Natural spectral line width and shape in the relativistic theory of the atom

L. N. Labzovskiĭ

A. A. Zhdanov Leningrad State University
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A relativistic theory of the spectral line shape is developed that is a generalization of the well-known results for one-electron atoms. The theory is based on the Gell-Mann and Low formalism for the evolution operator. The familiar Lorentz contour is obtained in the resonance approximation by taking into account the self-energy corrections to the electron line of the initial state to the emission diagram for a single photon. It is shown that diagrams with self-energy corrections to the final state electron lines make contributions to the probability only if the width of the final state vanishes. To obtain the probability formula in the case of a decay final state, the specific decay channels of the latter must be taken into account (e.g., the single-quantum decay channel) and the emission diagram for two photons must be considered. In this diagram, it is necessary to take into account the electron self-energy corrections to the inner electron line. Then integration over the frequency of one of the photons leads to a Lorentz contour with a width equal to the sum of the single-quantum widths of the initial and final states. In the case of two-electron atoms, in addition to the self-energy corrections to the electron lines, it is necessary to take into account ladder corrections that describe the electron interaction. This yields the frequency shift due to the interaction.

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1. INTRODUCTION

The problem of the natural width and shape of the spectral lines corresponding to transitions between the levels of a nonrelativistic atom[1)] has been solved, as is well known, in general terms with the use of quantum mechanics.[1] One can thus obtain the Lorentz shape of the spectral lines, for example. A rigorous theory of the shape of spectral lines can be developed, however, only on the basis of quantum electrodynamics. Such a theory has been constructed by Low[2] for the one-electron atom.

In quantum electrodynamics, in contrast to quantum mechanics, the transition from the one-electron atom to the many-electron atom is not trivial and requires special methods. Therefore, the problem of the shape of spectral lines in the case of a relativistic atom with several electrons must be looked at a new. This is especially important for the study of the spectra of multiply charged ions, which has important practical applications (diagnostics of high-temperature plasma). Multiply charged ions constitute a very clearly expressed case of the relativistic atom since, in view of the small screening, the effective charge of the nucleus in them $Z_e \approx Z$ (Z is the actual charge of the nucleus) and at sufficiently large values of Z, all the electrons become relativistic.

In the present work, the problem considered above is solved with the help of the adiabatic formalism of Gell-Mann and Low.[3] This formalism turns out to be extremely useful for the construction of the perturbation theory in nonrelativistic quantum mechanics.[4] In the relativistic theory of the atom it is used for the calculation of the level shift under the action of the interelectron interaction and for the calculation of the width of the levels.[5,6] At the present time, there is an extensive literature on the application of this formalism both in nonrelativistic and in relativistic theories of the atom.

In Sec. 2 of the present paper, the basic premises of the adiabatic approach are formulated. In Sec. 3, the expressions obtained previously for the natural single-quantum width of the level of a relativistic atom are put down. Equations for the contour of the line of a single-quantum transition in a one-electron atom are obtained in Secs. 4–6 with the help of the adiabatic method. Finally, in Sec. 7, on the basis of calculations carried out in the previous sections, an expression is obtained for the contour of the line of the single-quantum transition in a two-electron relativistic atom.

2. ADIABATIC FORMALISM

We shall consider the multi-electron atom as a set of electrons interacting with one another through the electromagnetic field and moving in the Coulomb field of the nucleus (the Furry picture). The Hamiltonian of the atom in the second-quantization representation has the form

$$\hat{H}=\hat{H}_0+\hat{H}_{int}, \tag{1}$$

where $\hat{H}_0$ corresponds to the noninteracting electrons and $\hat{H}_{\text{int}}$ is the interaction with the electromagnetic field. In the zeroth approximation, the energy of the N-electron atom is equal to

$$E^{(0)}=\sum_{i=1}^{N}\varepsilon_i, \tag{2}$$

where ε_i are the one-electron energies, determined by the Dirac equation

$$\hat{h}(\mathbf{x})\varphi_i(\mathbf{x})=\varepsilon_i\varphi_i(\mathbf{x}), \tag{3}$$

$$\hat{h}(\mathbf{x})=\boldsymbol{\alpha}\hat{\mathbf{p}}+\beta-eU(\mathbf{x}). \tag{4}$$

In (4), α and β are Dirac matrices, $U(\mathbf{x})$ is the Coulomb potential of the nucleus, $p\equiv i\nabla$. We use the relativistic units $\hbar=c=m=1$.

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For the calculation of the shift in the energy level under the effect of interaction of the electrons, we can use the equation of Gell-Mann and Low,[3] for which there are several equivalent representations:

$$\Delta E=\lim_{\lambda\to 0}{}^{1}/_{2}\, i\lambda e\langle\Phi^0|\hat{S}_\lambda(\infty,-\infty)|\Phi^0\rangle^{-1}\frac{\partial}{\partial e}\langle\Phi^0|\hat{S}_\lambda(\infty,-\infty)|\Phi^0\rangle$$

$$=\lim_{\lambda\to 0} i\lambda e\langle\Phi^0|\hat{S}_\lambda(0,-\infty)|\Phi^0\rangle^{-1}\langle\Phi^0|\hat{S}_\lambda(\infty,0)\frac{\partial}{\partial e}\hat{S}_\lambda(0,-\infty)|\Phi^0\rangle$$

$$=\lim_{\lambda\to 0} i\lambda e\langle\Phi^0|\hat{S}_\lambda(\infty,0)|\Phi^0\rangle^{-1}\langle\Phi^0|$$

$$\times\left(\frac{\partial}{\partial e}\hat{S}_\lambda(\infty,0)\right)\hat{S}_\lambda(0,-\infty)|\Phi^0\rangle. \qquad (5)$$

