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Dissolution of relativistic atoms into negative energy states

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The problem of atomic dissolution by means of decay to the negative energy continuum is discussed. The derivation of the one-electron central-field Hamiltonian from quantum electrodynamics is made as an example. It is found that the operators that project the Coulomb interaction into positive and negative energy states of the Dirac noninteracting Hamiltonian cause the eigenstates of the atomic Hamiltonian to break up into two sets. One set is expandable in the positive energy noninteracting states, and this set propagates forward in time. The other set is expandable in terms of the negative energy noninteracting states and propagates backward in time. There is, therefore, no danger that transitions will occur from the forward propagating eigenstates into the negative continuum with continued propagation in the forward direction, regardless of the magnitude of the nuclear charge.

I. INTRODUCTION

The interaction of *nonrelativistic* atoms with electromagnetic fields has long been understood, and many calculations have been made and compared successfully with experiments. The introduction of relativistic equations, however, has created problems related to the existence of negative energy atomic states.

What prevents an atom from dropping into the negative energy states while radiating electromagnetic energy? Dirac[1] proposed filling the negative energy states with electrons so that the Pauli exclusion principle could operate and keep the electrons out of these states. Feynman[2] translated this proposal into his propagators by requiring them to transmit only the positive energy eigenstates forward in time while the negative energy states propagate backward in time. These two equivalent restrictions on the theory refer to eigenstates of the noninteracting Dirac Hamiltonian

$$\underline{H}_D = -i\underline{\alpha}\cdot\nabla + m\underline{\gamma}^0 , \qquad (1.1)$$

where underlines indicate matrices.

Dirac[1] constructed a Hamiltonian for the hydrogen atom by adding a Coulomb potential to the above equation. Unfortunately, an expansion of the negative energy eigenstates of his Hamiltonian in terms of the eigenstates of $\underline{H}_D$ involves positive energies. Thus transitions to the negative energy states of the Coulomb Hamiltonian followed by forward propagation become possible. This opens the question of whether Dirac and Feynman's rules should apply to eigenstates of $\underline{H}_D$ or to the Hamiltonian of the entire system including interactions. The latter choice is actually ruled out if we use Dirac's Coulomb Hamiltonian and are to be consistent with quantum field theory as currently presented in textbooks and as used to compute the radiative corrections of the hydrogen atom.[3] Is it possible, then, that Dirac chose the wrong Hamiltonian for the hydrogen atom?

A similar problem has arisen when actual calculations of multielectron eigenfunctions have been attempted.[4] Although no difficulties of this nature occur when the Hartree-Fock approximation is used, efforts to include the correlation energy run into trouble. This is because the Coulomb interactions mix the negative energy Hartree-Fock eigenstates with the bound states. For example, a bound state would mix strongly with the state formed from it by moving one electron up into the positive energy continuum and a second electron into a negative energy continuum state in such a way that the energy is unchanged from that of the original bound state. Since these continuum states extend to infinity, the atom dissolves by electron emission.

This phenomenon of atomic disintegration has been called by Sucher,[4] the "continuum dissolution" or the "Brown-Ravenhall disease." It is the result of a poor choice for the interaction energy between electrons in the Hamiltonian of the relativistic atom. The means of avoiding it were first pointed out by Brown and Ravenhall.[5] They did not have this problem because their Hamiltonian had the Coulomb interaction sandwiched between projection operators into the positive energy states of $\underline{H}_D$. However, these operators are not convenient for calculations, and this has led Sucher and Mittleman[4] to consider alternative projection operators. As we shall see, these discussions arise from an uncertainty as to how the atomic Hamiltonian is to be chosen.

Brown and Reavenhall[5] and Bethe and Salpeter[6] derived the wave equation for the hydrogen atom from quantum electrodynamics many years ago. Bethe and Salpeter used Feynman's[2] techniques, and their work has recently been generalized to multielectron atoms.[7] These papers show that the Coulomb interaction terms in the wave equation should be preceded by operators that project into the positive or negative energy states of $\underline{H}_D$ in Eq. (1.1). We now seek to clarify how these projection operators prevent the dissolution of the atom into the negative energy continuum and how they effect the atomic eigenstates.

The wave equations derived by Salpeter[6] and Broyles[7] do not obviously arise from eigenequations for Hermitian Hamiltonians. We shall see, however, that the eigenfunctions themselves satisfy a condition that makes the Hamiltonian Hermitian.

