Dynamics of neutral vacuum decay

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A time-independent Hamiltonian formulation of relativistic atomic structure and scattering problems is developed in which virtual-pair creation and annihilation effects are explicitly included. The method is discussed in the context of a specific problem—the scattering of a positron by a system consisting of two electrons bound to a nucleus of charge Z. This provides the basis for a consistent treatment of spontaneous positron production that can occur when Z exceeds a critical value $Z_{cr} \approx 173$. For Z not too much greater than Z_{cr} the two-electron atom is stable and represents the (doubly charged) vacuum state. In the approach adopted here the one-electron state, which is unstable against spontaneous pair creation, is viewed as a resonance in the scattering of the positron by the two-electron target atom. The lifetime of the unstable state is determined, in the usual way, from a knowledge of the width of the resonance. The formal resonance theory required to carry out this analysis is developed here with the aid of an effective-potential description of the scattering problem of the type familiar from standard treatments of resonant processes in nonrelativistic atomic and nuclear reaction theories.

I. INTRODUCTION

The effect of virtual-pair creation on the structure of atoms is expected to be small, in general. Nevertheless, in calculations of high precision, on systems of high nuclear charge Z, this effect can be significant. In an earlier work[1] (referred to in the following as I) a time-independent Hamiltonian formulation of the bound-state problem in QED was developed in the context of the resolvent-operator method of many-body perturbation theory. The problem of including virtual-pair effects was addressed there for a model hydrogen atom in which the creation of only a single virtual pair is allowed. Here this study is extended to the consideration of a class of problems involving a one-electron atom in which Z is sufficiently large (greater than a critical value $Z_{cr} \approx 173$) so that *real* pair creation is possible. The effect is then rather more dramatic. The stability of the one-electron atom is destroyed owing to the fact that creation of a pair, with the additional electron filling the K-shell vacancy and the positron escaping in a continuum state, is energetically possible. It is not our purpose at this time to attempt a description of the physics of this process which is sufficiently realistic as to allow for a detailed comparison with experimental findings. Extensive studies of this nature, taking into account the dynamic effect of the motion of the pair of heavy ions which momentarily coalesce to form the superheavy nucleus, have been carried out.[2] It is, in fact, not clear at present whether the existence of the spontaneous positron production effect will be confirmed by the current round of experiments.[3] This issue, important as it is, will not be of concern to use here. Rather, the focus is on methodology. Of primary concern is the development of calculational techniques for describing relativistic few-electron systems in bound and continuum states. These techniques lend themselves very naturally to the study of the dynamical properties of the vacuum. This is a matter of fundamental interest the investigation of which is clearly warranted, quite aside from the current status of experiments.

The decay of the unstable neutral vacuum into the doubly charged vacuum state,[4] which is stable for Z less than the value at which the first excited state enters into the continuum ($Z \approx 185$), is studied here using standard resonance theory—the one-electron unstable state appears as a resonance in the scattering of a positron by the two-electron atom. The level-shift formalism developed in I, suitably modified to account for the fact that in the application considered here the level shift is complex, provides a convenient framework for the analysis. This formulation allows one to obtain explicit expressions for the complex level shift from whose imaginary part the decay rate into the positron continuum state is determined. It should be recognized at the outset that the main effect of the vacuum instability is likely to be described reasonably well by the lowest-order calculations given previously.[2] The work reported on here represents an attempt to apply the time-independent Hamiltonian approach, in the form outlined in I, to the problem of determining higher-order corrections in a systematic manner, with the instantaneous Coulomb interaction treated nonperturbatively.

The time-independent description of the supercritical one-electron atom is outlined in Sec. II; this allows us to introduce notation, to review the resolvent-operator approach, and to develop certain modifications in the formulation of I which are required when the external field is supercritical. The lowest-order approximation to the neutral vacuum decay rate[2] is rederived here as a simple illustration of the formalism, and the means for generating higher-order terms in a well-defined perturbation expansion is provided. A formal description of resonant positron scattering in a supercritical field is given in Sec. III and this is used as the basis for a more elaborate

"one-pair" approximation scheme which is worked out in Sec. IV. This procedure, which amounts to the neglect of the effect of two or more virtual electron-positron pairs, is based on the method developed previously.[1] The paper concludes with a discussion and summary of results obtained.

II. ONE-ELECTRON ATOM IN A SUPERCRITICAL FIELD

A. Formulation

To establish procedures we review the resolvent-operator method employed in I for the study of a one-electron atom, and introduce a modification made necessary by the fact that the positive- and negative-energy solutions of the Dirac equation, which were used previously as basis functions, can no longer serve that purpose when the external field is supercritical. That is, we consider a situation in which the ground state has entered the negative-energy sea and become a resonance as the nuclear charge is increased beyond the critical value. To construct an orthogonal basis under these circumstances we follow a method originally devised some time ago by Wang and Shakin[5] for use in nuclear reaction theory.[6,7] This is discussed first in the context of the first-quantized Dirac equation and then carried over to the hole-theoretic formulation adopted later on.

The Dirac Hamiltonian, in units with $\hbar=c=1$, is written, in standard notation, as

$$h(\mathbf{x})=\boldsymbol{\alpha}\cdot(-i\nabla)+\beta m+V_{\text{ext}} , \tag{2.1}$$

where V_{ext} has the Coulomb form $-Ze^2/|\mathbf{x}|$ away from the nucleus but will be modified, in general, close up. For Z sufficiently small a complete, orthogonal set of eigenfunctions may be constructed by solving the equations

$$h(\mathbf{x})u_p(\mathbf{x})=\varepsilon_p u_p(\mathbf{x}), \quad \varepsilon_p>0 , \tag{2.2a}$$

$$h(\mathbf{x})v_n(\mathbf{x})=\varepsilon_n v_n(\mathbf{x}), \quad \varepsilon_n<0 . \tag{2.2b}$$

[Boundary conditions must be specified to complete the definition of the continuum solutions. When, as above, no indication is given the solutions may be assumed to satisfy outgoing-wave boundary conditions at great distances. Later on it will be necessary to distinguish between outgoing- and incoming-wave solutions, and this will be done by labeling the functions with superscripts $(+)$ and $(-)$, respectively.] With Z now increased above the critical value the state u_1, formerly the positive-energy ground state, has disappeared, having effectively been replaced by a resonance in the negative-energy continuum. Let $r(\mathbf{x})$ be a normalized function which represents the resonant state to the extent that it resembles the positron continuum wave function at the energy of the resonance in the region close to the nucleus, falling off at great distances as required by the normalization condition. It will be assumed in the following that $r(\mathbf{x})$ has been chosen so that its overlap with the set of functions $\{u_2,u_3,\ldots\}$, whose energies all lie above $-mc^2$, is effectively zero. The Wang-Shakin prescription allows us to construct a modified set of negative-energy wave functions $y_n(\mathbf{x})$ which are orthogonal to the function $r(\mathbf{x})$. To describe this procedure, in the context of the present problem, we first introduce some notation.