Here $\hat{S}_\lambda(t,t')$ is the adiabatic evolution operator determined by perturbation theory:

$$\hat{S}_\lambda(t,t')=1+\sum_{n=1}^{\infty}S_\lambda^{(n)}(t,t'), \qquad (6)$$

$$\hat{S}_\lambda^{(n)}(t,t')=(i)^n e^n\int_{t'}^{t}\hat{H}_{\rm int}(t_1)e^{-\lambda|t_1|}dt_1,\ldots,\int_{t'}^{t_{n-1}}\hat{H}_{\rm int}(t_n)e^{-\lambda|t_n|}dt_n, \qquad (7)$$

$\hat{H}_{\rm int}(t)$ is the operator $\hat{H}_{\rm int}$ in the interaction representation, Φ^0 is the wave function of the atom in the zeroth approximation, λ is the parameter of adiabatic turning-on of the interaction. Equations (5) are applicable both for nondegenerate states and also for those degenerate states in which the correct linear combinations of the wave functions of zeroth approximation are determined by symmetry conditions (in real systems—atoms, multiply charged ions—such states are in the majority).

In some cases, a much simpler formula is obtained for the level shift. If the considered matrix element of the $\hat{S}_\lambda$ operator is such that the initial state Φ^0 is not encountered as an intermediate state, we shall call it irreducible. The contribution to the energy shift from the sum of irreducible matrix elements in nth order perturbation theory is equal to[7]

$$\Delta E_{\rm II}{}^{n}=\lim_{\lambda\to 0}{}^{1}/_{2}\, i\lambda n\langle\Phi^0|S_\lambda^{(n)}(\infty,-\infty)\Phi^0\rangle_{\rm II}=\lim_{\lambda\to 0} i\lambda n$$

$$\times\langle\Phi^0|S_\lambda^{(n)}(0,-\infty)|\Phi^0\rangle_{\rm irr}=\lim_{\lambda\to 0} i\lambda n\langle\Phi^0|S_\lambda^{(n)}(\infty,0)|\Phi^0\rangle_{\rm irr}, \qquad (8)$$

where the subscript "irr" of the matrix elements indicates their irreducibility.

3. NATURAL WIDTH OF THE LEVELS

For the calculation of the corrections of different orders by Eqs. (5) and (8), we can use the usual Feynman diagram technique in all the Furry representation. The electrons are pictured in the diagrams by solid vertical lines, with the initial state at the bottom. The photons are pictured by wavy lines. The external electron lines of the diagram correspond to the wave functions $\varphi_A(x)=\varphi_A(\mathbf{x})\exp(-i\varepsilon_A t)$, where $\varphi_A(\mathbf{x})$, $\varepsilon_A(x\equiv\mathbf{x},it)$ are determined by Eq. (3). The internal electron lines correspond to the propagator[2]

$$S(x_1x_2)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}d\omega\exp i\omega(t_1-t_2)\sum_n\frac{\varphi_n(\mathbf{x}_1)\bar{\varphi}_n(\mathbf{x}_2)}{\varepsilon_n(1-i0)+\omega}, \qquad (9)$$

where $\bar{\varphi}_n$ is the Dirac conjugate to the function φ_n. The external photon lines correspond to the potentials

$$A^{(k,s)}(x)=\left(\frac{2\pi}{\omega}\right)^{1/2}e_\nu^{(s)}\exp[i(\mathbf{kx}-\omega t)]$$

in the case of absorption of a quantum, and to $(A_\nu^{(k,s)}(x))^*$ in the case of emission; $e_\nu^{(s)}$ ($\nu=0,1,2,3$) is the polarization vector. Internal photon lines in the Feynman gauge correspond to the propagator[8]

$$D_{\mu\nu}(x_1x_2)=\frac{1}{2\pi i}\frac{\delta_{\mu\nu}}{r_{12}}\int_{-\infty}^{\infty}d\omega\exp[i\omega(t_1-t_2)+i|\omega|r_{12}], \qquad (10a)$$

where $r_{12}\equiv|\mathbf{x}_1-\mathbf{x}_2|$. It is convenient to use such a gauge for the photon lines that begin and end on the same electron line. In the case of photon lines that begin and end on different electron lines, it is expedient to distinguish between Coulomb and transverse photons. This can be done, since the each photon line is independently gauge invariant. The Coulomb photons (Coulomb interaction) is shown in the diagram by dashed lines. The internal Coulomb and transverse photon lines correspond to the propagators[7]

$$D_{\mu\nu}{}^{c}(x_1x_2)=-ir_{12}{}^{-1}\delta(t_1-t_2)\delta_{\mu 4}\delta_{\nu 4}, \qquad (10b)$$

$$D_{\mu\nu}{}^{t}(x_1x_2)=\frac{1}{2\pi i}\left\{\frac{\delta_{\mu\nu}}{r_{12}}\int_{-\infty}^{\infty}d\omega\exp[i\omega(t_1-t_2)+i|\omega|r_{12}]\right.$$

$$\left.-\nabla_{1\mu}\nabla_{2\nu}\frac{1}{r_{12}{}^{3}}\int_{-\infty}^{\infty}\exp i\omega(t_1-t_2)(\exp[i|\omega|r_{12}]-1)\frac{d\omega}{\omega^2}\right\}$$

$$\times(1-\delta_{\mu 4})(1-\delta_{\nu 4}). \qquad (10c)$$

The vertices of the diagrams correspond to the factors $\gamma_\nu\exp(-\lambda|t|)$, where γ_ν are the Dirac matrices. Finally, the factor $(-1)^n e^n$ is set in correspondence to the entire diagram.