We shall approach quantum electrodynamics as a boundary-value problem to be solved for the wave functions of electrons, nuclei, and photons.[8] Although such wave functions have frequently been used in the past,[2,5,6] the complete formulation of quantum electrodynamics in terms of differential equations solved by such wave functions is presented in Ref. 9. Of course, this formulation is equivalent to others,[10] but it has the advantage of using wave functions at every stage.

In order to illustrate the manner in which an atomic Hamiltonian arises in the treatment of a relativistic atom by means of quantum electrodynamics, we shall present the derivation for the electron in a central field, that is, the hydrogen atom with an infinitely heavy nucleus as a simple example. The projection operators that arise naturally in the derivation will present the electron from falling into the negative energy states. Properties of the eigenstates of the hydrogen Hamiltonian that result from the work of Bethe and Salpeter will be studied. We will then see how these properties generalize to the multielectron atom.

II. HYDROGEN ATOM WITH INFINITE NUCLEAR MASS

Although, as noted above, a relativistic Hamiltonian for the hydrogen atom was derived long ago by Salpeter,[6] a simplified derivation for the hydrogen atom in the limit of infinite nuclear mass will be presented here in order to show how a Hamiltonian is introduced in a particularly elementary case.

We begin with Eq. (9) in the paper by Salpeter and Bethe,[6]

$$\underline{K}(3,4;1,2)=\underline{K}_e(3,1)\underline{K}_n(4,6)+i\int\int\int\int\underline{K}_e(3,5)\underline{K}_n(4,6)\underline{G}(5,6;7,8)\underline{K}(7,8;1,2)d^4x_5d^4x_6d^4x_7d^4x_8\ , \tag{2.1}$$

where $\underline{K}(3,4;1,2)$ is the propagator for an electron and nucleus (proton), $\underline{K}_e$ and $\underline{K}_n$ are the dressed electron and nuclear propagators whose mass shell limits are given by

$$\underline{K}(\bar{x},\bar{y})=i\int(\not{p}-m)^{-1}e^{-i\bar{p}\cdot(\bar{x}-\bar{y})}d^4p(2\pi)^{-4}\ , \tag{2.2}$$

where $\bar{x}$, $\bar{y}$, and $\bar{p}$ are four vectors and where the appropriate experimental masses must be inserted for m. $\not{p}$ is the scalar product of $\bar{p}$ and $\bar{\underline{\gamma}}$. $\underline{G}$ represents the infinite series of irreducible terms involving photon exchanges between the electron and the nucleus. The first term of this series is

$$\underline{G}_a(5,6;7,8)=-e^2\underline{\gamma}_{e\mu}\underline{\gamma}_n^{\mu}\int e^{-\bar{k}\cdot\bar{x}}k^{-2}d^4k\,\delta(5,7)\delta(6,8)/2\pi^2\ , \tag{2.3}$$

where

$$\bar{x}=\bar{x}_5-\bar{x}_6\ .$$

We take odd numbered points to belong to the electron and even numbered to the nucleus.

Salpeter[6] has noted that a gauge transformation can replace this last expression for $\underline{G}_a$ with one involving a Coulomb potential added to a transverse contribution. Making use of his Eqs. (1) and (2) and a Fourier transform, we can show that

$$\underline{G}_a(5,6;7,8)=e^2\underline{\gamma}_{e0}\underline{\gamma}_n^0\delta(x_5^0-x_6^0)|\mathbf{x}_5-\mathbf{x}_6|^{-1}\delta(5,7)\delta(6,8)+\cdots\ , \tag{2.4}$$

where the center dots represent transverse terms. Since the δ functions cause this expression to vanish unless all the times are equal, it can provide the interaction between the electron and nucleus in an atomic Hamiltonian. The transverse terms and the higher-order terms, in $\underline{G}$, on the other hand, require two times to be specified. Although the transverse terms in $\underline{G}_a$ involve retardation, they can be approximated by the Breit interaction that is instantaneous. Since they are small, however, we shall include them with the higher-order components in the series expansion for $\underline{G}$ which are small correction terms that we shall not consider here.