Let $|r\rangle$ be the ket representing the resonant state and let $|r\rangle\langle r|$ be the projection operator on to that state. (The degeneracy associated with spin will be ignored here to simplify notation.) We define $Q\equiv L^{<}-|r\rangle\langle r|$, where

$$L^{<}=\sum_{\varepsilon_n<-m}|v_n\rangle\langle v_n| \tag{2.3}$$

projects on to the set of continuum solutions of the Dirac equation with energies less than $-m$. Here and in the following the sum over states is a generalized one, representing an intergration over the continuum along with a sum over any discrete states that might exist. We now introduce the resolvents g and g^Q which satisfy

$$Q(z-h)Qg^Q(z)=Q , \tag{2.4}$$

$$L^{<}(z-h)L^{<}g(z)=L^{<} , \tag{2.5}$$

respectively. Now observe that the solution of Eq. (2.4) may be represented in the form

$$g^Q=g-g|r\rangle(\langle r|g|r\rangle)^{-1}\langle r|g . \tag{2.6}$$

It then follows that a set of basis functions $\{y_n\}$ may be defined as

$$|y_n\rangle=\lim_{(z-\varepsilon_n)\to 0}(z-\varepsilon_n)g^Q(z)|v_n\rangle , \tag{2.7}$$

with energies $\varepsilon_n<-m$, where z approaches the real energy axis from below in the complex plane. These functions, which are orthogonal to $|r\rangle$ and satisfy $Q(\varepsilon_n-h)Q|y_n\rangle=0$, may be expressed in the form

$$|y_n\rangle=|v_n\rangle-g(z)|r\rangle[\langle r|g(z)|r\rangle]^{-1}\langle r|v_n\rangle , \tag{2.8}$$

with z approaching ε_n from negative imaginary values. The modified basis functions $|y_n\rangle$ satisfy the same orthonormality relations amongst themselves as do the original set $|v_n\rangle$.[5]

We have two mutually orthogonal sets of states $\{r,u_2,u_3,\ldots\}$ and $\{y_1,y_2,y_3,\ldots\}$, and may now identify the projection operator Q as

$$Q=\sum_{\varepsilon_n<-m}|y_n\rangle\langle y_n| . \tag{2.9}$$

These states provide a basis which proves to be convenient in the analysis of vacuum decay.[2] This will be seen below in the context of the Hamiltonian formulation of QED.

In the Schrödinger picture of QED the particle field operator, when expressed in the modified basis introduced above, may be expanded as

$$\psi_D(\mathbf{x})=\sum_{\varepsilon_p>-m}A_p u_p(\mathbf{x})+b^{\dagger}r(\mathbf{x})+\sum_{\varepsilon_n<-m}B_n^{\dagger}y_n(\mathbf{x}) . \tag{2.10}$$

The creation and annihilation operators are defined by the anticommutation relations

$$\{A_{p'}, A_p^\dagger\}=\delta_{p'p}, \quad \{B_{n'}, B_n^\dagger\}=\delta_{n'n}, \quad \{b, b^\dagger\}=1 , \tag{2.11}$$

with all other anticommutators vanishing, along with the specification of their action on the vacuum state. The latter is taken here to be the doubly charged supercritical vacuum, denoted as $|0\rangle$. We have

$$A_p|0\rangle=0, \quad B_n|0\rangle=0, \quad b|0\rangle=0 ; \tag{2.12}$$

the creation of a vacancy in the K shell is indicated, in this notation, by

$$b^\dagger|0\rangle=|r\rangle . \tag{2.13}$$

The QED Hamiltonian is of the form $H=H_0+V$, where the unperturbed part $H_0=H_D+H_{\rm rad}$ is the sum of the particle and radiation-field energy operators, and the perturbation $V=H_T+H_C$ represents the sum of the transverse radiation-field interaction and the instantaneous Coulomb interaction. With H_D expressed, in normal-ordered form, as

$$H_D=\int d^3x\, \psi_D^\dagger(\mathbf{x})h(\mathbf{x})\psi_D(\mathbf{x}) , \tag{2.14}$$

and with the field operator expanded as shown in Eq. (2.10), one obtains the representation

$$H_D=\sum_{\varepsilon_p>-m}\varepsilon_p A_p^\dagger A_p-\varepsilon_r b^\dagger b-\sum_{\varepsilon_n<-m}\varepsilon_n B_n^\dagger B_n - \sum_{\varepsilon_n<-m}\Delta_n b^\dagger B_n-\sum_{\varepsilon_n<-m}\Delta_n^* B_n^\dagger b . \tag{2.15}$$

The off-diagonal element

$$\Delta_n\equiv\langle y_n|h|r\rangle \tag{2.16}$$

plays the role of a transition amplitude for the decay of the neutral vacuum. Our main concern in the following will be to develop a procedure for calculating higher-order corrections to this decay amplitude in a systematic fashion. The energy $|\varepsilon_r|$, with

$$\varepsilon_r=\langle r|h|r\rangle , \tag{2.17}$$

represents the average energy of the resonant state.

Following the procedure of I, we study the resolvent operator $R(z)=(z-H)^{-1}$ whose iterative solution generates the expansion which serves as a convenient starting point for time-independent multiparticle perturbation theory. An arbitrary matrix element of $R(z)$ may be expressed as the convolution[1] of two terms, one representing the sum of all connected diagrams and the other, of the form $\langle 0|R(z)|0\rangle$, accounting for the totality of all vacuum components. In the following we analyze the connected part, from whose pole singularity the energy of the system, relative to that of the vacuum, may be determined.