We first consider a one-electron atom. In lowest order in the coupling constant, the imaginary increments to the energy appear first in the self-energy diagram of the electron (diagram 1). These increments yield the single-quantum radiation width connected with the emission of a single photon. Diagram 1 is irreducible, and we can use Eq. (8) for the calculation of the level shift. Substituting the expressions for the propagators (9) and (10a) in the matrix element, integrating over the times and calculating the limit $\lambda\to 0$ in (8), we obtain for the level shift of an atom in the state φ_A

$$\Delta E_A=\frac{e^2}{2\pi i}\sum_n\left(\frac{1-\alpha_1\alpha_2}{r_{12}}I_{nA}(r_{12})\right)_{AnnA}\equiv\delta E_A-\frac{i}{2}\Gamma_A, \qquad (11)$$

where

$$I_{nA}(r_{12})=\int_{-\infty}^{\infty}\frac{\exp(i|\omega|r_{12})d\omega}{\varepsilon_n(1-i0)-\varepsilon_A-\omega}, \qquad (12)$$

$\alpha_{1,2}$ are the Dirac matrices acting on the various one-electron wave functions. The real part of Eq. (11), δE_A, diverges and is subject to regularization. In the case of a relativistic atom, the regularized quantity $\delta_A E_A$ (the Lamb shift) was calculated in Refs. 9 and 10. The imaginary part of the shift (11), which determines the single-quantum radiative width of the level, is finite and, after calculation of the integral (12),

reduces to the expression

$$\Gamma_A=-\alpha\sum_n\theta(\varepsilon_n)\theta(\beta_{nA})\left(\frac{1-\alpha_1\alpha_2}{r_{12}}\sin(\beta_{nA}r_{12})\right)_{AnnA}, \quad (13)$$

where $\beta_{nA}=\varepsilon_A-\varepsilon_n$, $\theta(x)$ is the Heaviside step function. In the nonrelativistic limit at $\alpha Z\ll 1$, the usual expression for the single-quantum level width of a hydrogen-like atom follows from (13).

4. SINGLE-QUANTUM TRANSITION: RADIATIVE SHIFT AND WIDTH OF THE UPPER LEVEL

The amplitude of the single-quantum transition from level A to level B is determined in the lowest order in the coupling constant by diagram 2. In this case, when we are speaking of the decay of a quasistationary state, it is natural to use the evolution operator $\hat{S}_\lambda(\infty,0)$, assuming that the state is produced at the time $t=0$. The transition amplitude, calculated from the correspondence rules set forth in Sec. 3, is then equal to

$$\langle\Phi_B^0|S_\lambda^{(1)}(\infty,0)|\Phi_A^0\rangle=U_{BA}/(\varepsilon_A-\varepsilon_B-\omega_{\rm ph}-i\lambda), \quad (14)$$

$$U_{BA}=e\left(\frac{2\pi}{\omega}\right)^{1/2}[(\alpha\mathbf{e}^*)\exp(-i\mathbf{k}_{\rm ph}\mathbf{x})]_{BA} \quad (15)$$

where $|\mathbf{k}_{\rm ph}|=\omega_{\rm ph}$; $\omega_{\rm ph}$ is the frequency of the emitted quantum.

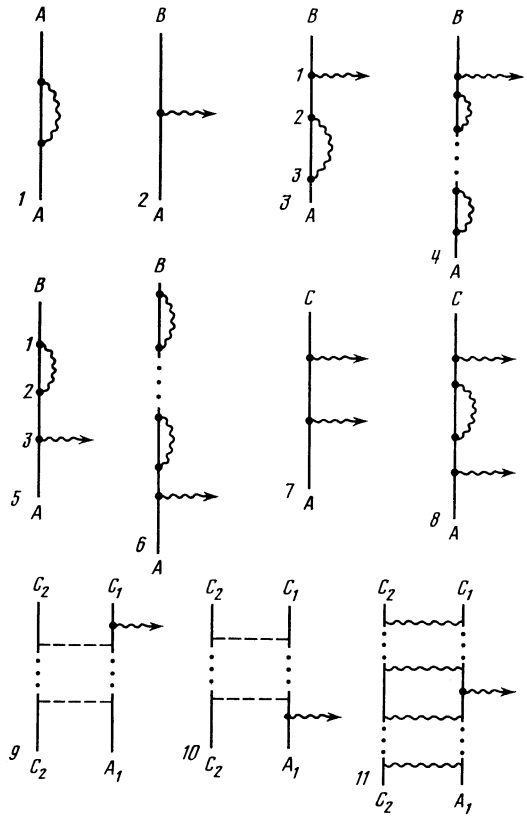
We now consider diagram 3 of the third order in the coupling constant. Substitution of the propagators [(9) and (10a)] lead to the equation

$$\langle\Phi_B^0|S_\lambda^{(3)}(\infty,0)|\Phi_A^0\rangle=\frac{ie^2}{(2\pi i)^3}\int dt_1\,dt_2\,dt_3\int d\omega\,d\omega_1\,d\omega_2$$
$$\exp[i(\varepsilon_B+\omega_{\rm ph}+\omega_1+i\lambda)t_1]\exp[i(\omega_2-\omega_1+\omega+i\lambda)t_2]$$
$$\exp[-i(\omega_2+\varepsilon_A+\omega-i\lambda)t_3]$$
$$\times\sum_{n_1}\sum_{n_2}\frac{U_{Bn_1}[r_{12}^{-1}(1-\alpha_1\alpha_2)\exp(i|\omega|r_{12})]_{n_1n_2n_2A}}{[\varepsilon_{n_1}(1-i0)+\omega_1][\varepsilon_{n_2}(1-i0)+\omega_2]}. \quad (16)$$