In the limit of infinite nuclear mass, contributions to Eq. (2.1) involving the backward propagation of the nucleus become negligible. This establishes the time ordering of the nuclear points so that $x_2^0<x_6^0<x_4^0$. We also take the initial times to be equal and the final times to be equal so that $x_1^0=x_2^0$, $x_3^0=x_4^0$, and $x_1^0<x_6^0<x_3^0$. Since we will include only the instantaneous Coulomb part of $\underline{G}$, contributions are nonvanishing only when the two lines involved in the photon propagator are the same, that is, when $x_5^0=x_6^0$. In this case, Eq. (2.1) will not include terms in the perturbation expansion with the electron traveling backward in time.

In the limit of a very heavy nucleus, the effect of the electron on it becomes negligible so that it propagates as though there were no interactions. Furthermore, the initial nuclear wave function at x_1^0, $\underline{\psi}_n(1)$ can be chosen to be sharply confined to the origin. Because of the large mass, this wave function will spread a negligible amount while it propagates to x_4^0 and becomes $\underline{\psi}_n(4)$. To remove the nuclear coordinates, we multiply Eq. (2.1) by $\underline{\psi}_n^\dagger(4)d^3x_4$ from the left and $\underline{\gamma}_n^0\underline{\psi}_n(2)d^3x_2$ from the right and integrate over $\mathbf{x}_2$ and $\mathbf{x}_4$. (A dagger indicates the complex conjugate transpose.) $\underline{K}_n(4,6)$ will then propagate $\underline{\psi}_n^\dagger(4)$ backwards from x_4^0 to x_6^0.

The expression on the left of Eq. (2.1) will then have the form

$$\underline{K}^c(3,1)=\int\int\underline{\psi}_n^\dagger(4)\underline{K}(3,4;1,2)\times\underline{\gamma}_n^0\underline{\psi}_n(2)d^3x_2d^3x_4\ . \tag{2.5}$$

This is the propagator that transports the initial wave function of the electron from time x_1^0 to x_3^0 in the presence of a point nucleus fixed at the origin. If we use this expression to identify $\underline{K}^c$, we have in place of Eq. (2.1)

$$\underline{K}^c(3,1)=\underline{K}_e(3,1)+i\int\int\int\int\int\underline{K}_e(3,5)\underline{\psi}_n^\dagger(6)\underline{G}(5,6;7,8)\underline{K}(7,8;1,2)\underline{\psi}_n(2)d^3x_2d^4x_5d^4x_6d^4x_7d^4x_8\ . \tag{2.6}$$

The expression in Eq. (2.4) now replaces $\underline{G}$ and introduces the $\underline{\gamma}^0$ corresponding to the one in Eq. (2.5) so that we can identify a $\underline{K}^c$. Integration over x_7 and x_8 then gives

$$\underline{K}^c(3,1)=\underline{K}_e(3,1)+ie^2\int\int\int\underline{K}_e(3,5)\underline{\psi}_n^\dagger(6)\underline{\gamma}_e^0\underline{\gamma}_n^0\delta(x_5^0-x_6^0)|\mathbf{x}_5-\mathbf{x}_6|^{-1}\underline{K}(5,6;1,2)\underline{\psi}_n(2)d^3x_2d^4x_5d^4x_6\ . \tag{2.7}$$

We note now that we can identify a $\underline{K}^c$ on the right-hand side with the aid of Eq. (2.5), integrate over x_6^0 to remove the delta function, and obtain

$$\underline{K}^c(3,1)=\underline{K}_e(3,1)+ie^2\int\underline{K}_e(3,5)\underline{\gamma}_e^0|\mathbf{x}_5|^{-1}\underline{K}^c(5,1)d^4x_5,\quad x_1^0<x_5^0<x_3^0\ . \tag{2.8}$$

The $\mathbf{x}_5-\mathbf{x}_6$ could be replaced by $\mathbf{x}_5$ because the wave function for the nucleus is confined to the origin. The restrictions on the times result from, as we have noted, an infinite nuclear mass and the instantaneous Coulomb interactions. This is the equation satisfied by the propagator for an electron moving in a Coulomb field.

We now seek to write this propagator in terms of the wave functions that diagonalize it, that is, a complete set of functions that are propagated so that their only time dependence is a phase factor whose phase changes linearly with time. A large amount of computational experience can be drawn upon if a Hamiltonian is found whose eigenfunctions form such a set. This, then, is the criterion that determines the atomic Hamiltonian. The eigenfunctions of this Hamiltonian provide the most economical way to write down the propagator which describes the atom between emissions of photons.