Let us suppose that the nuclear charge Z is increased continuously from below to just above the critical value. If one followed the position in the complex plane of the pole in the resolvent, one would see the pole move off the real axis onto the second Riemann sheet. We study the matrix element $\langle r|R(z)|r\rangle$, from which the pole position may be determined, using a standard projection operator procedure[8] which leads to a convenient expression for this matrix element. (It will be understood, without further burdening the notation, that only the connected part of the matrix element is retained in the calculation.) With the projection operator q defined as $1-|r\rangle\langle r|$, the identity which proves to be useful in this analysis is

$$R(z)=R^q(z)+[1+R^q(z)H]|r\rangle\langle r|R(z)|r\rangle \times\langle r|[1+HR^q(z)] , \tag{2.18a}$$

where

$$\langle r|R(z)|r\rangle=[z+\varepsilon_r-\langle r|V|r\rangle-\langle r|HR^q(z)H|r\rangle]^{-1} , \tag{2.18b}$$

and where $R^q(z)$ is defined by the resolvent equation

$$q(z-H)qR^q(z)=q . \tag{2.19}$$

From the analogous relation

$$q(z-H_0)qR_0^q(z)=q , \tag{2.20}$$

we obtain the integral equation

$$R^q(z)=R_0^q(z)+R_0^q(z)qVqR^q(z) , \tag{2.21}$$

which serves as the basis for a perturbation expansion of $R^q(z)$, and hence of the level-shift operator

$$T_{rr}^q(z)\equiv\langle r|V|r\rangle+\langle r|HR^q(z)H|r\rangle \tag{2.22}$$

which appears in Eq. (2.18b).

B. Lowest-order approximation

As a first approximation we ignore the interaction V, in which case, in the eigenfunction expansion of $R_0^q(z)$, only the states which span the modified negative-energy continuum need be retained. Consequently, $R_0^q(z)$ may be replaced by the modified positron propagator

$$QR_0^q(z)Q=\sum_{\varepsilon_n<-m}\frac{|y_n\rangle\langle y_n|}{z+\varepsilon_n} . \tag{2.23}$$

We then obtain the approximate level shift

$$T_{rr}^q(z)\approx\sum_{\varepsilon_n<-m}\frac{\langle r|h|y_n\rangle\langle y_n|h|r\rangle}{z+\varepsilon_n} . \tag{2.24}$$

An evaluation of the position of the pole in the complex plane of the matrix element (2.18b) is complicated by the fact that the level shift is z dependent. This pole position may be determined by an iterative procedure which generalizes to complex energies the standard perturbation expansion applicable to real eigenvalues.[9] The first approximation, appropriate when the pole is sufficiently close to the real axis, is obtained by replacing the imaginary part of z on the right-hand side of Eq. (2.24) by an infinitesimal positive quantity, and the real part by $|\varepsilon_r|$. In this approximation the pole appears at the complex energy $|\varepsilon_r|-i\Gamma/2$, where the width (or inverse lifetime) Γ of the unstable state associated with the resonance is determined as[10]

$$\Gamma=2\pi \sum_{\varepsilon_n<-m} |\Delta_n|^2\delta(\varepsilon_n-\varepsilon_r) , \tag{2.25}$$

in agreement with previous treatments.[2] In the following we outline a procedure for developing improved approximations, in a systematic way, taking into account the effect of higher-order QED perturbations.

III. RESONANT SCATTERING OF POSITRONS

A. Generalized unitarity relations

The view of a decay process as representing half a collision provides us not only with additional physical insight but also allows us to apply some of the powerful methods of formal scattering theory to the study of unstable states.[10] In following such an approach here we have a twofold objective. The primary goal is to set up a systematic procedure for generating higher-order corrections to the decay rate. At the same time we shall develop a framework for calculating positron-atom or electron-atom scattering amplitudes in the context of the time-independent Hamiltonian formulation of QED, analogous to that set up previously for the bound-state problem.[1] The relationship between the scattering and decay problems is perhaps most clearly seen in the generalized unitarity relations which couple the free-free, bound-free, and bound-bound transition amplitudes. We begin by summarizing these relations, following the development presented earlier,[7] in which the distortion of the basis states arising from the orthogonality constraint is fully accounted for.

The scattering matrix may be decomposed as

$$S_{n'n}=S^{(1)}_{n'n}+S^{(2)}_{n'n} , \tag{3.1}$$

where

$$S^{(1)}_{n'n}=\langle y^{(-)}_{n'}|y^{(+)}_n\rangle \tag{3.2}$$

represents the scattering due to the distortion of the basis states. In the following, to simplify notation, we write $|y^{(\pm)}_n\rangle\equiv|n^{(\pm)}\rangle$; as mentioned earlier the superscripts distinguish between outgoing-wave (+) and incoming-wave (−) boundary conditions. We have

$$S^{(2)}_{n'n}=-2\pi i\langle n'^{(-)}|T(\varepsilon+i\eta)|n^{(+)}\rangle , \tag{3.3}$$

where ε is the total energy and η is a positive infinitesimal. The unitarity relation satisfied by the S matrix may be expressed, in an abbreviated notation, as

$$\sum_c{}' S_{n'c}S^*_{nc}=\delta_{n'n} ; \tag{3.4}$$

here the prime on the summation sign is meant to indicate that only energy-conserving continuum states are included. The matrix $\underline{S}^{(1)}$ satisfies a unitarity relation of the same form, and this may be taken into account to simplify the matrix equation obtained by substituting the decomposition (3.1) into Eq. (3.4). One finds that

$$\underline{S}^{(2)\dagger}\underline{S}^{(1)}+\underline{S}^{(1)\dagger}\underline{S}^{(2)}+\underline{S}^{(1)\dagger}\underline{S}^{(2)}\underline{S}^{(2)\dagger}\underline{S}^{(1)}=\underline{0} . \tag{3.5}$$