We carry out integration in (16) over the times $\mathbf{t}_1$, $\mathbf{t}_2$, $\mathbf{t}_3$, and then integrate over the complex plane ω_1, ω_2. The results of such integration turn out to be different for positive and negative-frequency terms of the sums over n_1 and n_2 in (16). In what follows, we shall consider the contour of the spectral line in the resonance approximation, to which corresponds retention of only the single term $n_1=A$ in the sum over n_1 in (16). The nonresonant terms $n_1\neq A$ can be taken into account later as small increments by means of perturbation theory. Then

$$\langle\Phi_B^0|\hat{S}_\lambda^{(3)}(\infty,0)|\Phi_A^0\rangle=-\frac{e^2}{2\pi i}\frac{1}{[\varepsilon_A-\varepsilon_B-\omega_{\rm ph}-3i\lambda]}$$
$$\times\int d\omega\sum_{n_2}\frac{U_{Bn_1}[r_{12}^{-1}(1-\alpha_1\alpha_2)\exp(i|\omega|r_{12})]_{An_2n_2A}}{[\varepsilon_A-\varepsilon_B-\omega_{\rm ph}-i\lambda]}$$
$$\times\left\{\frac{\theta(\varepsilon_{n_2})}{\varepsilon_{n_2}(1-i0)-\varepsilon_B-\omega_\Phi-\omega-2i\lambda}+\frac{\theta(-\varepsilon_{n_2})}{\varepsilon_{n_2}(1-i0)-\varepsilon_A-\omega+i\lambda}\right\}. \quad (17)$$

In Eq. (17) we can also set $\lambda=0$ since, as will be shown below, the final result is finite for any value of the photon



DIAGRAMS: 1 through 11

frequency $\omega_{\rm ph}$. Setting $\varepsilon_B+\omega_{\rm ph}=\varepsilon_A$ in the nonresonant denominators in (17), and taking into account the definition (11) of ΔE_A, we can write down (17) in the form

$$\langle\Phi_B^0|\hat{S}_\lambda^{(3)}(\infty,0)|\Phi_A^0\rangle_{\rm res}=-U_{BA}\Delta E_A/(\varepsilon_A-\varepsilon_B-\omega_{\rm ph})^2. \quad (18)$$

Carrying out similar calculations, we can show that allowance for the nonresonant terms in all diagrams of type 4 leads to the following expression for the transition amplitude:

$$\langle\Phi_B^0|\hat{S}_\lambda(\infty,0)|\Phi_A^0\rangle_{\rm res}$$
$$=-U_{BA}(\varepsilon_A-\varepsilon_B-\omega_{\rm ph})^{-1}\sum_{n=0}^{\infty}\left(\frac{\Delta E_A}{\varepsilon_B-\varepsilon_A+\omega_{\rm ph}}\right)^n. \quad (19)$$

Summing the resultant progression, we obtain

$$\langle\Phi_B^0|\hat{S}_\lambda(\infty,0)|\Phi_A^0\rangle_{\rm res}=U_{BA}/(\varepsilon_A-\varepsilon_B-\omega_{\rm ph}+\Delta E_A). \quad (20)$$

Thus as $\lambda\to 0$ Eq. (20) has a finite limit also at the point of resonance $\omega_{\rm ph}=\varepsilon_A-\varepsilon_B$, at which each of the Eqs. (14), (18), etc., diverges. Equation (20) is the analytic continuation of the expansion (19) over the entire complex $\omega_{\rm ph}$ plane.

Allowance of the infinite series of diagrams 4 determines at the same time more accurately the location of the resonance and its width under the condition that the final state B has no width. We note that Eq. (20) is obtained directly from (14) if we replace ε_A in the wave function of the initial state by $\varepsilon_A+\Delta E_A$. This is the usual procedure of determining the line shape in quantum mechanics.

The approach used here permits us to take into account

(for relativistic atoms) those terms which determine the line contour far from resonance [the discarded terms of the sum over n_1 in (17).] In the first place, these terms contain a single resonant denominator, in which we must replace ε_A by $\varepsilon_A + \Delta E_A$. This substitution corresponds to the fact that the entire equation (17) can be regarded as a correction to the emission amplitude, and for this correction we can again take into account the entire sequence of self-energy insertions in the electron line of the initial state. Second, the terms in (17) that we have mentioned contain a more complicated dependence on ω_{ph} and, in particular, yield resonances also at $\omega_{ph} = \varepsilon_n - \varepsilon_B (n \neq A)$ i.e., at frequencies that are far removed from the center of the considered line. Here it is also necessary to take into account the self-energy insertion ΔE_n in the internal electron line in diagram 3. For a nonrelativistic atom, frequence regions so far from the center of the line are not of interest. However, this can be important in the case of multiply charged ions, whose natural line widths are relatively large and whose individual line contours can overlap.

