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LINE SHAPE AND POTENTIAL GAUGE

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1. Introduction

An unstable state is characterized by a distribution over energies. Its measurement is difficult, however it has been realized in Lamb-shift experiments. The microwave radiation of the frequency K induces transitions of the H-atoms from a metastable 2s-state to a short-lived $2\,^2P_{1/2}$ state. The number of survived metastable atoms is measured as a function of the difference $K-\varkappa$, where $\varkappa$ is the difference of the $2S$ and $2P$ level energies. The function is called the line shape.

Lamb [1] has pointed out that the observed line shape agrees with a calculation (performed in the Weisskopf-Wigner approximation), in which the microwave field is described by the external scalar potential equal to $\vec{E}\cdot\vec{q}$. Here $\vec{E}$ is the microwave electric field, q is the electron coordinate. But the similar calculation, in which the same field is described by the corresponding nonzero vector potential $\vec{A}$ and zero scalar potential (see below sect. 3.7 for details) gives another line shape which is in disagreement with experiments. Lamb writes [1]: "Of course, the difference between the perturbations $\vec{E}\vec{q}$ and $-\vec{A}\vec{p}/m$ just corresponds to a gauge transformation under which the theory is known to be invariant, so both perturbations must lead to the same physical predictions. Nevertheless, a closer examination shows that the usual interpretation of probability amplitudes is valid only in the former gauge ...".

The problem was discussed in a number of papers. Reasons were given in refs.[2,3,4] in favour of using just the $\vec{E}\cdot\vec{q}$ interaction. On the other hand, it was shown in refs.[5,6,4] that it is possible to obtain the same result using either of the interactions. I stress that the latter was demonstrated for the processes which are described by S-matrix, e.g., for reactions of scattering. I argue in Section 2 that the line shape measurement (and the very Lamb shift)

must not be of the kind. A refined experiment is proposed, in which the line shape should be measured. The experiment cannot be described by the S-matrix. Standard calculations give for it different line shapes in different gauges (see Sections 2 and 4 below). So, the problem is revived. Analogous problems hold for other observables, see part IV in ref. /3/.

Kuo Ho Yang /3/ has suggested a nonstandard approach to the line shape calculation. He describes atom states by means of eigenfunctions of a gauge-invariant operator, which do not coincide in general with the free part of the total Hamiltonian defined in the usual manner. The approach gives for any gauge the same result as the $\vec{E}\cdot\vec{q}$ -interaction (see below Section 3.6). This can be considered as a solution of Lamb's problem. However, Kuo Ho Yang considers the electron which interacts only with the external field.

I discuss in Section 3 the general case, when there is also the quantized electromagnetic field. I consider the form of quantum electrodynamics suggested in refs. /2,8,9,10/. Its Hamiltonian has the free part H_0 (defined in the usual manner) which is invariant under any gauge transformations. The eigenfunctions of H_0, which describe initial and final states, and interaction Hamiltonian $H_I = H - H_0$ also are gauge-invariant. Using such H_0 and H_I one gets gauge-invariant results for observables, which cannot be described by the S-matrix. In the Coulomb gauge the results may be obtained only in an intricate nonstandard way. At the same time the standard calculations give the same S-matrix in any gauge. We show how an interaction of the $\vec{E}\cdot\vec{q}$ type arises in the discussed form of the theory.

A new theoretical definition of the excitation probability of unstable states is given in Sec.4. It takes properly into account the so-called virtual processes. The proposed formula (30) is calculated exactly in a solvable model. As in the Weisskopf-Wigner approximation /1,2/, one gets different line shapes if one uses the same standard description of the excited atom in different gauges.

The gauge-invariant calculations of the line shape discussed in Sections 3 and 4 predict that in the experiment proposed in Sec. 2 one will measure the same line shape, as in the existing Lamb-shift experiments, see, e.g., refs. /11,12/.

2. Gauge Invariance of the S-Matrix and Line Shape

1. Z. Fried performed the following calculation of the line shape. The microwave photon is incident on the atom in the 2s-state. The probability amplitude T of the transition in the final state "$1S$ + Lyman photon γ" is calculated as a function of the incident photon frequency κ. It is the "resonance channel" $\kappa + 2S \to 2P \to 1S + \gamma$ which brings the main contribution to T. However, other intermediate channels are possible, e.g., $\kappa + 2S \to 3P \to 1S + \gamma$ which are characterized by the large energy nonconservation in the virtual transitions $\kappa + 2S \to 3P$ and $3P \to 1S + \gamma$. Denoting the contribution of all these "background" channels by B, we represent T as R+B in the case of $\vec{A}\cdot\vec{p}/m$ interaction. With the $\vec{E}\cdot\vec{q}$ interaction one has correspondingly $T' = R' + B'$. Fried showed (in the first nonvanishing approximation) that although $R \neq R'$, but $T = T'$. A similar result is declared in ref. /6/. It turns out that B' is small and practically $R + B \cong R'$.