Further simplification is achieved by applying the unitarity property of $\underline{S}^{(1)}$ once again to obtain

$$\sum_c{}' S^{(1)*}_{cn'}S^{(2)}_{cn}=-2\pi i\langle n'^{(+)}|T(\varepsilon+i\eta)|n^{(+)}\rangle \equiv-2\pi iT^{(+)}_{n'n} , \tag{3.6}$$

$$\sum_c{}' S^{(2)*}_{cn'}S^{(1)}_{cn}=2\pi i\langle n'^{(+)}|T(\varepsilon-i\eta)|n^{(+)}\rangle \equiv2\pi iT^{(-)}_{n'n} . \tag{3.7}$$

By combining these equations with Eq. (3.5) we arrive at the discontinuity relations

$$T^{(+)}_{n'n}-T^{(-)}_{n'n}=-2\pi i\sum_c{}' T^{(+)}_{n'c}T^{(-)}_{cn} . \tag{3.8}$$

We are interested here in the scattering of a positron by a stable target consisting of a nucleus of charge $Z>Z_{cr}$ to which two electrons are bound. The positron can annihilate with one of the bound electrons, leaving an unstable one-electron atom. In the second half of the collision the atom decays and the positron emerges in a stable continuum state. This separation of the collision into capture and decay processes may be represented formally through a (Breit-Wigner) decomposition of the $\underline{T}$ matrix as a nonresonant part $\underline{T}^q$ plus a resonant remainder. We write [with superscript (+) understood when no sign is given]

$$T_{n'n}=T^q_{n'n}+T^q_{n'r}(\varepsilon-|\varepsilon_r|-T^q_{rr})^{-1}T^q_{rn}, \quad n,n'\neq r . \tag{3.9}$$

One of the elements of the level-shift matrix $\underline{T}^q$ has been defined in Eq. (2.22) and the remaining elements will be specified more precisely later on. Here we observe that, as can readily be verified, the discontinuity relation (3.8) will be satisfied provided that $\underline{T}^q$ satisfies

$$T^{(+)q}_{\beta\alpha}-T^{(-)q}_{\beta\alpha}=-2\pi i\sum_c{}' T^{(+)q}_{\beta c}T^{(-)q}_{c\alpha} . \tag{3.10}$$

In this equation the channel indices β and α may refer to the discrete (resonant) state $|r\rangle$ as well as to the continuum states but the sum runs over continuum states only. The problem has now been shifted to devising a means of constructing $\underline{T}^q$, subject to the discontinuity constraint (3.10). This will be a simpler calculational problem, in general, since the rapid energy dependence associated with the resonance has been removed.

B. The level-shift matrix

Assuming the system to be in the state $|r\rangle$ at $t=0$, the probability amplitude for finding it in a continuum state, labeled by the index n, at $t=\infty$ is given by[10]

$$M_{nr}=\lim_{\eta\to0+}[i\eta\langle v^{(-)}_n|R(\varepsilon+i\eta)|r\rangle] , \tag{3.11}$$

with the limit understood here and in the following to be one in which η approaches zero through positive values. From the identity (2.18) we obtain the relation

$$R(z)|r\rangle=[1+R^q(z)H]|r\rangle[z-|\varepsilon_r|-T^q_{rr}(z)]^{-1} , \tag{3.12}$$

which in turn implies that

$$M_{nr}=T^q_{n^{(-)}r}[z-|\varepsilon_r|-T^q_{rr}(\varepsilon+i\eta)]^{-1} , \tag{3.13}$$

with

$$T^q_{n^{(-)}r} = \lim_{\eta\to 0+} [i\eta \langle v_n^{(-)}|R^q(\varepsilon+i\eta)H|r\rangle] . \quad (3.14)$$

(The notation anticipates the relationship, to be established below, between this T-matrix element and the level shift.) We are then led to study the state vector

$$|\Psi_n^{(-)q}\rangle = \lim_{\eta\to 0+} [-i\eta R^q(\varepsilon-i\eta)|v_n^{(-)}\rangle] . \quad (3.15)$$

The procedure now to be followed is analogous to that which led to Eq. (2.8), here restated in the language of hole theory. With $R_0(z)=(z-H_0)^{-1}$ we have, for the resolvent R^q_0 defined in Eq. (2.20), the representation

$$R^q_0 = R_0 - R_0|r\rangle(\langle r|R_0|r\rangle)^{-1}\langle r|R_0 . \quad (3.16)$$

Distorted basis states are defined as

$$|n^{(\pm)}\rangle = \lim_{\eta\to 0+} [\pm i\eta R^q_0(\varepsilon\pm i\eta)|v_n^{(\pm)}\rangle] ; \quad (3.17)$$

we then find that

$$|n^{(\pm)}\rangle = |v_n^{(\pm)}\rangle - R_0(\varepsilon\pm i\eta)|r\rangle \times[\langle r|R_0(\varepsilon\pm i\eta)|r\rangle]^{-1}\langle r|v_n^{(\pm)}\rangle . \quad (3.18)$$

[The compatibility of this representation with that shown in Eq. (2.8) follows from the fact that R_0, projected onto a one-body subspace, differs only by a sign from the Dirac propagator g.]

The combination of Eqs. (2.21) and (3.15) implies that

$$|\Psi_n^{(-)q}\rangle = |n^{(-)}\rangle + R^q(\varepsilon-i\eta)V|n^{(-)}\rangle . \quad (3.19)$$

From the definition

$$T^q_{n^{(-)}r} = \langle \Psi_n^{(-)q}|H|r\rangle$$

we are led to the expression

$$T^q_{n^{(-)}r} = \langle n^{(-)}|H + VR^qH|r\rangle . \quad (3.20)$$

The final state in the matrix element $T^q_{n^{(-)}r}$ satisfies the physically appropriate incoming-wave boundary conditions. The matrix elements which appear in the discontinuity relations (3.10), on the other hand, involve only outgoing-wave continuum states. Once these auxiliary amplitudes are determined the physical matrix elements, such as that which appears in Eq. (3.20), can be constructed by applying transformations, similar to those shown in Eq. (3.6) and (3.7), involving the (presumably known) matrix $\underline{S}^{(1)}$. One frequently deals with a particular partial wave, in which case the transformation from one form of T-matrix element to the other involves only multiplication by a phase factor.

