

# Decay law of unstable levels and spectral lineshape in the theory of a relativistic atom

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The time evolution of quasistationary atomic levels is derived taking into consideration the quantum-electrodynamic interaction. The method of single-time Green's functions and associated quasipotential equations is used. Renormalization is possible over finite times, on the order of the lifetime of a quasistationary level. Expressions for the probabilities for one- and two-photon transitions at a specified time  $t$  are derived with radiative corrections in the nondegenerate case. In the limit  $t \rightarrow \infty$  the spectral line has a purely Breit–Wigner shape. In the degenerate case, one-photon transitions are analyzed. The lineshape is found to depend on the method by which the initial state is specified: It is a Breit–Wigner lineshape if quasistationary levels are formed statistically, while it contains interference terms if close-lying quasistationary levels are produced coherently through the quantum-mechanical interaction.

## 1. INTRODUCTION

Since the development of covariant perturbation theory it has been known that the ultraviolet infinities which arise in relativistic quantum field theory can be eliminated through renormalization of the  $S$  matrix and the Green's functions, but not in quantities characterizing the time evolution of processes, e.g., the evolution operator  $\exp[-iH(t_2 - t_1)]$ , where  $H$  is a Hamiltonian. Additional surface infinities appear for this operator in perturbation theory because the interaction is turned on at the time  $t_1$  and off at  $t_2$  (Ref. 1). Because of this circumstance, a description of the time evolution has been abandoned in quantum field theory, and  $S$  matrices and Green's functions have been used exclusively. This is not always the best approach for studying unstable states. In principle, of course, it is clear that even processes involving unstable particles can be dealt with by the  $S$ -matrix approach, provided that the initial stage of the formation of the unstable entities is taken into account, and processes which go from stable particles to stable particles are studied. A description of that sort, however, would become unjustifiably complicated and would not include the time evolution. Accordingly, practical calculations usually either totally ignore the instability of the particles (in the course of their interactions), or in cases in which the instability is important (in a description of a decay probability), are restricted to lowest-order perturbation theory and analogies with quantum-mechanical problems. As the calculations become more accurate, and radiative corrections are taken into account, it becomes necessary to clearly distinguish the instability effects and to correctly describe the time evolution of an unstable state with the help of higher-order perturbation theories.

Higher-order corrections to the decay probability and to the spectral lineshape have been under study for a long time now because of practical problems in atomic physics. Researchers working in this field use the apparatus of a finite-time evolution operator or an adiabatic theory, ignoring the ultraviolet infinities. In that approach it becomes possible to derive the Lamb shift of the center of a spectral line and its Breit–Wigner shape through a summation of dia-

grams.<sup>2</sup> Estimates show, however, that surface terms arise because of the multiplicative renormalization of the wave function in the diagrams considered in Ref. 2 and remain infinite even after renormalization of the mass and charge of the electron (see the Appendix). In lowest-order perturbation theory, in the resonant approximation used in Ref. 2, these infinities are unimportant, but in higher orders they cannot be avoided.

In the present paper we develop an approach for studying unstable states in quantum electrodynamics which starts from the understanding of an unstable particle as a pole of the  $S$  matrix on a nonphysical sheet of the complex energy. The approach is essentially a translation of this concept into a time-evolution language. We systematically derive all the characteristics of an unstable state—its lifetime, mass, mixing ratios, and probabilities for decay by various mechanisms—in terms of renormalized Feynman diagrams. Simultaneous Green's functions in which all the initial particles and all the final particles are considered at the same times turn out in a natural way to be a key entity which is convenient for describing unstable particles. Green's functions of this sort have been used for a long time in the quasipotential method.<sup>3,4</sup> In the approach which we are proposing here the incorporation of higher-order corrections to the transition amplitudes, in particular, incorporating the Lamb shift and the mixing of unstable levels, turns out to be completely trivial, as we will see, in contrast with, say, the adiabatic approach, where complicated summations of series of diagrams are required in order to accomplish the same purpose.<sup>2</sup>

## 2. TIME EVOLUTION OF A QUASISTATIONARY STATE IN QUANTUM ELECTRODYNAMICS

Let us consider the quantum electrodynamics (QED) of an atom, taking the customary approach of replacing the nucleus by an external Coulomb potential. For simplicity we first consider atoms having a single electron outside a filled shell; the latter corresponds to the vacuum state. We denote by  $\varepsilon_n$  the unperturbed electronic levels, and by  $\varphi_n$  the wave functions. We are interested in the behavior of level  $n$  when

the complete QED interaction is taken into account; this interaction is known to render all levels except the ground state unstable.

The formal description of the dynamics of unstable states in quantum theory is well known. The unstable state (level  $n$ ) is described at the initial time by a wave function  $\Phi_n$ , while the decay products are described by wave functions  $\Phi_\alpha$ . The amplitude for nondecay by the time  $t$  is described to within a phase factor by the expression  $A_{nn}(t) = \langle \Phi_n | e^{-iHt} | \Phi_n \rangle$ , while the amplitude for decay by mechanism  $\alpha$  is described by the expression  $A_{\alpha n}(t) = \langle \Phi_\alpha | e^{-iHt} | \Phi_n \rangle$ . The entire problem is one of choosing the wave functions  $\Phi_n$  and  $\Phi_\alpha$ . In nonrelativistic quantum mechanics,  $\Phi_n$  and  $\Phi_\alpha$  are usually taken to be eigenstates of some unperturbed Hamiltonian  $H_0$ . In relativistic quantum field theory, it is not possible to find a suitable  $H_0$ .

We will accordingly attempt to choose wave functions  $\Phi_n$  and  $\Phi_\alpha$  without resorting to any unperturbed Hamiltonian, working exclusively from the physical interpretation of these functions and the renormalizability condition. The latter requirement dictates the choice of wave functions essentially unambiguously. We introduce Heisenberg operators which create (bare) electrons,  $\alpha_n^+(x_0)$ , and photons,  $c^+(k, x_0)$ , at the time  $x_0$ . For example,

$$a_n^+(x_0) = \int d^3x \psi^+(x) \varphi_n(x) e^{-i\epsilon_n x_0}, \quad (1)$$

where the operator  $\psi(x)$  represents the electron-positron field, and  $c^+(k, x_0)$  are determined in a corresponding way in terms of the electromagnetic field  $A(x)$ . We construct the states  $\Phi_n$  and  $\Phi_\alpha$  in the form

$$\Phi_n = a_n^+(0) \Psi_0, \quad \Phi_\alpha = c^+(k, 0) a_m^+(0) \Psi_0, \quad (2)$$