The equality $T = T'$ is a manifestation of the known property of the (renormalized) S-matrix: S is gauge-invariant. There are other examples of the equality of the results obtained with $\vec{A}\cdot\vec{p}/m$ and $\vec{E}\cdot\vec{q}$ interactions /5,6,7/. Let us stress that all of them deal with S-matrix processes.

2. However, it is just the resonance term which has the direct relevance to the Lamb shift: just the $2P$-state shift is of interest. If the "background" is essential, the experiment must be changed as to pick out just the resonance channel. For instance, one should measure the number of Lyman quanta (as a function of κ) which are radiated after the beam of H-atoms abandons the microwave field region. Then the contribution of the nonresonance channels will diminish because is does not increase with time unlike the resonance channel contribution (note that energy nonconservation in the transition $\kappa + 2S \to 3P$ is much greater than the $2P$ level width, which corresponds to the lifetime $1.6\ 10^{-9}$ sec).

The experiment cannot be described by the S-matrix because it provides information on the intermediate stage of the process $\kappa + 2S \to 1S + \gamma$ and not only on its initial and final stages. (In other words, only delayed γ-photons are measured in this experiment).

The $\vec{A}\cdot\vec{p}/m$ and $\vec{E}\cdot\vec{q}$ interactions predict different outcomes for the proposed experiment (R and $R' \cong T'$, respectively).

3. Let us note that it suffices to calculate, instead of R or R', the probability of the transition $\kappa + 2S \to 2P$ because the experiment can

be made so that the probability of a subsequent decay $2P \to 1S + \gamma$ will be practically equal to 1. Just the probability of $K + 2S \to 2P$ was calculated by Lamb and in ref. /11/ (see Sec. 4.2 therein) and will be calculated in Sec. 4.

3. New Gauge and $\vec{E}\cdot\vec{q}$ Interaction

A new form of quantum electrodynamics has been proposed in refs. /2,8,9,10/, which is applicable for localized charges. It has been shown in ref. /10/ that it can be considered as one more electrodynamical gauge (along with the Coulomb one, e.g.) with the gauge condition (9), see below. Here it will be generalized to the case when there is a time-dependent external electromagnetic field. Just such a field is usually used to describe the microwave radiation in the Lamb shift experiment. It will be sufficient for our purposes to consider only the single spinless electron, which interacts with the quantized electromagnetic field besides the external one (the level shifts and widths are caused by the former interaction). The generalization to the second-quantized Dirac electrons can be made in analogy with ref. /10/ and brings no problems.

1. We start with the Coulomb gauge for the quantized potentials and with an arbitrary gauge for the external ones A^{ex}_{μ}. The Hamiltonian is

$$H(t) = [\vec{p} - e\vec{A}_{\perp}(\vec{q}) - e\vec{A}^{ex}(\vec{q},t)]^2/2m + W(\vec{q}) + eA_0^{ex}(\vec{q},t) + \frac{1}{2}\int d^3x\,[\vec{E}_{\perp}^2(\vec{x}) + \vec{H}^2(\vec{x})]. \tag{1}$$

Let us perform the canonical transformation $\mathcal{O}' = S^{+}\mathcal{O}S$ of the theory operators $\mathcal{O}$

$$S = \exp\{(-ie)[\int_0^{\vec{q}} d\vec{\xi}\cdot\vec{A}_{\perp}(\vec{\xi}) + \int_0^{\vec{q}} d\vec{\xi}\cdot\vec{A}^{ex}(\vec{\xi})]\}. \tag{2}$$