5. SINGLE-QUANTUM APPROACH: RADIATIVE SHIFT OF THE LOWER (GROUND) LEVEL

Allowance for the radiative shift of the lower level is somewhat more complicated in the adiabatic theory. In this case, the diagrams which must be summed have singularities in the adiabatic parameter λ. We begin with the calculation of the diagram 5. In place of Eq. (16), we now have

$$\langle \Phi_B^0 | S_\lambda^{(3)}(\infty, 0) | \Phi_A^0 \rangle = \frac{ie^2}{(2\pi i)^3} \int dt_1\, dt_2\, dt_3 \times \int d\omega\, d\omega_1\, d\omega_2 \exp[i(\varepsilon_B + \omega_1 + \omega + i\lambda) t_1] \times \exp[i(\omega_2 - \omega_1 - \omega + i\lambda) t_2] \exp[i(\omega_{ph} - \varepsilon_A - \omega_2 + i\lambda) t_3] \times \sum_{n_1} \sum_{n_2} \frac{[r_{12}^{-1}(1 - \alpha_1\alpha_2) \exp(i|\omega|r_{12})]_{Bn_1n_2} U_{n_2A}}{[\varepsilon_{n_1}(1 - i0) + \omega_1][\varepsilon_{n_2}(1 - i0) + \omega_2]}. \quad (21)$$

Carrying out integration over the times and the frequencies ω_1 and ω_2, retaining in the sum over n_2 only the singular term, $n_2 = B$ and putting $\lambda = 0$ in the nonsingular and nonresonant factors, we obtain

$$\langle \Phi_B^0 | S_\lambda^{(3)}(\infty, 0) | \Phi_A^0 \rangle = \frac{e^2}{2\pi i} \frac{1}{(\varepsilon_A - \varepsilon_B - \omega_{ph} - 3i\lambda)} \times \frac{1}{(-2i\lambda)} \int d\omega \sum_{n_1} \frac{[r_{12}^{-1}(1 - \alpha_1\alpha_2) \exp(i|\omega|r_{12})]_{Bn_1n_1B} U_{BA}}{\varepsilon_{n_1}(1 - i0) - \varepsilon_B - \omega}. \quad (22)$$

Again using the definition (11), we write down (22) in the form

$$\langle \Phi_B^0 | \hat{S}_\lambda^{(3)}(\infty, 0) | \Phi_A^0 \rangle_{sing} = -\frac{1}{2i\lambda} \frac{U_{BA}\, \Delta E_B}{\varepsilon_A - \varepsilon_B - \omega_{ph} - 3i\lambda}. \quad (23)$$

Similar calculations in the higher-order perturbation theory (diagram 6) with account of only singular terms give

$$\langle \Phi_B^0 | \hat{S}_\lambda(\infty, 0) | \Phi_A^0 \rangle_{sing} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i\Delta E_B}{2\lambda} \right)^n \frac{U_{BA}}{\varepsilon_A - \varepsilon_B - \omega - (2n+1) i\lambda}. \quad (24)$$

Setting $\lambda = 0$ in the nonsingular factor in (24), we arrive at the equation

$$\langle \Phi_B^0 | \hat{S}_\lambda(\infty, 0) | \Phi_A^0 \rangle_{sing} = \frac{U_{BA}}{\varepsilon_A - \varepsilon_B - \omega_{ph}} \exp\left(-\frac{i\Delta E_B}{2\lambda} \right). \quad (25)$$

However, we need to take it into account that expansion of the nonsingular factor of (24) in powers of λ results in terms that do not depend on λ and give a nonzero contribution to (24). We expand the nonsingular factor in a series:

$$\frac{1}{\varepsilon_A - \varepsilon_B - \omega_{ph} - (2n+1) i\lambda} = \frac{1}{\varepsilon_A - \varepsilon_B - \omega_{ph}} \sum_{k=0}^{\infty} \left[\frac{(2n+1) i\lambda}{\varepsilon_A - \varepsilon_B - \omega_{ph}} \right]^k \quad (26)$$

and substitute initially the first term of the series (26) in (24) at $k = 1$ [at $k = 0$ the zeroth term yields (25)]. We obtain

$$\frac{i\lambda}{(\varepsilon_A - \varepsilon_B - \omega_{ph})^2} \sum_{n=0}^{\infty} \left(-\frac{i\Delta E_B}{2\lambda} \right)^n \frac{2n+1}{n!} = \frac{i\lambda}{(\varepsilon_A - \varepsilon_B - \omega_{ph})^2} \left\{ -\frac{i\Delta E_B}{\lambda} + 1 \right\} \exp\left(-\frac{i\Delta E_B}{2\lambda} \right) \quad (27)$$

The term of series (26) at $k = 2$, after substitution in (24), gives

$$\frac{(i\lambda)^2}{(\varepsilon_A - \varepsilon_B - \omega_{ph})^3} \sum_{n=0}^{\infty} \left(-\frac{i\Delta E_B}{2\lambda} \right)^n \frac{(2n+1)^2}{n!} = \frac{(i\lambda)^2}{(\varepsilon_A - \varepsilon_B - \omega_{ph})^3} \left\{ \left(-\frac{i\Delta E_B}{\lambda} \right)^2 - \frac{4i\Delta E_B}{\lambda} + 1 \right\} \exp\left(-\frac{i\Delta E_B}{2\lambda} \right). \quad (28)$$