where  $\Psi_0$  is the physical vacuum. We have specified only the simplest type of states  $\alpha$ : an electron in state  $m$  and a photon with a momentum  $k$ . More-complex states can be found by using several operators  $c^+$  and, possibly, operators of electron-positron (or hole) pairs. All of the Heisenberg operators are taken at the same time and are applied to the physical vacuum. The latter circumstance is responsible for the renormalizability of the theory. Substituting (1) and (2) into the definition of the amplitudes for nondecay and decay by mechanism  $\alpha$ , we find

$$A_{nn}(t) = \int d^3x d^3y \varphi_n^*(x) e^{i\epsilon_n t} \langle \Psi_0 | T\{\psi(x)\psi^+(y)\} | \Psi_0 \rangle \varphi_n(y),$$

$$A_{\alpha n}(t) = (2\pi)^{-3/2} \int d^3x d^3y d^3z \varphi_m^*(x) e^{i\mu(k)} e^{i(kz + i\epsilon_m t)}$$

$$\cdot i\vec{\partial}_0 \langle \Psi_0 | T\{\psi(x)\psi^+(y)A_\mu(z)\} | \Psi_0 \rangle \varphi_n(y),$$

$$x_0 = z_0 = t, \quad y_0 = 0, \quad (3)$$

etc., for more-complex states  $\Phi_\alpha$ . We see that the amplitudes are expressed in terms of Green's functions in which the time of the initial operator,  $\psi^+$ , is zero, while the times of all the final operators are identical, equal to  $t$ . These are simultaneous Green's functions: They depend on only one time,  $t$ , the final-state time, and their Fourier  $t$  transform depends on only the total energy  $E$ . It is not difficult to rewrite (3) in terms of simultaneous Green's functions in the energy representation,  $G_{\alpha n}(E)$  ( $\alpha = n$  or  $\alpha$ ):

$$A_{\alpha n}(t) = \int (dE/2\pi i) e^{-iEt} G_{\alpha n}(E). \quad (4)$$

The amplitude (3) or (4) has the advantage that the renormalization procedure is simple: it reduces to the elimination of the vacuum diagrams and a further multiplication by the required number of factors  $Z^{-1/2}$  for the electrons and photons. Now let us look at the disadvantages of these amplitudes. An explicit and formal disadvantage of the system  $\Phi_n, \Phi_\alpha$  is that it is not orthonormal. It might seem a straightforward matter to correct this situation through orthogonalization, but this procedure does not work. The quantities  $\langle \Phi_a / \Phi_b \rangle = A_{ab}(0)$  remain infinite even after renormalization since the integral of the renormalized  $G_{\alpha n}$  over  $E$  in (4) diverges at  $t=0$  for large values of  $E$ . The reason for this result and a physical interpretation of it can be understood better by considering the spectral characteristics of the state  $\Phi_n$ , which are determined in accordance with  $B_{\alpha n} = \langle \Psi_a / \Phi_n \rangle$ , where  $\Psi_a$  are eigenstates of Hamiltonian  $H$  (among the one-electron states, only one—the ground state—appears in them). The amplitudes  $B$  are found from expressions similar to (3) in which all of the final-particle times become infinite in a manner independent of each other. These are covariant Green's functions that are truncated on the side of the final particles which lie on the mass shell. On the initial-particle side we are left with an ordinary tail, which corresponds to the one-electron Green's function  $G_{nn}$  for the total energy of the final state,  $E_\alpha$ . For the simplest spectral function  $B_{\alpha n}$  with a single photon, the entire dependence on  $E_\alpha$  is specifically in this Green's function, so the distribution in the energy of state  $\Phi_n$ , described by  $|B_{\alpha n}|^2$ , is a slowly decreasing function  $\propto 1/E_\alpha^2$ . Renormalization makes this distribution finite, but its integral over the photon momentum, with allowance for the phase volume, remains divergent.

The slowly decreasing tail on the energy distribution is a result of an unsuccessful choice of the initial state  $\Phi_n$  and is not pertinent to the observable physical picture. This point can be seen best in the behavior of the nondecay amplitude  $A_{nn(t)}$ . We write

$$A_{nn}(t) = \sum_a |B_{\alpha n}|^2 e^{-iE_\alpha t} = \int dE \rho_n(E) e^{-iEt}.$$

It is clear from a comparison with (4) that we have  $\rho_n = \text{Im } G_{nn}$  for  $E > E_{\min}$ , where  $E_{\min}$  is the lowest energy of an intermediate state. The contribution to  $\rho_n$  is the sum of a possible pole corresponding to the ground state,  $E = E_{n0}$  and a cut from the intermediate states  $\Psi_a$  of the continuum. The pole contribution is of no interest. It is a consequence of the nonorthogonality of  $\Phi_n$  and  $\Psi_{n0}$ ; it must be removed through orthogonalization. A rotation of the contour makes it possible to break up the contribution from the cut into a contribution from poles on a second sheet, at the points  $E_p = W_p - i\Gamma_p/2$ , which correspond to the previous stable unperturbed levels, and one from cuts which run parallel to the negative imaginary axis away from the branch points. Some of these branch points coincide with these poles for the case of zero photon mass, and some stem from the boundaries of the continuum of the electrons and pairs (the points  $E = m, 2m + E_{nn}, 3m$  etc.; Fig. 1). The discontinuities in  $G_{nn}$  at the cuts which are associated with the complex poles at the points  $E_p$  fall off rapidly (as  $1/E^3$ ) in the limit  $E \rightarrow \infty$ .

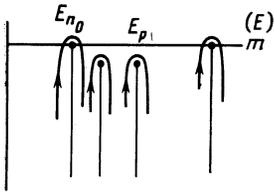


FIG. 1. Integration contour in the complex energy plane.

A slow decrease in  $\rho_n(E)$  is observed on cuts which run away from the boundaries of the electron continuum. One can verify, however, that in a description of the dynamics of unstable states the entire contribution from the cuts is devoid of physical meaning, as in standard decay theory in the nonrelativistic theory.<sup>5</sup> This contribution takes the form