The identification of $T^q_{n^{(+)}r} \equiv T^q_{nr}$, as just defined, with the bound-free element of the level-shift matrix is established by showing that the discontinuity relations (3.10) are satisfied. This is easily done using the resolvent equation

$$R^q(\varepsilon+i\eta) - R^q(\varepsilon-i\eta) = -2\pi i \sum_c{}' |\Psi_c^{(+)q}\rangle\langle\Psi_c^{(+)q}| . \quad (3.21)$$

It is also necessary to complete the definition of the level-shift matrix with the relations

$$T^q_{rn^{(+)}} = \langle r|H + HR^q(\varepsilon+i\eta)V|n^{(+)}\rangle , \quad (3.22)$$

and

$$T^q_{n'^{(+)}n^{(+)}} = \langle n'^{(+)}|V + VR^q(\varepsilon+i\eta)V|n^{(+)}\rangle . \quad (3.23)$$

As remarked earlier, an iterative solution of the integral equation (2.21) for the resolvent R^q can serve as the basis for a perturbative construction of the level shift. Equivalently, elements of the matrix $\underline{T}^q$ may be shown to satisfy a set of coupled integral equations to be solved perturbatively, or perhaps in some more general fashion. These latter equations are obtained by combining the integral equations for R^q with the relations which define $\underline{T}^q$ and then employing the eigenfunction expansion

$$R^q_0(\varepsilon) = \sum_c \frac{|c^{(+)}\rangle\langle c^{(+)}|}{\varepsilon+i\eta-|\varepsilon_c|} . \quad (3.24)$$

The resulting set of equations are of the form

$$T^q_{\beta\alpha} = B_{\beta\alpha} + \sum_c B_{\beta c}\frac{1}{\varepsilon+i\eta-|\varepsilon_c|}T^q_{c\alpha} . \quad (3.25)$$

The " Born" amplitudes are defined as

$$B_{c'c} = \langle c'^{(+)}|V|c^{(+)}\rangle , \quad (3.26)$$

$$B_{cr} = \langle c^{(+)}|H|r\rangle = B^*_{rc} , \quad (3.27)$$

$$B_{rr} = \langle r|V|r\rangle . \quad (3.28)$$

It is readily verified that the solutions of Eq. (3.25) satisfy the appropriate discontinuity relations (3.10). We note that Eq. (3.25) may be put in the alternative form

$$T^q_{\beta\alpha} = B_{\beta\alpha} + \sum_c T^q_{\beta c}\frac{1}{\varepsilon+i\eta-|\varepsilon_c|}B_{c\alpha} . \quad (3.29)$$

Since the intermediate continuum states which appear in the integral equations involve arbitrarily large numbers of particles in general, these equations do not serve as the basis for calculation as they stand. Let us suppose that the sum over states has been truncated in some fashion. (A specific model which accomplishes this is proposed in Sec. IV.) Suppose further that the (now finite) set of equations obtained by allowing β and α in Eqs. (3.25) to range over all continuum channel indices has been solved. It then follows from the form of Eqs. (3.25) and (3.29) that the remaining elements of $\underline{T}^q$, those involving the resonant state $|r\rangle$, can be constructed by quadratures. Specifically, we have

$$T^q_{rr} = B_{rr} + \sum_c B_{rc}\frac{1}{\varepsilon+i\eta-|\varepsilon_c|}T^q_{cr} . \quad (3.30)$$

The elements T^q_{cr} which appear on the right-hand side can be evaluated as

$$T^q_{cr} = B_{cr} + \sum_{c'} T^q_{cc'}\frac{1}{\varepsilon+i\eta-|\varepsilon_{c'}|}B_{c'r} \quad (3.31)$$

once the submatrix $T^q_{cc'}$ has been determined. From this point of view the problem of the decay of the neutral vac-

uum has been converted into one requiring the solution of a nonresonant positron-atom scattering problem, with radiative corrections included. This idea is developed further in Sec. IV.

The discontinuity equation

$$T_{rr}^{(+)q}-T_{rr}^{(-)q}=-2\pi i\sum_c{}' T_{rc}^{(+)q}T_{cr}^{(-)q} , \tag{3.32}$$

when combined with the reciprocity relation

$$T_{\beta\alpha}^{(-)q}=(T_{\alpha\beta}^{(+)q})^* , \tag{3.33}$$

leads to a more general expression for the resonance width than that given earlier in Eq. (2.25), allowing, in particular, for radiative decay modes. We find that, under the assumption that the width is sufficiently small,

$$\Gamma=2\pi\sum_c{}'|T_{rc}^{(+)q}|^2 , \tag{3.34}$$

with the energy parameter ε in the definition of the level shift evaluated at the resonance energy $|\varepsilon_r|$. [Recall that the sum in Eq. (3.34) is over energy-conserving states only so that channels with threshold energies lying above $|\varepsilon_r|$ are not included. As mentioned earlier, corrections introduced when the assumption concerning the width is relaxed can be calculated by a successive approximation procedure,[9] but we shall not pursue this matter further here.] The importance of conforming to the constraints imposed by the requirements of unitarity and reciprocity in developing approximations to the level-shift matrix should be clear from the derivation of Eq. (3.34). These constraints are automatically satisfied in the calculational method to be described below.

IV. ONE-PAIR APPROXIMATION

A. Integral equations of the Dyson-Schwinger type

Further progress in the analysis of the level-shift matrix can be made only after the dynamical model is specified in more detail. To begin this process we examine Eq. (3.30) for the element T_{rr}^q. The continuum states which appear in the sum over channels are just those for which the Born amplitudes B_{rc} are nonvanishing. This is then an appropriate place to recall the form of the particle-field interaction $V=H_C+H_T$. We have

$$H_C=\tfrac{1}{2}\int\psi_D^\dagger(\mathbf{x})\psi_D(\mathbf{x})\frac{e^2}{4\pi|\mathbf{x}-\mathbf{x}'|}\psi_D^\dagger(\mathbf{x}')\psi_D(\mathbf{x}')d^3x\,d^3x' , \tag{4.1}$$

and

$$H_T=e\int\psi_D^\dagger(\mathbf{x})\boldsymbol{\alpha}\psi_D(\mathbf{x})\cdot\mathbf{A}(\mathbf{x})d^3x . \tag{4.2}$$