The integrals in (2) are along the straight line, connecting $\vec{q}$ with the origin which is chosen in the centre of the binding potential W. We have

$$\vec{q}' = S^{+}\vec{q}\,S = \vec{q}\,, \quad \vec{A}_{\perp}' = \vec{A}_{\perp}\,, \quad \vec{H}' = \vec{H}\,, \tag{3}$$

$$\vec{p}' = S^{+}\vec{p}\,S = \vec{p} + e\vec{\nabla}_q\Lambda(\vec{q}) + e\vec{\nabla}_q\Lambda^{ex}(\vec{q},t)\,,$$

$$\Lambda(q) \equiv -\int_0^{q} d\vec{\xi}\cdot\vec{A}_{\perp}(\vec{\xi})\,, \quad \Lambda^{ex}(q,t) \equiv -\int_0^{q} d\vec{\xi}\cdot\vec{A}^{ex}(\vec{\xi},t), \tag{4}$$

$$E_{\perp m}(\vec{x}) = E_{\perp m}(\vec{x}) + e\int_0^{q}\sum_n d\xi_n\,\delta^{tr}_{nm}(\vec{\xi}-\vec{x})\,, \quad m = x,y,z\,, \tag{5}$$

$$\delta^{tr}_{nm}(\vec{y}-\vec{x}) \equiv \delta_{mn}\,\delta^{(3)}(\vec{y}-\vec{x}) - \frac{1}{4\pi}\frac{\partial}{\partial y_n}\frac{\partial}{\partial x_m}\frac{1}{|\vec{y}-\vec{x}|}\,. \tag{6}$$

From eq. (3) we obtain

$$\vec{p} - e\vec{A}_{\perp} - e\vec{A}^{ex} = \vec{p}' - e(\vec{A}_{\perp} + \vec{\nabla}\Lambda) - e(\vec{A}^{ex} + \vec{\nabla}\Lambda^{ex}) \equiv \equiv \vec{p}' - e\vec{a} - e\vec{a}^{ex}. \tag{7}$$

Here $\vec{a}$ and $\vec{a}^{ex}$ can be considered as new potentials. It was shown in ref. /8,10/ that

$$\vec{a}(\vec{x}) \equiv \vec{A}_{\perp}(\vec{x}) + \vec{\nabla}\Lambda(\vec{x}) = -\int_0^1 \alpha\,d\alpha\;\vec{x}\times\vec{H}(\alpha\vec{x})\,,$$
$$a^{ex}(\vec{x},t) \equiv A^{ex} + \nabla\Lambda^{ex} = -\int_0^1 \alpha\,d\alpha\;\vec{x}\times\vec{H}^{ex}(\alpha\vec{x},t)\,. \tag{8}$$

Eqs. (3) and (8) show that the operators $\vec{p}'$ and $\vec{a}$ are connected with $\vec{p}$ and $\vec{A}$ by a gauge transformation. The potentials $\vec{A}_{\perp}$ have satisfied the gauge condition $div\,A_{\perp} = 0$, no conditions have been imposed on A^{ex}_{μ}. We can and do impose the following conditions on $\vec{a}$ and $\vec{a}^{ex}$

$$\int_0^{\vec{x}} d\vec{\xi}\cdot\vec{a}(\vec{\xi}) = 0\,, \quad \int_0^{\vec{x}} d\vec{\xi}\cdot\vec{a}^{ex}(\vec{\xi},t) = 0 \qquad \forall\,\vec{x}\,. \tag{9}$$

It is easy to verify that middle parts of eqs. (8) satisfy these conditions.

2. All operators in eqs. (1)-(8) are Schroedinger ones. But new operators $\vec{p}'$ depend upon the time t explicitly if A^{ex} do depend upon t, see (3). No such operators appeared in refs. /2,8,9,10/. The corresponding Heisenberg operators

$$\vec{p}'_H(t) = \mathcal{U}^{+}(t,0)\,\vec{p}'\,\mathcal{U}(t,0)\,, \quad i\,\partial\mathcal{U}(t,0)/\partial t = H(t)\,\mathcal{U}(t,0)$$

therefore satisfy the equation

$$\frac{\partial}{\partial t}\vec{p}'_H(t) = \frac{\partial}{\partial t}\{\mathcal{U}^{+}(t,0)[\vec{p} + e\vec{\nabla}\Lambda(\vec{q},) + e\vec{\nabla}\Lambda^{ex}(\vec{q},t)]\,\mathcal{U}(t,0)\} = -i[\vec{p}'_H(t),\, H_H(t)] + \mathcal{U}^{+}\frac{\partial}{\partial t}e\vec{\nabla}\Lambda^{ex}(\vec{q},t)\,\mathcal{U}\,. \tag{10}$$

It can be rewritten in the canonical form

$$\frac{\partial}{\partial t}\vec{p}'_H(t) = -i\left[\vec{p}'_H(t),\, H'_H(t)\right], \qquad H' = H - e\frac{\partial}{\partial t}\Lambda^{ex}(\vec{q}',t). \tag{11}$$

As we see, the additional dependence of $\vec{p}'_H(t)$ upon time can be fully taken into account if we substitute H' for H and then consider $p'_H(t)$ to be the usual Heisenberg operator (i.e., the one corresponding to the Schroedinger operator which does not depend explicitly upon time). It was shown in Sec. 3 of ref. /13/ how the replacement $H \to H'$ can be obtained within the Schroedinger picture.