$$\int_{E_0}^{\infty} dE \rho_n(E) e^{-iEt},$$

where  $\rho_n$  is a smooth function which contains the quantity  $E_0 \sim E_n$  as a dimensional parameter; i.e., we have  $\rho_n(E) = E^{-1} f(E/E_0)$ . Clearly, the contribution is a dimensionless function of  $E_0 t$ , which varies at times  $t \sim 1/E_0$  and approaches a power-law asymptotically for  $t \sim 1/E_0$ . The specific asymptotic form is determined by the behavior of  $\rho_n(E)$  at  $E = E_0$ ; for intermediate states with a single photon and a single electron, it is determined by the behavior of this function  $E_0: \rho_n \sim E - E_0$ . The contribution from the cut at  $t \gg 1/E_0$  is thus  $1/(E_0 t)^2$  in order of magnitude. For a large number of particles in the intermediate state the degree of the denominator is larger. If the imaginary part of the poles on the second sheet is  $\Gamma \ll E_0$  in order of magnitude, there exists a region of intermediate times  $t \sim 1/\Gamma \ll 1/E_0$  in which the contribution from the cuts is negligibly small in comparison with that from complex poles. The latter is  $\exp(-\Gamma t)$  in order of magnitude, while the contribution from the cuts in this region is found to be of order  $(\Gamma/E_0)^2$ . At times  $t \sim 1/\Gamma$  the contribution from the cuts can thus be ignored. If the condition  $\gamma \ll E_0$  does not hold, the contribution from the cuts will be comparable to that from the poles, and the behavior of the nonstationary state will depend strongly on the contribution from the cuts, i.e., on  $\rho_n$ . As we have seen, the specific choice of  $\rho_n$  reflects the behavior of the nonstationary state at times  $t \sim 1/E_0$ , i.e., the method by which the initial state is formed. Different methods for preparing the initial state will correspond to different forms of  $\rho_n$ . The contribution from the cuts thus tells us nothing about the dynamics of the quasistationary state; it simply reflects the details of the formation of this dynamics for the specific choice of  $\Phi_n$ .

We arrive at a description of the nonstationary state which is of the sort usually found in nonrelativistic quantum mechanics. An unstable particle is an approximate asymptotic entity, defined at small values of the imaginary parts  $\Gamma/2$  of the complex poles in the energy plane below the unitary cut to within corrections on the order of  $\Gamma/E_0$ , where  $E_0$  is the typical spacing between levels. All of the physical information is in these poles. From the time-evolution standpoint, the picture is this: Immediately after the initial state  $\Phi_0$  is specified at  $t = 0$ , this state begins to decay rapidly. By the time  $t \sim 1/m$ , all of the contributions from the slowly

decreasing energy distribution  $\rho_n(E)$  at  $E \gg m$  have died out. By  $t \sim 1/m$ , all of the contributions from the cuts, without exception, have died out. Thereafter, the decay amplitudes go into an exponential stage and exhibit a behavior  $\exp(-\Gamma t/2)$ , where  $\Gamma/2$  is a typical imaginary part of the poles. In this stage the amplitudes vary up to very large values of  $\Gamma t$ , at which nonexponential terms associated with the details of the formation come back into play. In this picture it becomes clear that the norm of  $\Phi_n$ , which is specified rigorously at  $t = 0$ , is not related to the unstable particle; it simply gives us a measure of the increment of extraneous states, which all die out by the beginning of the dynamics of the actual unstable particle. It might thus be a correct procedure to measure relative probabilities of the type  $|A_{an}(t_2)|^2 / |A_{an}(t_1)|^2$  under the assumption  $t_2 > t_1 \gg 1/E_0$ , i.e., under the assumption that both measurements are taken after all of the extraneous states have died out, and we are left with the actual unstable particle. One could also take the simpler approach of setting the time  $t_1$  equal to zero, after retaining in  $A_{an}(t)$  only those terms which arise because of the pole contribution to  $\Gamma_{an}(E)$ . The meaning here is that we extend the asymptotic behavior of the process at times  $t \sim 1/\Gamma$  smoothly into the region of smaller values of  $t$ . This is the approach we will take below. As a result, for the physical amplitudes  $A_{an}(t)$  we are left with our previous expression, (4), in which only the pole contribution  $\Gamma_{an}$  is retained. In the following sections of this paper we carry out specific studies of the amplitudes for nondecay and decay by a given mechanism.

### 3. NONDECAY AND DECAY PROBABILITIES OF NONDEGENERATE UNSTABLE STATES

The retention of only the pole contribution in the Green's function in (4) makes a calculation of transition probabilities in the QED of an atom essentially identical to the corresponding problem in nonrelativistic quantum mechanics.<sup>5</sup> The final expressions for the probabilities naturally turn out to be of the same nature. All the radiative corrections to the energy shift and the width and also to the vertex functions for transitions are taken into account in these expressions. In this sense the expressions are exact, not based on perturbation theory. We will go into more detail on the problem of diagonalizing the states and on the one- and two-photon decays of unstable atomic levels.

After renormalization in QED, the residues at the poles of Green's function  $G_{an}$  become finite. The one-electron Green's function  $G_{mn}(E)$  satisfies the Dyson matrix equation  $G = G_0 + G_0 \Sigma G$ , where  $(G_0)_{mn} = \delta_{mn} (\epsilon_n - E)^{-1}$ , and  $\Sigma_{mn}$  is the self-mass with the incorporated intermediate states of an electron for the continuing. Continuing this equation onto the second energy sheet below the cut, and taking the residue at the complex point  $E_n$ , we find that it has a structure

$$\text{Res}_{E=E_n} G_{kl}(E) = -\bar{f}_k^{(n)} \bar{f}_l^{(n)}, \quad (5)$$

where  $\bar{f}$  is found from  $f$  through time reversal, and  $f$  satisfies a quasipotential equation:

$$(\epsilon_k - E_n) f_k^{(n)} = \Sigma_{kl}(E_n) f_l^{(n)}. \quad (6)$$

From this we determine both  $f^{(n)}$  and  $E_n$ . Since  $\Sigma$  is not Hermitian and depends on  $E$ , the wave functions  $f^{(n)}$  for

different values of  $n$  are not orthogonal.

From this point on the calculations depend on the separations in energy between unstable states having identical quantum numbers. In this section of the paper we discuss the case in which there are no unstable states with identical quantum numbers and approximately equal energies. For one-electron states in an atom, this condition holds for all levels. For multielectron levels, on the other hand, the non-degeneracy condition may be violated.

In the nondegenerate case we are justified in assuming  $f^{(n)}$  to be real. At the cut,  $\text{Im}\Sigma$  is on the order of  $\Gamma$ , and  $\text{Im}\Sigma$  at the complex point  $E_n$  is of the same order of magnitude. It follows that the adjoint of Eq. (6) differs from Eq. (6) by terms on the order of  $\Gamma$ , and in terms of the nondegeneracy  $\text{Im}f$  is of order  $\Gamma$ . Since the overall accuracy of our analysis is limited specifically by terms of order  $\Gamma/E_0$ , we can ignore this imaginary part. From  $T$  invariance we have  $\Sigma_{kl} = \Sigma_{ik}$  and  $\bar{f}^{(n)} = f^{(n)}$ . It thus becomes possible to avoid the complex pole structure of the Green's function in an extremely simple way. We choose a system of real vectors  $g^{(n)} = \bar{f}^{(n)}$  which have the property  $\Sigma_k g_k^{(n)} f_k^{(m)} \equiv g^{(n)} f^{(m)} = \delta_{nm}$ . Multiplying the Green's function from the right by  $G^{(n)}$  and from the left by  $G^{(m)}$ , we can then diagonalize the matrix of residues: If  $G^{(mn)} = g_k^{(m)} G_{kl} g_i^{(n)}$ , then

$$\text{Res}_{E=E_n} G^{(mp)} = -\delta_{mp} \delta_{mn}. \quad (7)$$

As a result we find from (4) that in the pole approximation we have  $A_{mn}(0) = \sigma_{mn}$  so this part of the normalization has been carried out.