Continuing these calculations and gathering the terms that differ from zero as $\lambda = 0$, we obtain

$$\langle \Phi_B^0 | S_\lambda(\infty, 0) | \Phi_A^0 \rangle_{sing} = \frac{U_{BA}}{\varepsilon_A - \varepsilon_B - \omega_{ph}} \exp\left(-\frac{i\Delta E_B}{2\lambda} \right) \sum_{k=0}^{\infty} \left[\frac{\Delta E_B}{\varepsilon_A - \varepsilon_B - \omega_{ph}} \right]^k = \frac{U_{BA} \exp(-i\Delta E_B/2\lambda)}{\varepsilon_A - \varepsilon_B - \Delta E_B - \omega_{ph}}. \quad (29)$$

We now take simultaneous account of the contributions of the resonant terms in diagrams 4 and of the singular terms in diagrams 6. According to (20), it suffices here to replace ε_A, in (29) by $\varepsilon_A + \Delta E_A$, since we can assume that the calculations in (29) are carried out from the very beginning with the corresponding wave function.

We now write down the transition probability defined by the equation

$$dW_{AB}(\mathbf{k}_{ph}, \mathbf{e}) = |\langle \Phi_B^0 | \hat{S}_\lambda(\infty, 0) | \Phi_A^0 \rangle|^2 d\mathbf{k}_{ph}, \quad (30)$$

where $\mathbf{k}_{ph}$ and $\mathbf{e}$ are the momentum and polarization of the emitted photon. When substituting (29) in (30) it is necessary to distinguish between two cases. In the first case, B is the ground state. Then $\Gamma_B = 0$, $\Delta E_B = \delta_R E_B$ and $|\exp(-i\Delta E_B/2\lambda)|^2 = 1$. Equation (30) in this case gives the usual Lorentz contour (after summation over the polarization and integration over the directions of emission of the photon $\nu \equiv \mathbf{k}_{ph}/\omega_{ph}$):

$$dW_{AB} = \frac{\Gamma_{BA}\, d\omega_{ph}}{(\omega_{AB} - \omega_{ph})^2 + {}^1/_4 \Gamma_A^2}, \quad (31)$$

where

$$\Gamma_{BA}=\omega_{ph}^2\sum_s\int dv|U_{BA}|^2 \tag{32}$$

is the partial width of state A, connected with transition to state N; $\omega_{AB}=\varepsilon_A+\delta_R E_A-\varepsilon_B-\delta_R E_B$ is the distance between the levels with account of the Lamb shift for the upper and lower states. We note that although we have considered the diagram of the self-energy of the electron in lowest-order perturbation theory, everything that has been said above applies to any irreducible insertion in the external electron lines and in particular to the vacuum-polarization diagram. To obtain regularized equations, it suffices to expand these insertions in powers of the field, generated by the nucleus, and to single out the first few terms of the expansion, which are divergent. The diverging terms are regularized according to standard rules without fundamental difficulty.[2]

Allowance of all possible irreducible insertions in the external lines leads to the result that the initial wave functions of the initial and final states (the solutions of the Dirac equation (3)) are replaced by solutions of a Schrödinger equation that contains the exact mass operator.[2]

A different result is obtained if the lower state B itself has width. In this situation, $|\exp(-i\Delta E_B/2\lambda)|^2=\exp(-\Gamma_B/2\lambda)$. As $\lambda\to 0$, this quantity is exponentially small, i.e., the contributions of all the resonant terms vanish. The contributions of all remaining terms that stem from the nonsingular terms in (22) and also from the nonresonant terms in (17) also vanish. Actually, as has been mentioned previously, such terms can be regarded as corrections to the emission amplitude and we can again take account of the sequence of diagrams 6, which leads to the appearance of the exponential $\exp(-\Gamma_B/2\lambda)$. Thus, the diagrams 4 and 6 do not describe the evolution of the Lorentzian line contour at $\Gamma_B\neq 0$. Such a result for the decay state B is connected with the fact that we have not taken into account explicitly the dynamics of its decay. In fact, the decay of the states A and B can be considered simultaneously,[11] as will be done in the next section.

6. SINGLE-QUANTUM APPROACH: ALLOWANCE FOR THE WIDTH OF THE LOWER LEVEL

We now particularize the problem by assuming, as in Ref. 11, that the lower level B can in turn go over to the ground state C via single-quantum decay. We consider the diagram 7, which describes the transition of the atom from state A to state C with the emission of two quanta. The corresponding amplitude is

$$\langle\Phi_C^0|S_\lambda^{(2)}(\infty,0)|\Phi_A^0\rangle=\frac{1}{\varepsilon_A-\varepsilon_C-\omega_{ph}-\omega_{ph}'-2i\lambda}\sum_n\frac{U_{Cn}U_{nA}}{\varepsilon_n-\varepsilon_C-\omega_{ph}'-i\lambda}. \tag{33}$$

In the sum over n in (33) we are interested in the term resonant at $n=B$:

$$\langle\Phi_C^0|S_\lambda^{(2)}(\infty,0)|\Phi_A^0\rangle_{res}=\frac{U_{CB}U_{BA}}{[\varepsilon_A-\varepsilon_C-\omega_{ph}-\omega_{ph}'][\varepsilon_B-\varepsilon_C-\omega_{ph}']} \tag{34}$$

(we have set $\lambda=0$).