The equation for the wave function propagated by $\underline{K}^c$ can be obtained by multiplying the last equation from the right by $\underline{\gamma}^0\underline{\psi}(1)d^3x_1$ and integrating over $\mathbf{x}_1$. The result is (dropping the subscript e's)

$$\underline{\psi}(3)=\underline{\psi}^f(3)+ie^2\int\underline{K}(3,5)\underline{\gamma}^0|\mathbf{x}_5|^{-1}\underline{\psi}(5)d^4x_5\ ,\quad x_5^0<x_3^0\ , \tag{2.9}$$

where $\underline{\psi}^f$ is the wave function that would result if no Coulomb interaction were present.

If now we apply the operator $(i\not{\partial}_3-m)$, the $\underline{K}(3,5)$ will be replaced by $i\delta(3,5)$. If we take the limit of infinite mass for the nucleus *after* the integration over $\bar{x}_5$ is performed, the result is

$$(i\not{\partial}-m)\underline{\psi}=-\underline{\gamma}^0|\mathbf{x}|^{-1}\underline{\psi}\ . \tag{2.10}$$

This is the equation studied by Dirac for the hydrogen atom. However, the solutions usually found for it are not solutions of the previous equation.

To see this, we substitute $\underline{K}$ in Eq. (2.2) into (2.9) and carry out the integrations. We note first that Eq. (2.2) multiplied from the right by $\underline{\gamma}^0$ is equivalent to

$$\underline{K}(\bar{x},\bar{y})\underline{\gamma}^0=i\int(p-\underline{H}_D)^{-1}\delta(\mathbf{x}-\mathbf{y})e^{ip(x^0-y^0)}dp/2\pi\ . \tag{2.11}$$

Substituting this into Eq. (2.9) and integrating over $\mathbf{x}_5$ leaves

$$\underline{\psi}(3)=\underline{\psi}^f(3)-e^2\int\int(p-\underline{H}_D)^{-1}e^{-ip(x_3^0-x_5^0)}|\mathbf{x}_3|^{-1}\times\underline{\psi}(x_5^0,\mathbf{x}_3)dx_5^0dp/2\pi,\quad x_5^0<x_3^0\ . \tag{2.12}$$

As we have noted, we are restricting the wave functions to the form

$$\underline{\psi}(x_5^0,\mathbf{x}_3)=\underline{\phi}(\mathbf{x}_3)e^{-iEx_5^0}\ . \tag{2.13}$$

Substituting this into Eq. (2.12) then gives

$$\underline{\psi}(3)=\underline{\psi}^f(3)+e^2J|\mathbf{x}_3|^{-1}\underline{\psi}(3)\ , \tag{2.14}$$

where

$$J=-\int\int(p-\underline{H}_D)^{-1}e^{iy(p-E)}dy\,dp/2\pi,\quad y<0\ . \tag{2.15}$$

Integrating first over p and then over y with a negative imaginary component of m in $\underline{H}_D$ produces

$$J=(\underline{H}_D-E)^{-1}\underline{\Lambda}_+\ , \tag{2.16}$$

where $\underline{\Lambda}_+$ is the projection operator into positive energy eigenstates of $\underline{H}_D$. Substituting this into Eq. (2.14) then results in

$$\underline{\psi}(\bar{x})=\underline{\psi}^f(\bar{x})+e^2\underline{\Lambda}_+(\underline{H}_D-E)^{-1}|\mathbf{x}|^{-1}\underline{\psi}(\bar{x})\ . \tag{2.17}$$

We note that the equation derived by Salpeter[6] for hydrogen also has a $\underline{\Lambda}_-$ operator that has been eliminated because the infinitely heavy nucleus and the instantaneous Coulomb interactions have removed backward propagation of electron wave functions.

As we have noted, the Feynman propagators transmit only components of the wave function consisting of positive energy eigenfunctions of $\underline{H}_D$ forward from the initial surface of the space-time volume in which we are to determine the wave function. These positive energy eigenstates contribute to $\underline{\psi}^f$ in the last equation. The $\underline{\Lambda}_+$ in the last term prevents any contribution of negative energy states of $\underline{H}_D$ to $\underline{\psi}$ on the left. Thus the positive energy states propagated from the initial time surface will be part of a solution to Eq. (2.17) with no negative energy state component. We can, therefore, replace $\underline{\psi}(\bar{x})$ by $\underline{\Lambda}_+\underline{\psi}$ for these solutions in that equation. This component propagates forward in time.