In the pole approximation the nondecay amplitude  $A_{nn}$  is  $A_{nn}(t) = \exp(-E_n t)$ ; from this expression we find the usual expression for the probability for the nondecay of level  $n$ :  $p_n(t) = \exp(-\Gamma t)$ .

We turn now to the amplitude for a decay by mechanism  $\alpha$ . The Green's function  $G_{\alpha n}$  for a state  $\alpha$  which contains a photon with momentum  $k$  and an electron in state  $m$  is found from the covariant Green's function by integrating over the relative energy  $\varepsilon$  of the final particles

$$G_{\alpha n}(E) = \int (d\varepsilon/2\pi i) G_{m\alpha}(E-\varepsilon) \Delta(k, \varepsilon) (\varepsilon + k_0) \cdot V_{m\alpha}^{(1)}(E-\varepsilon, E, k) G_{nn}(E). \quad (8)$$

Here  $V^{(1)}$  is the vertex part of the emission of a photon accompanied by the transition of an electron from state  $n$  to state  $m$ , and  $\Delta$  is the complete renormalized Green's function of the photon. We have not written out the Lorentzian indices explicitly. We are interested in only the pole part of  $G_{\alpha n}$ , which stems from collisions of pole singularities of the integrand in (8). Accordingly, only the diagonal parts of the electron Green's function have been retained in (8). Taking the residue at  $\varepsilon = k_0$ , we find

$$G_{\alpha n}(E) = (E_m + k_0 - E)^{-1} V_{m\alpha}^{(1)}(E - k_0, E, k) (E_n - E)^{-1}. \quad (9)$$

Substituting this expression into (4), we find

$$A_{\alpha n}(t) = (E_n - E_m - k_0)^{-1} [V_{m\alpha}^{(1)}(E_m, E_m + k_0, k) e^{-i t(E_m + k_0)} - V_{m\alpha}^{(1)}(E_n - k_0, E_n, k) e^{-i t E_n}]. \quad (10)$$

By virtue of the difference between the arguments of  $V^{(1)}$ , the

quantities  $A_{\alpha n}(0)$  are nonzero. The difference, however, is less than the accuracy with which the quasistationary states have been determined (on the order of  $\Gamma/E_0$ ).

Let us find the probability for a one-photon transition from level  $n$  to level  $m$ , which is equal to  $w_{mn}^{(1)}(t)$ . This probability is found by integrating the square of the absolute value of (10) over all the photon momenta  $k$ . We are interested only in the leading terms with respect to  $\Gamma/E_0$ . At this accuracy level we can ignore the difference in the arguments of the vertex parts of  $V^{(1)}$  in the two terms in (10). We can then write

$$w_{mn}^{(1)}(t) = \int (d^3k/2k_0) |V_{m\alpha}^{(1)}(E_n - k_0, E_n, k)|^2 |E_n - E_m - k_0|^{-2} \cdot |e^{-i t(E_m + k_0)} - e^{-i t E_n}|^2. \quad (11)$$

In the integration over  $k$  we can, to leading order in  $\Gamma/E_0$ , set  $k_0 = W_n - W_m$  in the smooth factors and extend the integration over  $k_0$  to the entire axis. Introducing a deviation from resonance,  $\varphi = W_m + k_0 - W_n$ , we find

$$w_{mn}^{(1)}(t) = \Gamma_{m\alpha}^{(1)} \pi^{-1} \int d\kappa f(\kappa), \quad (12)$$

where

$$f(\kappa) = \left\{ e^{-\Gamma_m t} + e^{-\Gamma_n t} - 2 \exp\left[-\frac{1}{2}(\Gamma_m + \Gamma_n)t\right] \cos \kappa t \right\} \cdot \left[ \kappa^2 + \frac{1}{4}(\Gamma_m - \Gamma_n)^2 \right]^{-1} \quad (13)$$

and

$$\Gamma_{m\alpha}^{(1)} = \int (d^3k/2k_0) 2\pi \delta(W_m + k_0 - W_n) |V_{m\alpha}^{(1)}|^2. \quad (14)$$

Integration over  $\varphi$  yields

$$w_{mn}^{(1)}(t) = \Gamma_{m\alpha}^{(1)} (e^{-\Gamma_m t} - e^{-\Gamma_n t}) (\Gamma_n - \Gamma_m)^{-1}. \quad (15)$$

It is not difficult to see that expression (15) is equivalent to the conservation of probability in the one-photon approximation. Let us assume that  $m$  is the ground state and that  $n$  is the closest excited state, so there are no cascade transitions through intermediate states. We then have  $\Gamma_m = 0$  and

$$w_{mn}^{(1)}(t) = (\Gamma_{m\alpha}^{(1)}/\Gamma_n) (1 - e^{-\Gamma_n t}). \quad (16)$$

This result will satisfy the probability conservation condition  $p_n + W_{mn}^1 = 1$  if  $\Gamma_{m\alpha}^{(1)} = \Gamma_n \equiv -2 \text{Im} E_n$ . We can show that this is the case. After diagonalization of the pole part of the Green's function, Eq. (6) becomes

$$Z_n(\bar{\varepsilon} - E_n) = \Sigma_{nn}(E_n), \quad (17)$$

where  $Z_n = f^{(n)} f^{(n)}$ ,  $Z_{n\bar{n}} = \Sigma_k \varepsilon_k f_k^{(n)} f_k^{(n)}$  and the renormalization condition  $Z_n = 1 - \Sigma_{n\bar{n}}(E_n)$  which follows from (6) holds. As we have seen, we can assume  $Z_n$  to be real. We then find  $Z_n \text{Im} E_n = -\text{Im} \Sigma_{nn}(E_n)$  from (17). Expanding the right side in terms of the small width, we find that the terms which are linear in the width cancel out the  $S'_{nn}(E_n)$ , so that  $G_n = 2 \text{Im} S_{nn}(W_n)$ . The right side of this expression is equal to  $G_{mn}^{(1)}$  according to (14) if we consider only intermediate states with a single photon and an electron in state  $m$ . Probability is thus conserved to within terms of order  $\Gamma/E_0$ .

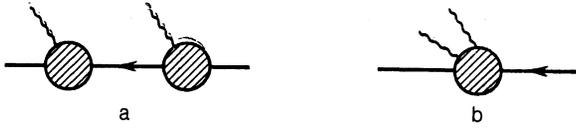


FIG. 2. Pole contributions to the Green's function from two-photon transitions.