The vector potential $\mathbf{A}(\mathbf{x})$ has (in the notation of I) the plane-wave expansion

$$\mathbf{A}(\mathbf{x})=\sum_s(2k_s)^{-1/2}[a_s\mathbf{U}_s(\mathbf{x})+a_s^\dagger\mathbf{U}_s^*(\mathbf{x})] , \tag{4.3}$$

where $a_s^\dagger$ and a_s are the photon creation and annihilation operators as usually defined and s is an index which specifies both the photon momentum $\mathbf{k}_s$ and the double-valued polarization index λ_s. With the radiation field quantized in a box of volume L^3 the photon wave function is of the form

$$\mathbf{U}_s(\mathbf{x})=L^{-3/2}\mathbf{e}^{\lambda_s}\exp(i\mathbf{k}_s\cdot\mathbf{x}) , \tag{4.4}$$

with $\mathbf{k}_s\cdot\mathbf{e}^{\lambda_s}=0$ in the Coulomb gauge which has been adopted here. Matrix elements of these interactions are evaluated with the aid of eigenfunction expansions of the field operators, such as the one shown in Eq. (2.10). Alternatively, we may write

$$\psi_D(\mathbf{x})=\sum_{\varepsilon_p>-m}A_pu_p(\mathbf{x})+\sum_{\varepsilon_n<-m}D_n^\dagger v_n(\mathbf{x}) , \tag{4.5}$$

in which the resonant state has not been explicitly separated off, as it was in Eq. (2.10). This alternative form is the appropriate one to use in dealing with multiparticle intermediate states since then there is no requirement that resonant and nonresonant states be separated.

In order to work with a reasonably tractable model we do not consider all possible virtual excitations but only those in which the original positron is accompanied by an additional photon or an additional electron-positron pair. (This is essentially the one-pair approximation adopted in I.) We introduce three channel labels—c_1, c_2, and c_3—to denote the class of intermediate states which, in this model, appear in the integral equation (3.30). These states are of the form

$$\begin{aligned}&|n\rangle=B_n^\dagger|0\rangle \quad \text{for } c_1 ,\\ &|n,s\rangle=D_n^\dagger a_s^\dagger|0\rangle \quad \text{for } c_2 ,\\ &|p,n,n'\rangle=A_p^\dagger D_n^\dagger D_{n'}^\dagger|0\rangle \quad \text{for } c_3 .\end{aligned} \tag{4.6}$$

It is the Coulomb interaction H_C which connects the state $|r\rangle$ to the three-particle states of type c_3. There is, however, a simplifying feature, based on the introduction of a "Coulomb photon," which allows us to treat the one-step process of pair creation as a two-step process in which a Coulomb photon, having first been emitted by the positron, then creates the pair. The fact, which was pointed out previously in I, that we may formally combine Coulomb and transverse photons, is more than a calculational convenience since the combined photon propagator is covariant, and this is of crucial importance in the renormalization program. For our present purposes, however, the essential point is that, anticipating the introduction of the Coulomb photon, we may omit the sum over states of class c_3 in Eq. (3.30), which for convenience we now rewrite as

$$T_{rr}^q=B_{rr}+\sum_{i=1}^{2}\int B_{ri}g_iT_{ir}^q . \tag{4.7}$$

Here B_{r1}, for example, is the Born matrix element connecting the continuum channel c_1 with the resonant state and g_1 represents the propagator for channel c_1. (Integration variables for the intermediate-state channels c_1 and c_2 are suppressed to simplify notation.) Similar reasoning allows us to reexpress Eq. (3.31) as

$$T^q_{ir}=B_{ir}+\sum_{j=1}^{2}\int T^q_{ij}g_jB_{jr},\quad i=1,2\ . \tag{4.8}$$

These equations are noncovariant and approximate, but are in other respects analogous to the standard Dyson-Schwinger equations of covariant QED. As pointed out earlier in the more general context of Eqs. (3.29)–(3.31), the elements T^q_{rr} and T^q_{ir}, $i=1,2$, may be constructed by quadratures once the scattering amplitude $T^q_{22'}$ has been determined. Here we shall show this directly by deriving explicit and calculationally convenient representations of the amplitudes T^q_{rr} and T^q_{ir}.

To begin the analysis we look at the integral equation for $T^q_{1'1'}$. It is readily verified that the solution may be expressed in terms of T^q_{12} and an auxiliary amplitude $t^q_{1'1'}$ defined as the solution of the one-body equation

$$t^q_{1'1'}=B_{1'1'}+\int t^q_{1'1''}g_{1''}B_{1''1'}\ . \tag{4.9}$$

The solution is

$$T^q_{1'1'}=t^q_{1'1'}+\int T^q_{12}g_2B_{21'}+\int\int T^q_{12}g_2B_{21''}g_{1''}t^q_{1''1'}\ . \tag{4.10}$$

Since a numerical solution of Eq. (4.9) is relatively easy to obtain we next focus our attention on the matrix element T^q_{12}. The relevant integral equation may be written as

$$T^q_{12}=t^q_{12}+\int t^q_{11'}g_{1'}t^q_{1'2}\ , \tag{4.11}$$

where we defined

$$t^q_{12}=B_{12}+\int B_{12'}g_{2'}T^q_{2'2}\ . \tag{4.12}$$

The remaining matrix elements to be determining (taking into account the fact that reciprocity may be used to relate pairs of off-diagonal elements) are T^q_{1r} and T^q_{2r}, and these may also be expressed in terms of $T^q_{2'2}$, as may been seen immediately by inspection of Eq. (4.8).

The preceding analysis has shown that the essence of the dynamical problem lies in the construction of the amplitude for positron-photon scattering (modified by the removal, in the manner described, of resonance effects) in the presence of the target atom. This problem is addressed below.