Taking into account the results of the previous sections, we can state that the summation of the self-energy insertions with resonant terms into the lowest electron line on diagram 7 leads to the replacement of ε_A by $\varepsilon_A+\Delta E_A$ in (34). The summation of self-energy insertions in the upper electron line in diagram 7 leads, when account is taken of the fact that C is the ground state, to replacement of ε_C by $\varepsilon_C+\delta_R E_C$. Thus, there remains to be taken into account only the self-energy insertion in the internal electron line of diagram 7, i.e., the radiative shift of the state B.

We consider diagram 8 with this in mind. The substitution of the expressions for the propagators and integration over the times and frequencies leads, after elimination of the resonant terms $n_1=n_3=B$, to the equation (we set $\lambda=0$ here)

$$\langle\Phi_C^0|\hat S_\lambda^{(4)}(\infty,0)|\Phi_A^0\rangle_{res}=\frac{e^2}{2\pi i}\frac{1}{\varepsilon_A-\varepsilon_C-\omega_{ph}-\omega_{ph}'}\cdot\int d\omega\sum_{n_2}\frac{U_{CB}[r_{12}^{-1}(1-\alpha_1\alpha_2)\exp(i|\omega|r_{12})]_{Bn_2n_2B}U_{BA}}{[\varepsilon_B-\varepsilon_C-\omega_{ph}'][\varepsilon_{n_2}(1-i0)-\varepsilon_C-\omega_{ph}'-\omega][\varepsilon_B-\varepsilon_C-\omega_{ph}']} \tag{35}$$

or, with account taken of (11), to

$$\langle\Phi_C^0|\hat S_\lambda^{(4)}(\infty,0)|\Phi_A^0\rangle_{res}=\frac{U_{CB}U_{BA}\Delta E_B}{[\varepsilon_A-\varepsilon_C-\omega_\Phi-\omega_{ph}'][\varepsilon_B-\varepsilon_C-\omega_{ph}']^2}. \tag{36}$$

Summing all the self-energy insertions with the resonant terms in the internal line on diagram 8, and also taking into account the results of summation of such insertions for the external lines, we obtain

$$\begin{aligned}\langle\Phi_C^0|\hat S_\lambda(\infty,0)|\Phi_A^0\rangle_{res}&=\frac{U_{CB}U_{BA}\exp(-i\delta_R E_C/2\lambda)}{[\varepsilon_A+\Delta E_A-\varepsilon_C-\delta_R E_C-\omega_{ph}-\omega_{ph}'][\varepsilon_B-\varepsilon_C-\delta_R E_C-\omega_{ph}']}\\&\cdot\sum_{n=0}^{\infty}\left[\frac{\Delta E_B}{\varepsilon_C+\delta_R E_C-\varepsilon_B+\omega_{ph}'}\right]^n\\&=\frac{U_{CB}U_{BA}\exp(-i\delta_R E_C/2\lambda)}{[\omega_{AC}-\omega_{ph}-\omega_{ph}'-i\Gamma_A/2][\omega_{BC}-\omega_{ph}'-i\Gamma_B/2]}.\end{aligned} \tag{37}$$

Transforming from amplitude to probability by the for-

mula

$$dW_{AB,\,BC}(\mathbf{k}_{\rm ph},\ \mathbf{e};\ \mathbf{k}_{\rm ph}'\mathbf{e}') = |\langle\Phi_C{}^0|\,\hat{S}_\lambda(\infty,\ 0)\,|\,\Phi_A{}^0\rangle|^2 d\mathbf{k}_{\rm ph} d\mathbf{k}_{\rm ph}', \tag{38}$$

integrating over the directions of the photon emission and summing over the polarizations, we get

$$dW_{AB,BC} = \frac{\Gamma_{CB}\Gamma_{BA}\,d\omega_{\rm ph}d\omega_{\rm ph}'}{[(\omega_{AC}-\omega_{\rm ph}-\omega_{\rm ph}')^2+{}^1/_4\Gamma_A{}^2][(\omega_{BC}-\omega_{\rm ph}')^2+{}^1/_4\Gamma_B{}^2]}. \tag{39}$$

Equation (39) is the well-known formula for the resonance contour of the two-quantum-transition line.[11] As has already been noted, our method makes it also possible to consider the nonresonant part of this contour.

Integrating (39) over $\omega_{\rm ph}'$ and assuming that the partial width Γ_{CB} is identical with the total width Γ_B of level B, we obtain the expression for the line contour of a single-quantum transition from state A to state B with account of the width Γ_B:

$$dW_{AB} = \frac{\Gamma_A+\Gamma_B}{\Gamma_A}\frac{\Gamma_{BA}\,d\omega_{\rm ph}}{[(\omega_{AB}-\omega_{\rm ph})^2+{}^1/_4(\Gamma_A+\Gamma_B)^2]}. \tag{40}$$