We also consider two-photon transitions. In this case the final state  $\beta$  contains two photons, with momenta  $k_1$  and  $k_2$ , and an electron in state  $m$ . The corresponding Green's function  $\Gamma_{\beta n}$  will contain two types of pole terms, which correspond to the diagrams in Fig. 2. The part which comes from the intermediate electronic state  $p$  (Fig. 2a) has three poles:

$$G_{\beta n}^{(4)} = (E_m + k_{10} + k_{20} - E)^{-1} V_{mp}^{(4)}(k_2) (E_p + k_{10} - E)^{-1} \cdot V_{pn}^{(4)}(k_1) (E_n - E)^{-1}. \quad (18)$$

We are not specifying the electron energies on which the vertices  $V^{(i)}$  depend, since they are all on the mass shell to lowest order in the limit  $\Gamma \rightarrow 0$ . In addition to (18),  $G_{\beta n}$  contains a contribution from two poles from the one-particle-irreducible two-photon vertex  $V^{(2)}$ :

$$G_{\beta n}^{(2)} = (E_m + k_{10} + k_{20} - E)^{-1} V_{mn}^{(2)}(k_1, k_2) (E_n - E)^{-1}. \quad (19)$$

Substituting these expressions into (4), we find the time-dependent transition amplitudes  $A_{\beta n}(t)$ . The complete probabilities for two-photon transitions are found by integrating  $|A_{\beta n}|^2$  over the momenta of the two photons. The probability  $w_{mpn}^{(2)}$  takes the following form by virtue of (18):

$$w_{mpn}^{(2)}(t) = \Gamma_{mp}^{(4)} \Gamma_{pn}^{(4)} \pi^{-2} \int d\chi_1 d\chi_2 f(\chi_1, \chi_2), \quad (20)$$

where we have introduced the deviations from resonance  $\chi_1 = W_p + k_{10} - W_n$  and  $\chi_2 = W_m + k_{20} - W_p$ . The function  $f(\chi_1, \chi_2)$  is of the form

$$f(\chi_1, \chi_2) = e^{-\Gamma_m t} (\chi_2^2 + \xi_2^2)^{-1} (\chi_3^2 + \xi_3^2)^{-1} + e^{-\frac{1}{2}(\Gamma_n + \Gamma_p) t} 2 \operatorname{Re} e^{-i\chi_1 t} (\chi_1^2 + \xi_1^2)^{-1} (\chi_3 + i\xi_3)^{-1} (\chi_2 - i\xi_2)^{-1} + \text{cyclic permutations of (123)}. \quad (21)$$

Here the states  $mpn$  have been numbered in the order 132;  $\chi_3 = -\chi_1 - \chi_2$ ;  $\xi_1 = \frac{1}{2}(\Gamma_p - \Gamma_n)$  etc. Integration over  $\chi_1$  and  $\chi_2$  yields

$$w_{mpn}^{(2)}(t) = \Gamma_{mp}^{(4)} \Gamma_{pn}^{(4)} (e^{-\Gamma_m t} |\Gamma_m - \Gamma_n|^{-1} |\Gamma_m - \Gamma_p|^{-1} + e^{-\Gamma_n t} |\Gamma_n - \Gamma_m|^{-1} |\Gamma_n - \Gamma_p|^{-1} - e^{-\Gamma_p t} |\Gamma_p - \Gamma_n|^{-1} |\Gamma_p - \Gamma_m|^{-1}). \quad (22)$$

The rest of the two-photon transition probability comes from (19) and from the interference of contribution (18) with (19) and of (18) with the interchange of photons. This remaining part of the probability is similar in form to the one-photon decay probability (15), with the one-photon width  $\Gamma_{mn}^{(1)}$  being replaced by the two-photon width,  $\Gamma_{mn}^{(2)}$ . The latter quantity as  $1/i$  times the discontinuity in the self-mass  $\Sigma_{nn}$  at the cut made with intermediate states with two photons and with an electron in state  $m$ , from which the part corresponding to diagrams like Fig. 3 has been removed. It is not difficult to verify that expressions (15) and (22) satisfy the probability conservation condition when we note that the total width of state  $n$  is the sum of the one-photon and two-photon widths. The contribution  $w_{mpn}$  incorporates cascade transitions.

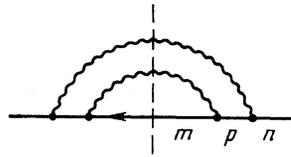


FIG. 3. The part of the self-mass of an electron corresponding to cascade transitions.

Let us examine the spectral lineshape. At a given observation time, this shape is specified by the quantity  $|A_{\alpha n}(t)|^2 = \text{const} f(\chi)$ , where  $f(\chi)$  is given by (13). For a given  $t$ , the line has a Breit-Wigner shape on which oscillations are superimposed. The frequency of these oscillations grows with time. They evidently stem from the determination of the decay probability over a finite time, i.e., from nonconservation of energy by an amount of order  $1/t$ . After a long time, the line acquires an exact Breit-Wigner shape. For two-photon cascade transitions, the lineshape at time  $t$  is described by the function  $f(\chi_1, \chi_2)$  in (21). After a long time we are left with only the first term for the stable state  $m$  in (21); as a result we find the familiar distribution.<sup>6</sup>

The formalism constructed here could be generalized without difficulty to the case in which an atom has several electrons. Let us consider the case of two electrons. As the initial state we now use

$$\Phi_n = \chi_n^{n_1 n_2} a_{n_1}^+(0) a_{n_2}^+(0) \Psi_0, \quad (23)$$

where  $n$  numbers the two-electron levels of the atom (the QED interaction is being ignored), and  $n_1$  and  $n_2$  are one-electron levels which have an identical total energy  $\varepsilon_n = \varepsilon_{n_1} + \varepsilon_{n_2}$ . Among the final states of the continuum,  $\Phi_\alpha$ , are states which differ from (23) by the addition of Heisenberg photon-creation operators. More-complex simultaneous Green's functions appear in the expressions for transition amplitudes  $A_{nn}$  and  $A_{\alpha n}$ . This change does not, however, alter either (a) the fundamental points associated with the possibility of renormalization, with the separation of the contribution of the pole terms, and with the limitation of the accuracy to quantities of order  $\Gamma/E_0$  or (b) the technical side of the description of the dynamics, which is reflected by the equations above, starting with (4). The only difference is that the Dyson equation for the one-electron Green's function is replaced by a corresponding quasipotential equation for a two-electron Green's function. From this equation we find, in place of (6),

$$(e_k - E_n) f_k^{(n)} = U_{ki}(E_n) f_i^{(n)}. \quad (24)$$

The properties of quasipotential  $U(E)$  do not differ from those of the self-mass of the electron, so all of the properties of  $f$  which were used above remain in force for the multielectron case if there is no degeneracy. The final expressions for the probabilities, (15) and (22), turn out to be the same. The conclusion regarding the spectral lineshape also remains in force.