By combining results we can arrive at a more concise representation of the matrix element T^q_{rr} with which we are here chiefly concerned. We observe, firstly, that the wave operator Ω, with elements

$$\Omega_{11'}=\delta_{11'}+\int g_{11''}t^q_{1''1'}\ , \tag{4.13}$$

appears throughout premultiplying the basis states $|n\rangle$. The "potential" $B_{11'}$ represents the effect of vacuum polarization on the propagation of the positron in the Coulomb field of the nucleus. (Since the vacuum is doubly charged[4] the Coulomb contribution to vacuum polarization has the effect of shielding the nucleus, so that the positron at great distances "sees," as it should, a charge of $Z-2$ rather than Z.) To take this self-energy correction into account in the formalism developed thus far we need merely replace the basis states $|n\rangle$ (which, it will be recalled, are themselves distorted by the orthogonality constraint) by the doubly distorted waves

$$|\bar{n}\rangle=\Omega|n\rangle\ . \tag{4.14}$$

In the following it will be understood, without the imposition of additional notation to indicate it explicitly, that this replacement has been made. Accordingly, we drop all terms in which the factor $t^q_{1'}$ appears. Then, after combining Eqs. (4.7)–(4.12), we have

$$T^q_{rr}=B_{rr}+\int B_{r1}g_1B_{1r}+\int\bar{B}_{r2}g_2\bar{B}_{2r}+\int\int\bar{B}_{r2}g_2T^q_{22'}g_{2'}\bar{B}_{2'r}\ , \tag{4.15}$$

where we introduced the abbreviations

$$\bar{B}_{r2}\equiv B_{r2}+\int B_{r1}g_1B_{12} \tag{4.16}$$

and

$$\bar{B}_{2r}\equiv B_{2r}+\int B_{21}g_1B_{1r}\ . \tag{4.17}$$

One easily sees how the lowest-order approximation shown in Eq. (2.24) is recovered by ignoring all radiative corrections in the more general result just derived. In a similar way one finds the representations

$$T^q_{1r}=B_{1r}+\int B_{12}g_2\bar{B}_{2r}+\int\int B_{12}g_2T^q_{22'}g_{2'}\bar{B}_{2'r} \tag{4.18}$$

and

$$T^q_{2r}=\bar{B}_{2r}+\int T^q_{22'}g_{2'}\bar{B}_{2'r}\ , \tag{4.19}$$

as well as representations of the elements T^q_{r2} and T^q_{r1} which we do not write explicitly. As already mentioned, the dynamical complexity of the model is seen to be contained, essentially, in the amplitude $T^q_{22'}$ describing positron-photon scattering in the presence of the external supercritical field. The structure of this amplitude is examined in greater detail in the following.

B. Further reduction of the level-shift matrix

In Eq. (3.9) an expression for the $\underline{T}$ matrix is displayed in which the resonant state $|r\rangle$ is "subtracted out," leaving a level-shift matrix which is a smoothly varying function of energy in the neighborhood of the resonance. This subtraction process may be carried one step further by removing all one-body intermediate continuum states, the states $|n\rangle$ belonging to channel c_1, from the level-shift submatrix $T^q_{\alpha\beta}$ $(\alpha,\beta=1,2)$. This leaves a reduced matrix, $W_{\alpha\beta}$, which has a simpler structure. This latter matrix plays the role of an effective potential in a linear integral equation

$$T^q_{\alpha\beta}=W_{\alpha\beta}+\int W_{\alpha1}g_1T^q_{1\beta}\ . \tag{4.20}$$

One readily verifies that the discontinuity relations for $T^q_{\alpha\beta}$ [they are of the form shown in Eq. (3.10) with only channels c_1 and c_2 appearing in the sum in the model considered here] will be satisfied provided that the simpler relations

$$W^{(+)}_{\alpha\beta}-W^{(-)}_{\alpha\beta}=-2\pi i\sum_{c_2}{}'W^{(+)}_{\alpha2}W^{(-)}_{2\beta}\ , \tag{4.21}$$

in which channel c_1 is missing in the sum over states, are satisfied by the effective-potential matrix. Once the effective potential has been determined one would solve the one-body integral equation (4.20) for the element T^q_{12}, at which point the element $T^q_{22'}$ could be obtained by quadratures from Eq. (4.20).

The equations which determine the effective potential, in a manner such that the discontinuity relations (4.21) are satisfied, are similar in form to those for the level shift, but with channel c_1 eliminated from the sum over intermediate states. Let us suppose, to begin, that the element $W_{22'}$ has been determined. (A procedure for doing this, in the context of the one-pair model, is outlined in Sec. IV C.) One then has

$$W_{21}=B_{21}+\int W_{22'}g_{2'}B_{2'1}\ , \tag{4.22}$$

$$W_{12}=B_{12}+\int B_{12'}g_{2'}W_{2'2}\ , \tag{4.23}$$

and

$$W_{11'}=B_{11'}+\int W_{12}g_2B_{21'}\ . \tag{4.24}$$

To be consistent with our earlier discussion leading to Eqs. (4.15)–(4.19) we will drop the self-energy term $B_{11'}$ in Eq. (4.24) with the understanding that the basis states $|n\rangle$ are to be replaced by the distorted waves defined in Eqs. (4.13) and (4.14). The problem has been shifted to that of constructing the matrix element $W_{22'}$, and we now turn our attention to this matter.

C. The K matrix

To begin we note, for the sake of orientation, that with $W_{22'}$ set equal to zero a very simple expression for the level shift is obtained. The positron-photon interaction, in such a model, is one in which the photon is absorbed and reemitted, an arbitrary number of times, and this amounts to the introduction of a renormalized positron propagator accounting for this radiative correction. To include the effect of virtual-pair creation one must choose a nonvanishing form for the element $W_{22'}$. In the one-pair model introduced in I and adopted here, a photon, in the presence of a spectator positron, can be transformed into a positron-electron pair. The Born matrix element for this transition from channel c_2 to c_3 is denoted as B_{32}. There are two types of interactions that can take place in channel c_3 under the constraints of the model—the pairwise Coulomb interaction is one type and pair annihilation and creation is the other. Let G_3 denote the propagator which fully accounts for these interactions. The system makes the transition from channel c_3 back to c_2 by pair annihilation; the relevant matrix element is B_{23}. An explicit notation for these propagators and vertex functions is given in I. In the more schematic (and, one hopes, transparent) notation employed here the expression for the effective-potential matrix element $W_{22'}$ takes the form