This can be shown more formally by iterating Eq. (2.17) to obtain

$$\begin{aligned}\underline{\psi}=\underline{\Lambda}_+\underline{\psi}^f+e^2(\underline{H}_D-E)^{-1}\underline{\Lambda}_+|\mathbf{x}|^{-1}\underline{\Lambda}_+\underline{\psi}^f\\ +e^4(\underline{H}_D-E)^{-1}\underline{\Lambda}_+|\mathbf{x}|^{-1}\underline{\Lambda}_+(\underline{H}_D-E)^{-1}|\mathbf{x}|^{-1}\underline{\psi}\ ,\end{aligned} \tag{2.18}$$

where we have replaced $\underline{\psi}^f$ by $\underline{\Lambda}_+\underline{\psi}^f$. We can now make use of the fact that a projection operator is equal to its square and rearrange this equation to obtain

$$\begin{aligned}\underline{\psi}=\underline{\Lambda}_+\underline{\psi}^f+e^2(\underline{H}_D-E)^{-1}\underline{\Lambda}_+|\mathbf{x}|^{-1}\underline{\Lambda}_+\\ \times[\underline{\Lambda}_+\underline{\psi}^f+e^2(\underline{H}_D-E)^{-1}\underline{\Lambda}_+|\mathbf{x}|^{-1}\underline{\psi}]\ .\end{aligned} \tag{2.19}$$

The bracketed quantity is immediately recognizable from Eq. (2.17) so that

$$\underline{\psi}(\bar{x})=\underline{\psi}^f(\bar{x})+e^2\underline{\Lambda}_+(\underline{H}_D-E)^{-1}|\mathbf{x}|^{-1}\underline{\Lambda}_+\underline{\psi}(\bar{x})\ , \tag{2.20}$$

where $\underline{\psi}^f$ involves only the positive energy states. It is clear that a $\underline{\Lambda}_+$ factors to the left on the right-hand side so that this is really the equation for $\underline{\Lambda}_+\underline{\psi}$.

On the other hand, the solutions transmitted backward in time from the final surface by the Feynman propagators can consist only of negative energy noninteracting states. They receive no contribution from the last term in Eq. (2.17) so that, for them, we can ignore the Coulomb interaction. We can show this more formally by operating on Eq. (2.17) from the left by $\underline{\Lambda}_-$. Since the Coulomb term is annihilated, no harm is done if we insert a $\underline{\Lambda}_+$ in front of the $\underline{\psi}(\bar{x})$ in that term and leave it in the last term of Eq. (2.20). Thus, Eq. (2.20) holds for both components of $\underline{\psi}$. We can then multiply by $(\underline{H}_D-E)$ and transpose to obtain

$$\underline{H}_c\underline{\psi}=E\underline{\psi}\ , \tag{2.21}$$

where

$$\underline{H}_c=\underline{H}_D-e^2\underline{\Lambda}_+|\mathbf{x}|^{-1}\underline{\Lambda}_+\ . \tag{2.22}$$

This Hamiltonian has two sets of eigenstates. One is composed of states that can be expanded in terms of the positive energy eigenstates of $\underline{H}_D$ alone and are propagated forward in time by $\underline{K}^c$. The other involves only the negative energy eigenstates, and they are unaffected by the Coulomb interaction because of the $\underline{\Lambda}_+$'s. They are clearly propagated by $\underline{K}^c$ and must move backward in time. The atom cannot dissolve by radiative transitions from the bound states in the first set to the negative energy states in the second set since $\underline{K}^c$ does not transmit the latter set forward in time. Thus an atom with this Hamiltonian is stable and does not suffer from the problem of continuum dissolution.