#### 4. THE DEGENERATE CASE

We now consider the case, encountered in two- and multielectron atoms, in which two unstable states appear with identical quantum numbers and approximately equal energies,  $W_n \approx W_m$ . The degenerate case is analogous to the problem of  $K^0 \bar{K}^0$  transitions in elementary particle theory, with the distinction that in atomic theory we do not have the

approximate conservation of strangeness which considerably simplifies the analysis of the  $K^0\bar{K}^0$  system. On the other hand,  $T$  invariance holds very accurately in an atom.

At the formal level, difficulties in making a comparison with the earlier analysis arise because the mixing coefficients  $f$  become complex in the case of degenerate states, and it is not possible to transform to a new basis by multiplying by  $g$  vectors. Let us assume that all of the other states—all except the pair  $n, m$ —are nondegenerate. The pole part of the Green's function which corresponds to them can then be diagonalized as before, and all of the nondiagonal aspects of the poles are associated exclusively with the pair of degenerate states. We assign these states the indices 1 and 2. The mixing coefficients  $f^{(1,2)}$  satisfy the quasipotential equation (24); the degeneracy means  $E_1 - E_2 \sim \Gamma$ . The quasipotential  $U$  in a real atom depends weakly on the energy because of retardation. The main, and energy-independent, real part of  $U$  can be diagonalized by a standard unitary transformation. We assume that the energy shifts found in this manner are incorporated in the seed energies  $\varepsilon_k$ , so  $U$  in (24) refers to only that part of the quasipotential which depends strongly on the energy. We then have  $U_{kl} \sim G$  in order of magnitude, and we find from (24) that two unperturbed levels should approximately coincide. Denoting them as levels 1 and 2, we have  $e_1 - e_2 \sim G$ . It is thus clear that (24) is dominated by  $k, l, = 1, 2$  and that  $f_k^{(1,2)}$  for  $k \neq 1, 2$  are of order  $\Gamma/E_0$ . We will ignore them. We also note that to the same accuracy we can ignore the difference  $E_1 - E_2$  in the argument of  $U$ . As a result, the two-dimensional vectors  $f_k^{(1,2)}$  are found to be eigenvectors of the same non-Hermitian Hamiltonian:

$$H_{kl} f_l^{(1,2)} = (\varepsilon_k \delta_{kl} + U_{kl}) f_l^{(1,2)} = E_{1,2} f_k^{(1,2)}. \quad (25)$$

Here  $U_{kl} = U_{kl}(E_{1,2})$  and  $k, l = 1, 2$ . From  $T$  invariance we find  $U_{kl} = U_{kl}$ . Expression (25) then leads to the orthogonality of  $f^{(1)}$  and  $f^{(2)}$  in a symmetric metric (without conjugation):  $\sum_k f_k^{(1)} f_k^{(2)} = 0$ . Normalizing  $f$  to 1 in this metric, we find orthonormality and completeness relations:

$$\sum_k f_k^{(m)} f_k^{(n)} = \delta_{mn}; \quad \sum_n f_i^{(n)} f_k^{(n)} = \delta_{ik}; \quad i, k, m, n = 1, 2. \quad (26)$$

The pole part of the Green's function  $G_{ik}$ , which corresponds to states 1 and 2, can be written

$$G_{ik} = \sum_n f_i^{(n)} f_k^{(n)} (E_n - E)^{-1} = [(H - E)^{-1}]_{ik}. \quad (27)$$

According to (4), the nondecay amplitude can be written  $A_{ik}(t) = (e^{-iHt})_{ik}$ .

Let us analyze the nondecay and decay probabilities. In the degenerate case there is no possibility of a separate determination of any specific 1 or 2 at a finite time, since a time  $t \sim (W_1 - W_2)^{-1} \sim 1/\Gamma$  is required. The only question that can be asked is that of the probability for observing either of states 1 and 2. With regard to the initial state, we specify it by means of the density matrix  $\rho$ , which describes the distribution among states 1 and 2:  $\text{tr} \rho = 1$ ,  $\rho^+ = \rho$ . The nondecay probability can then be written

$$p(t) = \sum_{i,k,l} A_{ik}(t) \rho_{kl} A_{li}^*(t). \quad (28)$$

Using representation (27), we find

$$p(t) = \sum_{i,k,l,m,n} f_i^{(m)} f_k^{(m)} f_l^{(n)*} f_l^{(n)*} \rho_{kl} \exp[-it(E_m - E_n^*)]. \quad (29)$$

We introduce the matrices  $t^{(mn)} = f^{(m)} f^{(n)*}$  and  $\rho^{(mn)} = f^{(m)} \rho f^{(n)*}$ . From (26) we find  $\frac{1}{2} \text{tr}(t t^T) = \text{tr}(\rho t^T) = 1$ . For brevity we use the notation  $t^{(nn)} = t^{(nn)}$ ,  $\rho^{(n)} = \rho^{(nn)}$ ,  $t^{(0)} = t^{(12)} = t^{(21)*}$ ,  $\rho^{(0)} = \rho^{(12)} = \rho^{(21)*}$ ,  $\Gamma = \frac{1}{2}(\Gamma_1 + \Gamma_2)$ ,  $\Delta = W_1 - W_2$ . From (29) we find

$$p(t) = t^{(1)} \rho^{(1)} e^{-\Gamma_1 t} + t^{(2)} \rho^{(2)} e^{-\Gamma_2 t} + e^{-\Gamma t} 2 \text{Re} t^{(0)} \rho^{(0)} e^{-i\Delta t} \quad (30)$$

The quantities  $T^{(n)}$  can be expressed in terms of the parameters of Hamiltonian  $H$  (Ref. 7). In the case of  $T$  invariance, these quantities can be expressed in terms of the single complex parameter

$$\delta = (\Gamma_1 - \Gamma_2 + 2iH_{12}) / i(H_{11} - H_{22}).$$

Solutions of Eq. (25) are written in the form

$$f_1^{(1)} = f_2^{(2)} = (1 + \delta) / [2(1 + \delta^2)]^{1/2}, \\ f_1^{(2)} = -f_2^{(1)} = (1 - \delta) / [2(1 + \delta^2)]^{1/2}, \quad (31)$$

from which we find

$$t^{(1)} = t^{(2)} = (1 + |\delta|^2) / |1 + \delta^2|, \quad t^{(0)} = 2i \text{Im} \delta / |1 + \delta^2|. \quad (32)$$

According to (30), the nondecay probability  $p(t)$  contains oscillations at a frequency  $\Delta$  which are well known in  $K^0\bar{K}^0$  decay theory. The phase of the oscillations depends on  $\rho$ , i.e., on the method by which the initial state is specified. We will discuss the most characteristic choices of  $\rho$  after we examine the decay probability.