7. RADIATIVE TRANSITIONS IN A TWO-ELECTRON ATOM

In two-electron atoms, in addition to the radiative corrections to diagram 2, it is necessary to take into account the interelectron interaction. This problem can also be solved using the adiabatic formalism. For simplicity, we limit ourselves to such states of the two-electron atom in which only one electron is excited. We first consider diagrams 9, which describe the transition from the excited state C_2A_1 to the ground state C_2C_1 with account taken of the Coulomb interaction of the electrons in the initial state. Using Eq. (10b) for the Coulomb propagator and summing the resonant contributions in a manner similar to what was done in Sec. 4, we arrive at an equation of the form

$$\langle\Phi^0_{C_2C_1}|\hat{S}_\lambda(\infty,0)\,|\,\Phi^0_{C_2A_1}\rangle_{\rm res} = U_{C_1A_1}/(\varepsilon_{A_1}-\varepsilon_{C_1}-\omega_{\rm ph}+\Delta E^{(c)}_{C_2A_1}). \tag{41}$$

Here $\Delta E^{(c)}_{C_2A_1}$ is the first-order perturbation-theory correction, for the interelectron interaction, to the energy of the ground state:

$$\Delta E^{(c)}_{C_2A_1} = (1/r_{12})_{C_2A_1C_2A_1} - (1/r_{12})_{C_2A_1A_1C_2}. \tag{42}$$

The second term in (42) arises from the exchange diagrams, which are obtained from diagram 9 by the exchange of the subscripts $A_1 \leftrightarrow C_2$.

Considering diagrams 10, which describe the Coulomb interaction of the electrons in the final state, and using the same methods as in Sec. 5 (summation of the contributions of the singular terms), we find that Eq. (41) must be replaced by

$$\langle\Phi^0_{C_2C_1}|\hat{S}_\lambda(\infty,0)\,|\,\Phi^0_{C_2A_1}\rangle_{\rm sing} = \frac{U_{C_1A_1}\exp(-i\Delta E_{C_2C_1}/2\lambda)}{\varepsilon_{A_1}-\varepsilon_{C_1}-\omega_{\rm ph}+\Delta E^{(c)}_{C_2A_1}-\Delta E^{(c)}_{C_2C_1}}. \tag{43}$$

The contributions of both diagrams 9 and 10 are taken into account in (43). It is also clear from the results of the calculations in Secs. 4 and 5 that the self-energy insertions in diagrams 9 and 10 lead to the appearance of additions to the denominator of Eq. (43). The Lamb shift can, however, be neglected in comparison with the correction to the Coulomb interaction of the electrons. Then the addition to the denominator reduces to $1/2\,i\Gamma_A$, where the quantity Γ_A is determined by Eq. (13).

It remains to consider the contribution of the transverse-photon exchange diagram 11. With account taken of all the previous calculations, we can state that allowance for the principal terms in the sequence of diagrams 11 leads to the appearance in the denominator of (43) of the increment $\Delta E^{Br}_{C_2A_1} - \Delta E^{Br}_{C_2C_1}$, where ΔE^{Br}_{AB} is the correction to the energy levels of the two-electron atom for the Breit interaction. A expression for this correction is obtained by substituting the transverse photon propagator (10c) in the corresponding matrix element. We shall only take into account the contribution ΔE^{Br}_{AB} to the level width, neglecting for simplicity the real part of the Breit correction (although, at $\alpha Z \sim 1$, the Breit and Coulomb interactions are of the same order of magnitude). Then an increment $1/2\,i\Gamma_{C_2A_1}$ arises in the denominator of (43), where[7]

$$\Gamma_{C_2A_1} = -\alpha\left[\frac{1-\alpha_1\alpha_2}{r_{12}}\sin(\beta_{A_1C_2}r_{12})\right]_{C_2A_1A_1C_2} \tag{44}$$

(the minus sign in (44) is explained by the fact that the increment arises from the exchange diagram, since the entire contribution of the direct diagram is real). The increment $\Gamma_{C_2A_1}$ to Γ_{A_1} has a simple physical meaning: it cancels that term in Eq. (13) for Γ_{A_1} which corresponds to the transition to the state C_2 (which is occupied in the two-electron atom).

Finally, we obtain for the transition probability an equation similar to (31):

$$dW_{A_1C_2,C_1C_2} = \frac{\Gamma_{C_1A_1}\,d\omega_{\rm ph}}{(\omega_{A_1C_2,C_1C_2}-\omega_{\rm ph})^2+{}^1/_4\Gamma^2_{A_1(C_1)}}, \tag{45}$$

where $\omega_{A_1C_2C_1C_2}$ is the transition frequency with account taken of corrections of the first-order perturbation-theory in the Coulomb interaction of the electrons, $\Gamma_{A_1(C_1)} = \Gamma_{A_1} - \Gamma_{C_2A_1}$. Thus, we can take into account in Eq. (45) the Coulomb interaction of the electrons in second and higher order perturbation theories.

In conclusion, we note that we could dispense completely with Eqs. (5) and (8) for the energy shift. The approach developed in this work allows us to find right away the dependence of the radiation intensity on the frequency of the photon, i.e., on a measurable quantity, without first calculating either the correction to the energy level or the transition probabilities per unit time. Furthermore, since the nonresonant terms distort the shape of the Lorentz contour, calculation of the energy levels and transition probabilities (i.e., the location of the resonance and its width) have meaning only with the same accuracy with which we take into account the contribution of the nonresonant terms.

[1)]We can tentatively call the atom nonrelativistic if the inequality $\bar{v}/c \approx \alpha Z_e \ll 1$, is satisfied, where $\bar{v}$ is the mean speed of the electron in the atom, c is the speed of light, $\alpha = e^2/\hbar c \approx 1/137$ is the fine structure constant, e is the charge of the electron, $\hbar$ is Planck's constant, and Z_e is the effective charge of the nucleus.

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