$$W_{22'}=\int B_{23}G_3B_{32'}\ . \tag{4.25}$$

Only a brief outline of the formal procedure for constructing the matrix element $W_{22'}$ will be given here in order to avoid repetition of material presented earlier.[1] The point we wish to emphasize is that the analysis draws heavily on techniques introduced originally in the context of the integral equation approach to nonrelativistic three-body scattering theory, in the form developed by Faddeev[11] and others some years ago. The Faddeev equations effectively sum up successive scatterings of different pairs. Each two-body collision is described by the interacting Green's function for the pair. This is particularly convenient for our present purposes since it facilitates the separation of the pair interaction into a Coulombic contribution and a part, involving pair annihilation and creation, which can be expressed in terms of the renormalized photon propagator. Correspondingly, the effective potential in this three-body model can, after some formal manipulations (of the type employed in earlier studies of the analogous nonrelativistic problem[12]), be shown to satisfy an integral equation in which Coulomb and pair annihilation interactions are separately summed and introduced as input to the equations. The result is of the form

$$W_{22'}=K_{22'}+\int K_{22''}g^{\rm ren}_{2''}W_{2''2'}\ . \tag{4.26}$$

Here $g^{\rm ren}_2$ represents the photon propagator, renormalized by the inclusion of self-energy corrections associated with virtual-pair creation and annihilation, in the presence of a spectator positron. [See Eq. (3.3) of I for a more explicit definition. Note that in I we were dealing with a system consisting of two electrons and a positron, while here we have two positrons and an electron, so that some rather trivial changes must be made in transcribing the formulas of I to the problem under present consideration.] The kernel $K_{22'}$ was referred to in I as the $\underline{K}$ matrix. As shown there [see Eq. (3.20) of I] the $\underline{K}$ matrix can be expressed in terms of the Green's function of a system of three particles interacting through Coulomb pair potentials. It was also shown how variational methods of the Rayleigh-Ritz type could be used to obtain approximations to the $\underline{K}$ matrix which allow for systematic improvement by suitable choice of trial functions. Such methods, which include the availability of a rigorous minimum principle, are applicable in the present problem as well. Let us recall that the validity of the minimum principle follows directly from the fact that the three-body intermediate states appearing in the construction of the $\underline{K}$ matrix have a spectrum of energy eigenvalues lying above the energy parameter in the Green's function, which is the resonance energy $|\varepsilon_r|$ in the case at hand.

There is another important consequence of the above-mentioned spectral property, which is that the $\underline{K}$ matrix, evaluated at the resonance energy, satisfies the particularly simple discontinuity relation

$$K^{(+)}_{22'}-K^{(-)}_{22'}=0\ . \tag{4.27}$$

It is not difficult to ensure that approximations to the $\underline{K}$ matrix will satisfy this relation, in which case the complete set of generalized unitarity relations, Eqs. (4.21), (3.10), and (3.8), are guaranteed (by the structure of the integral equations from which they are determined) to be

satisfied. It is clear that the Hermiticity property of the $\underline{K}$ matrix [which follows from Eq. (4.27) and the reciprocity condition] is its most essential feature with regard to the development of approximation methods for bound-state and scattering problems.

If one were primarily interested in positron-atom scattering, rather than the decay problem, construction of the effective-potential matrix element $W_{11'}$ would be of primary concern. Once this element is known the scattering parameters can be determined by solving the relatively simple one-body integral equation (4.20) and then making use of Eqs. (3.9). From Eqs. (4.22)–(4.24) we find that

$$W_{11'} = \int B_{12} g_2 B_{21'} + \int\int B_{12} g_2 W_{22'} B_{2'1'} \ . \qquad (4.28)$$

Evidently, our discussion of the decay problem, which focused on the determination of the element $W_{22'}$, is directly applicable to the scattering problem; the intimate connection between the two becomes particularly clear from this point of view. We remark that when a virtual pair is produced the positron is created in a state which may be thought of as a superposition of resonant and nonresonant components. Production of the resonant component corresponds, physically, to a scattering process in which the incident positron collides with one of the bound electrons in the target; this electron makes a transition to an excited state, leaving behind a vacancy in the target. One is dealing here with a fundamental mechanism for the interaction of projectile and target, the dynamics of which is completely contained in the $\underline{K}$ matrix. Indeed, the particle-hole excitation mechanism is an important one under the more general circumstances of positron or electron scattering from a target which, by suitable choice of Fermi level, is taken as the ground state of the system. The formalism developed here should provide the basis for the analysis of relativistic scattering and decay problems in which the Coulomb interaction is accounted for beyond the lowest orders of perturbation theory.

V. SUMMARY

While it has a major drawback—the lack of manifest covariance—the Hamiltonian formulation of QED has distinct advantages as well, and these make its continued study worthwhile. This is particularly so with regard to atomic bound-state and scattering problems where nonperturbative treatments of the Coulomb interaction are of crucial importance. An earlier study of the bound-state problem in a one-pair approximation[1] has been extended here to scattering processes, and this provides an additional illustration of the applicability of the time-independent approach to relativistic atomic physics. To provide focus to the discussion we have examined the problem of neutral vacuum decay in a supercritical field. By treating this process as the second stage of a resonant collision one is able to bring to bear on the problem some of the formal apparatus of collision theory. Specifically, the unitarity property has been used here as a means for systematically "subtracting off" one- and two-body states, thereby allowing us to introduce a Hermitian kernel, the $\underline{K}$ matrix, which contains the essential dynamics of a system of three particles interacting Coulombically. The structure of the $\underline{K}$ matrix is precisely that studied previously[1] and we have not reproduced that analysis here. One finds that the procedure for constructing the $\underline{K}$ matrix can be formulated in terms of a Rayleigh-Ritz variational principle. Here we have shown how the $\underline{K}$ matrix enters into the determination of scattering and decay amplitudes.

A fairly general expression for the decay rate of the neutral vacuum is given in Eq. (3.34). The decay amplitudes appearing there are defined explicitly, in Sec. IV, in the context of the one-pair model. This allows for the introduction, in a manner consistent with unitarity, of corrections to the lowest-order formula, Eq. (2.25), which arise from the virtual creation and annihilation of a single photon and of a single electron- positron pair. In the course of the analysis we have obtained, in Eq. (4.26) and (4.28), the basis for an effective-potential treatment of relativistic atomic scattering which allows for extensions beyond the Dirac-Hartree-Fock techniques that have been used for the most part up till now.

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