Let us consider a one-photon transition from states 1 and 2 to the nondegenerate state 3. The transition probability is

$$w(t) = \sum_{i,k} A_{\alpha i}(t) \rho_{ik} A_{\alpha k}^*(t). \quad (33)$$

The amplitudes  $A_{\alpha i}$ , for a transition to a state  $\alpha$  which contains a photon with a momentum  $k$  and electrons in state 3, are found in the usual way. These amplitudes differ from (10) in that the energy  $E_n$  is replaced by the operator  $H$ . Using representation (27), we find

$$w(t) = \sum_{n=1,2} \rho^{(n)} |V^{(n)}|^2 a^{(n)}(t, \kappa) + 2 \text{Re} \rho^{(0)} V^{(1)} V^{(2)*} a^{(0)}(t, \kappa). \quad (34)$$

Here

$$a^{(n)} = \{ e^{-\Gamma_3 t} + e^{-\Gamma t} - 2e^{-1/2(\Gamma_3 + \Gamma_1)t} \cos[t(\kappa + \Delta_n)] \} \\ \cdot \left[ (\kappa + \Delta_n)^2 + \frac{1}{4}(\Gamma_3 - \Gamma_1)^2 \right]^{-1}, \\ a^{(0)} = [ e^{-\Gamma_3 t} + e^{-\Gamma t} e^{-i\Delta t} - e^{-1/2(\Gamma_3 + \Gamma_1)t} e^{i\kappa t} - e^{-1/2(\Gamma_3 + \Gamma_2)t} e^{-i(\kappa + \Delta)t} ] \\ \cdot \left[ \kappa + \frac{i}{2}(\Gamma_1 - \Gamma_3) \right]^{-1} \left[ \kappa + \Delta - \frac{i}{2}(\Gamma_2 - \Gamma_3) \right]^{-1}. \quad (35)$$

We have introduced a deviation  $\kappa = W_3 + k_0 - W_1$ , and we have  $\Delta_1 = 0$  and  $\Delta_2 = \Delta$ . Here we also have  $V^{(n)} = \sum_k f_k^{(n)} \times V_{3k}$  where  $V_{3k}$  is the matrix element for a transition involving the emission of a photon from basis level  $k = 1, 2$  to level 3. In the integration over the photon momentum, we set  $\kappa = 0$  in the slowly varying factors. After integrating  $k$  over

angle, we obtain the quantities  $I^{(n)} = I^{(nn)}$  and  $I^{(0)} = I^{(12)}$ , where

$$I^{(mn)} = \int (d^3k/2k_0) \pi \delta(W_3 + k_0 - W_1) V^{(m)} V^{(n)*}; \quad (36)$$

Here  $I^{(mn)}$  are related to the contribution of  $I$  to the imaginary part of  $H$  due to transitions to state 3 by the relation  $I^{(mn)} = f^{(m)} I^{(n)*}$ . If 3 is the ground state, and there are no other transitions,  $I$  is the imaginary part of  $H$ . Using Eq. (25), we can express  $I^{(n)}$  in terms of  $t^{(n)}$  in this case:

$$2I^{(n)} = \Gamma_n t, \quad n=1,2; \quad 2I^{(0)} = (\Gamma + i\Delta) t^{(0)}. \quad (37)$$

If state 3 is not a unique final state in transitions from 1 and 2, Eqs. (37) continue to hold if we substitute into them the partial widths and shifts of levels which arise because of intermediate state 3 in the quasipotential.

After integration over photon emission angles, the decay probability (34) takes the form  $w = \pi^{-1} \int d\kappa f(\kappa)$ , where

$$f(\kappa) = \sum_{n=1,2} \rho^{(n)} I^{(n)} a^{(n)}(t, \kappa) + 2 \operatorname{Re} \rho^{(0)} I^{(0)} a^{(0)}(t, \kappa) \quad (38)$$

and the quantities  $a^{(n)}$  are given by (35). Integration over  $\kappa$  yields the total transition probability:

$$w(t) = \sum_{n=1,2} \rho^{(n)} I^{(n)} (e^{-\Gamma_n t} - e^{-\Gamma_n t}) (\Gamma_n - \Gamma_3)^{-1} + 2 \operatorname{Re} \rho^{(0)} I^{(0)} (e^{-\Gamma_3 t} - e^{-\Gamma t} e^{-i\Delta t}) (\Gamma - \Gamma_3 + i\Delta)^{-1}. \quad (39)$$

If 3 is the ground state, and there are no other decay channels, then we have  $\Gamma_3 = 0$ ; using (37), we find

$$w(t) = \sum_{n=1,2} t^{(n)} \rho^{(n)} (1 - e^{-\Gamma_n t}) + 2 \operatorname{Re} t^{(0)} \rho^{(0)} (1 - e^{-\Gamma t} e^{-i\Delta t}). \quad (40)$$

Comparing this result with expression (30) for the nondecay probability, we find  $p(t) + w(t) = 1$ ; i.e., we find that the probability is conserved at each time.

The shape of the spectral line is extremely complicated at finite times [expression (38) for  $f(\kappa)$ ]. In the limit  $t \rightarrow \infty$  we find, assuming that level 3 is the ground level and using (37),

$$f(\kappa) = -\operatorname{Im} \left( \frac{t^{(1)} \rho^{(1)} + t^{(0)} \rho^{(0)}}{\kappa + i\Gamma_1/2} + \frac{t^{(2)} \rho^{(2)} + t^{(0)*} \rho^{(0)*}}{\kappa + \Delta + i\Gamma_2/2} \right). \quad (41)$$

The  $\kappa$  distribution depends on how the initial state is specified. We can imagine two basic versions: a purely statistical version, in which the initial state contains an equilibrium mixture of states 1 and 2, and a coherent version, in which the initial state is formed as the result of a specific quantum-mechanical interaction.