III. MULTIELECTRON ATOM

The equation for the multielectron atom corresponding to that for hydrogen derived by Salpeter[6] has been presented in Ref. 7. This equation was derived from Eqs. (6.7) and (6.9) of that reference. They can be combined to give (omitting the Breit interaction)

$$\begin{aligned}\underline{\psi}(X^0,\mathbf{x}_1\ldots\mathbf{x}_n)=\underline{\psi}^f(X^0,\mathbf{x}_1\ldots\mathbf{x}_n)\\ -e^2[\underline{\Lambda}_+-(-1)^n\underline{\Lambda}_-]\left[\textstyle\sum_k\underline{H}_{Dk}-E\right]^{-1}\\ \times V\underline{\psi}(X^0,\mathbf{x}_1\ldots\mathbf{x}_n)\ ,\end{aligned} \tag{3.1}$$

where

$$\underline{\Lambda}_\pm=\textstyle\prod_k\underline{\Lambda}_{k\pm} \tag{3.2}$$

and

$$V=\textstyle\sum_{i<k}Z_iZ_j|\mathbf{x}_i-\mathbf{x}_j|^{-1} \tag{3.3}$$

and where there are n spin-$\frac{1}{2}$ fermions with charges Z_i times the electron charge. The summations and products with subscripts k are over the indices k from 1 to n. The symbol $\sum_{i<j}$ represents summation over all pairs of values of i and j where i and j range from 1 to n. Z_i is -1 for electrons and a positive integer for a nucleus. We define $\underline{\Lambda}_{k\pm}$ to project into the positive or negative energy states of $\underline{H}_D$ for the kth fermion.

The first term on the right-hand side of Eq. (3.1) is generated from positive energy eigenstates of $\underline{H}_D$ that are transmitted forward from the initial time surface and the negative energy eigenstates that are transmitted backwards from the final surface by the Feynman propagators. These states propagate to the in-between surface at X^0 to form $\underline{\psi}^f$. Contributions consisting entirely of positive eigenstates of $\underline{H}_D$ or entirely of negative eigenstates are added from the second term of Eq. (3.1) to form $\underline{\psi}$. This is because of the projection operator $[\underline{\Lambda}_+-(-1)^n\underline{\Lambda}_-]$. Since the last term in Eq. (3.1) contributes only to those states, a set of solutions can be found by similarly restricting $\underline{\psi}^f$ so that

$$\underline{\psi}=(\underline{\Lambda}_++\underline{\Lambda}_-)\underline{\psi}\ . \tag{3.4}$$

Since the projection operator in the last equation can be inserted in front of $\underline{\psi}$, it can also be inserted after the potential energy term in the Hamiltonian. Thus the Hamiltonian for an atom can be written in the form

$$\underline{H}_m=\textstyle\sum_k\underline{H}_{Dk}+\alpha[\Lambda_+-(-1)^n\underline{\Lambda}_-]V(\underline{\Lambda}_++\underline{\Lambda}_-)\ . \tag{3.5}$$

A more formal proof of this may be made in steps analogous to Eqs. (2.18)–(2.20).

The terms in Eq. (3.5) that involve $\underline{\Lambda}_+|\mathbf{x}_i-\mathbf{x}_j|^{-1}\underline{\Lambda}_-$ and $\underline{\Lambda}_-|\mathbf{x}_i-\mathbf{x}_j|^{-1}\underline{\Lambda}_+$ vanish. This is because each of them will contain one of the factors, $\underline{\bar{w}}^+\underline{w}^-$ or $\underline{\bar{w}}^-\underline{w}^+$, where the eigenfunctions of $\underline{H}_D$ have the form

$$\underline{\psi}^{\pm}=\underline{w}^{\pm}e^{-i(\pm Et-\mathbf{p}\cdot\mathbf{x})}\,, \tag{3.6}$$

and ± indicates the sign of the energy. As a result

$$\underline{H}_m=\sum\nolimits_k\underline{H}_{Dk}+\alpha\underline{\Lambda}_+V\underline{\Lambda}_+-(-1)^n\alpha\underline{\Lambda}_-V\underline{\Lambda}_-\;. \tag{3.7}$$

This form of the Hamiltonian is obviously Hermitian.

As we have already noted, only wave functions that satisfy Eq. (3.4) are affected by the interaction. The eigenvalue equation for the Hamiltonian in Eq. (3.7) can be separated so that the two components $\underline{\Lambda}_+\underline{\psi}$ and $\underline{\Lambda}_-\underline{\psi}$ satisfy the two independent energy eigenvalue equations

$$\begin{aligned}\underline{H}_m(\underline{\Lambda}_+\underline{\psi})&=\sum\nolimits_k\underline{H}_{Dk}(\underline{\Lambda}_+\underline{\psi})+\underline{\Lambda}_+V\underline{\Lambda}_+(\underline{\Lambda}_+\underline{\psi})\\&=E_+(\underline{\Lambda}_+\underline{\psi})\end{aligned} \tag{3.8}$$

and

$$\begin{aligned}\underline{H}_m(\underline{\Lambda}_-\underline{\psi})=&\sum\nolimits_k\underline{H}_{Dk}(\underline{\Lambda}_-\underline{\psi})\\&-(-1)^n\underline{\Lambda}_-V\underline{\Lambda}_-(\underline{\Lambda}_-\underline{\psi})=E_-(\underline{\Lambda}_0\underline{\psi})\;.\end{aligned} \tag{3.9}$$

