. **42**, 1582 (1979); **43**, 176(E) (1979); **44**, 619(E) (1980).
[2]C. K. Au and Y. Aharonov, Phys. Rev. A **20**, 2245 (1979).
[3]C. K. Au and G. W. Rogers, Phys. Rev. A **22**, 1820 (1980).
[4]V. S. Polikanov, Zh. Eksp. Teor. Fiz. **52**, 1326 (1967) [Sov. Phys. JETP **25**, 882 (1967)]; Theoret. Math. Phys. (USSR) **24**, 230 (1975).
[5]R. J. Price, Proc. Phys. Soc. London **67**, 383 (1954).
[6]A. I. Mikhailov and V. S. Polikanov, Zh. Eksp. Teor. Fiz. **54**, 175 (1968) [Sov. Phys. JETP **27**, 95 (1968)].
[7]J. O. Hirshfelder, J. Chem. Phys. **39**, 2009 (1963).
[8]C. K. Au, Phys. Lett. A **77**, 221 (1980).
[9]C. K. Au and Y. Aharonov, Phys. Rev. A **22**, 328 (1980).
[10]H. Feshbach and F. Villars, Rev. Mod. Phys. **30**, 24 (1958).
[11]Also see, for example, G. Baym, *Lectures on Quantum Mechanics* (Benjamin, New York, 1969).