In the statistical version we have  $\rho_{ik} = (1/2)$  and thus  $\rho^{(n)} = (1/2) t^{(n)}$ . The numerators in (41) are identical and equal to  $1/2$ , so we have

$$f(\kappa) = -\frac{1}{2} \operatorname{Im} \{ (\kappa + i\Gamma_1/2)^{-1} + (\kappa + \Delta + i\Gamma_2/2)^{-1} \}. \quad (42)$$

In this case the lineshape is thus the mean of two Breit-Wigner distributions. The nondecay probability becomes

$$p(t) = \frac{1}{2} (t^{(1)})^2 (e^{-\Gamma_1 t} + e^{-\Gamma_2 t} - 2ae^{-\Gamma t} \cos \Delta t), \quad (43)$$

where

$$a = |(t^{(0)})^2| / (t^{(1)})^2 > 0.$$

In the coherent version we can imagine the formation of unstable states, e.g., intermediate states in the Compton effect involving the atom and ground state 3. The matrix is then proportional to the product  $V_{3i}^* V_{3k}$ , where  $V_{3i}$  is the operator (which we introduced above) which represents the emission of a photon accompanied by a transition of the atom from states  $i = 1, 2$  to the ground state. Integration of this product over the photon emission angles gives us a common factor which preserves the factorization with respect to indices  $i$  and  $k$ ; on the other hand, this integration gives us the imaginary part  $I_{ik}$  of Hamiltonian  $H_{ik}$  near the resonance (if, as we are assuming, there are no other mechanisms for the decay of states 1 and 2). In this case we thus have  $\rho_{ik} = c I_{ik}$ , where  $c$  is a constant; furthermore, we have  $\det I = 0$ . The latter condition is a consequence of our assumption that the decay mechanism is unique. This condition relates the parameter  $\delta$  to the masses and widths of states 1 and 2:

$$(t^{(0)})^2 = -\Gamma_1 \Gamma_2 / |E_1 - E_2|^2. \quad (44)$$

The constant  $c$  is determined by the condition  $\operatorname{tr} \rho = 1$  and is equal to  $1/\Gamma$ . We thus find the following result for the distribution  $f(\kappa)$

$$f(\kappa) = -\frac{1}{4} \operatorname{Im} \{ \Gamma_1 (1 - i\Gamma_2 (E_1 - E_2)^{-1}) (\kappa + i\Gamma_1/2)^{-1} + \Gamma_2 (1 + i\Gamma_1 (E_1 - E_2)^{-1}) (\kappa + \Delta + i\Gamma_2/2)^{-1} \}. \quad (45)$$

The residues at the poles have acquired imaginary parts, so the distribution is more complicated than simply the sum of two Breit-Wigner distributions. One can verify that (45) corresponds precisely to the scattering amplitude in a given mechanism in the presence of two complex energy poles, when the unitarity condition is taken into account. From unitarity we find

$$S(E) = \prod_n (W_n + i\Gamma_n/2 - E) (W_n - i\Gamma_n/2 - E)^{-1}$$

(the product is over all the poles). For the amplitude we thus find an expression which is the same as (45), to within a coefficient. The nondecay probability in the coherent version is expressed unambiguously in terms of the masses and widths of the unstable states:

$$p(t) = \frac{1}{2} c (t^{(1)})^2 [\Gamma_1 e^{-\Gamma_1 t} + \Gamma_2 e^{-\Gamma_2 t} - 2\Gamma_1 \Gamma_2 (\Delta^2 + \Gamma^2)^{-1/2} e^{-\Gamma t} \cos(\Delta t + \varphi)]. \quad (46)$$

Here  $(t^{(1)})^2 = (\Delta^2 + \Gamma^2) / |E_1 - E_2|^2$ . The phase shift is  $\varphi = -\tan^{-1} \Delta/\Gamma$ .

## 5. CONCLUSION

We have found that all properties of the unstable states can be determined from the renormalized quasipotential equation (6) or (24). The probabilities for decay by various mechanisms are determined in the usual way, in terms of vertex parts which are constructed in standard  $S$ -matrix theory with energy conservation. The indefiniteness regarding the specification of the energy of an unstable state and the complex nature of the corresponding pole in terms of the energy do not affect the magnitude of the probability, since

they are at the same level as the corrections which are discarded in defining the concept of an unstable particle and in establishing probability conservation.

These considerations seriously restrict the possibility of refining the transition vertices for relativistic electrons in an atom. If there are no special rules which forbid certain events in a strong field, the width is on the order of  $\alpha(Z\alpha)^4$ , and the distance between levels turns out to be of order  $(Z\alpha)^2$  (in units of the mass of an electron). The error in the determination of the dynamics of a nonstationary level is thus on the order of  $\alpha(Z\alpha)^2$ . We thus see that it would be meaningful to refine the transition vertex for allowed transitions only in the case  $(Z\alpha)^2 \ll 1$ . At large values of  $Z$  the refinement would go beyond the overall accuracy of the analysis and would be pointless.

## APPENDIX

Let us consider the simplest of the diagrams for an  $S$  matrix in the semi-infinite time integral  $[0, \infty]$  with self-mass insertions, as shown in Fig. 4. These are the diagrams which were analyzed in Ref. 2 for the purpose of extracting the Lamb shift of an initial or final level. For simplicity we restrict the discussion to intermediate state  $C$  which coincides with state  $A$  (as in Ref. 2). It is convenient to use a mixed representation in which the states of an electron are specified by its quantum numbers in the Coulomb nuclear field, and the time is retained. We then find the contribution

$$M_{BA} = iV_{BA}^{(1)}(k) \int_0^\infty dt_1 dt_2 dt_3 e^{it_1(\epsilon_B + k_0) - it_3 \epsilon_A} s_B(t_1 - t_2) \Sigma_A(t_2 - t_3).$$

Here  $s_B(t) = i\theta(t)e^{-i\epsilon Bt}$  is the propagator of an electron in state  $B$  with a positive energy,  $V_{BA}^1$  is the radiation operator in lowest order, and  $\Sigma_A(t)$  is the (unrenormalized) self-mass for state  $A$ . Writing it as a Fourier integral of the usual self-mass  $\Sigma_A(E)$  in the energy representation, we find

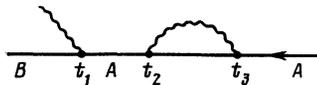


FIG. 4.

$$M_{BA} = iV_{BA}^{(1)}(k) (\kappa + i0)^{-1} \cdot \int \frac{dE}{2\pi} \Sigma_A(E) (E - \epsilon_A + i0)^{-1} (\epsilon_A + \kappa - E + i0)^{-1},$$

where  $\kappa$  is the deviation from resonance:  $\kappa = \epsilon_B + k_0 - \epsilon_A$ . In Ref. 2 the quantity  $\Sigma_A(E)$  was taken out from under the integral sign at the point  $E = E_A$ ; in that case, it is true that no difficulties were seen. Actually, however, an attempt to renormalize  $\Sigma_A$  runs into complications in connection with the convergence of the integral at large values of  $E$ . These complications are a manifestation of the surface infinities which we mentioned earlier. We see that renormalization of the mass does not run into any difficulties, but in renormalization of the wave function requires us to subtract from the regularized unrenormalized  $\Sigma_A$  terms which are linear in  $E$  and which contribute infinities to the integral. As a consequence, the renormalized self-mass  $\Sigma_A^{\text{ren}}$  varies as  $E \ln E$  in the limit  $E \rightarrow \infty$ , and the integral diverges. Some even more unpleasant infinities of this type are observed in renormalization of the photon wave function in connection with the vacuum polarization.

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