Thus there are two sets of energy eigenstates, one expandable in positive energy eigenstates of $\underline{H}_D$, the other expandable in negative energy states. Since the eigenstates of the Coulomb Hamiltonian propagate in the same direction as their $\underline{H}_D$ components would be individually propagated, we conjecture that the first set will be transmitted forward in time and the other backwards in time. Thus an atom in one of the first set of eigenstates will not be able to transfer into one of the other sets by radiation and then continue forward in time.

IV. SUMMARY

The Feynman restriction that only positive energy noninteracting states can propagate forward in time while the negative energy states propagate backward leads to Hamiltonians for atoms with Coulomb interaction terms sandwiched between projection operators. These projection operators (into positive and negative energy states of the Hamiltonian for a noninteracting system) assure that the atomic eigenstates can be divided into two sets, one set being expandable in terms of positive energy eigenstates of the Hamiltonian for a noninteracting system, the other in terms of negative energy eigenstates of the same Hamiltonian. The first set contains the bound states for an atom, and they are propagated forward in time. They cannot decay (by any means, Coulomb or transverse interactions) into the second set of states and propagate forward because the second set can only propagate backward in time. This is true even if some of the state of the first set becomes degenerate with some of those in the second set as a result of a very strong charge on the atomic nucleus. An atom in the lowest state of the forward-propagating states cannot decay by any process into the states of the other set and continue propagating forward in time. Thus a dissolution of the atom from its ground state in this manner cannot take place. It is the direction of propagation in time that separates these two sets of states, not a difference in sign of energy eigenvalues.

Since the bound states contain only positive energy plane-wave states while the other set (that extends to negative infinity in energy) involves only negative energy plane-wave states, a proper calculation of bound-state eigenfunctions will not mix the two so that true bound states of the Hamiltonian for the atom will exist.

The early derivations of quantum electrodynamics[1,11] allowed the Coulomb fields to remain unquantized. This was formalized for computing the properties of bound states by Furry.[12] In the case of atoms, the field of an infinitely heavy nucleus is generally taken[13] to be Coulomb. The electrons are then treated by quantum field theory in this external classical field. This is, however, not consistent with Eq. (2.22) where the projection operators sandwich the Coulomb potential. As we have seen, Eq. (2.22) was derived from the Feynman formalism which quantizes all components of the electromagnetic field.

The use of the Coulomb field in the Furry picture would introduce problems as we have noted since an expansion of a negative energy eigenstate involves positive energy eigenstates of the noninteracting Hamiltonian. This would allow components of these negative energy states to be propagated forward in time by the Feynman propagators. This is avoided in the Furry picture by using Coulomb propagators for the electrons that transmit positive energy states of the Coulomb Hamiltonian forward in time and the negative energy states of this Hamiltonian backward in time. The question arises as to whether the Furry picture with the Coulomb interaction produces the same description of an atom as do the equations derived from the Feynman formalism. If the answer is no, which set of equations is correct?

Let us compare the two methods for the case of an electron moving in the field of an infinitely heavy point nucleus. In this case, the Furry picture introduces a different electron propagator than that proposed by Feynman. It is clear, however, that the wave function describing the universe in our neighborhood cannot be derived using just any set of Green's functions that are consistent with the differential equations in Ref. 9. As Feynman[2] has pointed out, the Green's function propagating both positive and negative energy states forward in time would satisfy the differential equations. It would, however, allow electrons to drop into the negative energy states and propagate forward in time. Since this is not observed to happen, any Green's function propagating negative energy states forward in time is inconsistent with the boundary conditions that determine the physical wave function. Thus the Green's function chosen by Feynman seems to be the only one that will produce the wave function that we observe. This suggests that we are not free to choose between the Feynman propagator and that of the Coulomb Furry picture.

An example from classical electromagnetic theory may help to make this fact more evident. If a radio transmitter is turned on and then off, an electromagnetic pulse will be emitted. The motion of this pulse can best be calculated with the aid of the retarded Green's function. None of the pulse will move backward in time. Of course the advanced or half-advanced and half-retarded Green's functions will produce solutions of Maxwell's equations, but they do not represent the wave emitted from a source such as a radio transmitter. Wheeler and Feynman[14] have shown how the direction of propagation of a radio wave in time is related to the rest of the universe. This direction seems to be determined in a manner similar to the direction of increasing entropy.

If the choice of propagators is set by the nature of the wave function of the universe, then which of the two, Feynman's or the Coulomb Furry picture propagator, is the proper one? There are some obvious problems with the Furry picture. For one, it assumes a fixed center. Although the nucleus of an atom is much heavier than the electrons, it is by no means fixed. The Feynman propagators do not have this problem since they are related only to the kinetic energy rather than the entire Hamiltonian. The Furry picture introduces propagators that depend upon the charge of the nucleus while the Feynman propagators are independent of this charge. The Furry picture selects one constituent of an atom (the nucleus) to have a special position at the center of the classical potential. Although its mass and charge may be greater than the electrons, these differences do not seem to be sufficient to produce such a unique position for one of the elements of the theory. For these reasons, the Feynman propagator seems to be more likely to be the correct one.

The difference between the results of the calculations of the hydrogen energy levels using the Bethe-Salpeter equation and using the Coulomb Furry picture have, in fact, been considered by Salpeter[6] when he compared the Breit equation with the Bethe-Salpeter equation. He found that the higher-order term involving two Coulomb photons appearing in the kernel G in our Eq. (2.1) makes a correction of -0.037 Mc/s in the $2S$ level of hydrogen. In the limit of infinite proton mass, this diagram just cancels the difference in the eigenvalues of the Bethe-Salpeter Hamiltonian [see our Eq. (2.22)] and the Breit Hamiltonian [our Eq. (2.22) without the projection operators]. Thus, if we could omit the corrections due to this diagram when we use the Coulomb Furry picture, we would have agreement in the two eigenvalues (although not the eigenfunctions) to this order. However, the Coulomb Furry picture requires us to include this diagram (although Coulomb propagators must be used). This throws the calculation of the energy eigenvalue off by a measurable amount when the Coulomb Furry picture is used. Since the Bethe-Salpeter result is in agreement with experiment, we conclude that the use of the Furry picture with the Coulomb external potential is inconsistent with experiment.

We have considered the Hamiltonians that arise from the summation of the ladder diagrams with Coulomb rungs. It is possible to include, in the Hamiltonian for an atom, contributions that arise from portions of the higher-order irreducible diagrams in the kernel G of the Bethe-Salpeter equation. The Breit interaction[7,15] is a contribution from the transverse components of the ladder rungs. The lowest-order vacuum polarization diagram contributes the Uehling[16] potential. These additional terms are added directly to the Coulomb potentials in Eqs. (2.22) and (3.7) and are sandwiched in between the same projection operators. We see this in Eq. (6.11) of Ref. 7 for the Breit interaction. Since the above considerations about the eigenfunctions of an atomic Hamiltonian depend only upon the presence of the projection operators sandwiching the potential, they will still apply after these additional potentials are added.

The Hamiltonians considered in Secs. II and III do not include diagrams involving positrons. Thus the only point that can be made here about positron production is that it cannot result from the static field of a charged particle no matter how large the charge. Increasing the charge may cause the two sets of states to become degenerate, but it will not change the character that one set propagates forward in time while the other propagates backward. Even this statement is limited to the eigenstates of the Hamiltonian and does not include all of the effects of the higher order diagrams in G.

In summary, let us conclude the following: (1) The Hamiltonian's derived by summing Feynman diagrams in the manner of Bethe, Salpeter, and Broyles producing potentials sandwiched between projection operators is to be preferred over the Furry picture with an external Coulomb potential. (2) The Hamiltonian eigenstates separate into sets, one expandable in positive energy Dirac plane-wave states alone propagating forward in time, the other expandable in negative plane-wave states and propagating backward in time. (3) Statement (2) holds regardless of the charge on the atomic nucleus. (4) Bound eigenstates of the above atomic Hamiltonians are members of the forward propagating set. Since their expansions involve none of negative energy plane-wave states, they are not required to have a component extending to infinity.

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