3. Using eqs. (3)–(7) one can write H' in terms of the new (primed) operators

$$\begin{aligned} H' = H - e\,\partial\Lambda^{ex}/\partial t = \left[\vec{p}' - e\vec{A}(\vec{q}) - e\vec{A}^{ex}(\vec{q},t)\right]^2/2m + W(\vec{q}') + \\ + e\,A_0^{ex}(\vec{q}',t) - e\frac{\partial}{\partial t}\Lambda^{ex}(\vec{q}',t) - e\int_0^{q} d\vec{\xi}\cdot\vec{E}'_{\perp}(\vec{\xi}) + \\ + \frac{1}{2}\int d^3x\left[\vec{E}'^2_{\perp} + \vec{H}'^2\right] + \frac{e^2}{2}\sum_{n,m}\int_0^{q'} d\xi_n \int_0^{q'} d\xi_m\, \delta^{tr}_{nm}(\vec{\xi}-\vec{\xi}'). \end{aligned} \tag{12}$$

The last (divergent) term in the eq. was considered in Sec. 4.2. of ref. /2/.

4. The theory described by the Hamiltonian (1) is invariant under an independent gauge transformation of the quantized and external potentials

$$\vec{A}_{\perp} \to \vec{A}_{\perp} + \vec{\nabla}\chi(\vec{x}), \tag{13}$$

$$A^{ex}_{\mu} \to A^{ex}_{\mu} - \partial_{\mu}\eta(\vec{x},t), \tag{14}$$

$$\vec{P} \to \vec{P} + e\vec{\nabla}\chi + e\vec{\nabla}\eta \quad , \quad H \to H - e\,\partial\eta/\partial t. \tag{15}$$

Usually one writes, instead of (15), the corresponding transformation of the wave function: $\phi \to \phi\, exp\, ie(\chi+\eta)$. When electrons are second-quantized, one transforms only operators, and it is convenient to do so in the considered case.

While $\eta(\vec{x},t)$ can be an arbitrary smooth function, the function $\chi(\vec{x})$ must be harmonic $\vec{\nabla}\cdot\vec{\nabla}\chi = 0$ because $div\, A_{\perp} = 0$. If the potentials $\vec{A}_{\perp}$ and $\vec{A}_{\perp} + \vec{\nabla}\chi$ are required to vanish at infinity (their matrix elements are implied, of course), then

$\vec{\nabla}\chi \to 0$ as $\vec{x} \to \infty$. Then $\vec{\nabla}\chi = 0$ for all $\vec{x}$ if $\Delta\chi = 0$ holds everywhere.

However, usually we consider physical systems which are localized in a finite volume V (e.g., inside a laboratory). If (13) holds only for the points $\vec{x}$ which belong to a part V of the whole space, then $\Delta\chi = 0$ not everywhere and $\vec{\nabla}\chi$ can vanish at infinity not being zero everywhere. For example, the infinite solenoid with a current induces outside itself a nonzero gradient-like potential $\vec{A}_{\perp}$. Another example is the "quasigradient transformation" (26) in /10/.

Let us show that even such a gauge freedom is absent when one considers the new electron momentum $\vec{P}'$ and the potentials $\vec{A}, \vec{A}^{ex}$ satisfying the condition (9). Indeed, let us try to write

$$\tilde{\vec{A}} = \vec{A}(\vec{x}) + \vec{\nabla}\chi'(\vec{x}) \qquad \vec{x} \in V. \tag{16}$$

As (9) must be true both for $\tilde{\vec{A}}$ and $\vec{A}$, one must have

$$0 = \int_0^{q} d\vec{\xi}\cdot\vec{\nabla}\chi'(\xi) = \chi'(\vec{q}) - \chi'(0)$$

if V covers completely the region V_e, where the electron is localized. We see that $\chi'(q)$ is a constant and $\vec{\nabla}\chi' = 0$.

The gauge transformation (16) with $\vec{\nabla}\chi \neq 0$ can be shown to exist only if V does not cover V_e. But such a transformation is accompanied inevitably by a change of observables. For instance, let (16) be induced by a solenoid, the magnetic field $\vec{H}$ of which is equal to zero outside V (it follows from eq. (8) that $\vec{A}$ must be a gradient in the region where $\vec{H} = 0$). In the considered case the region, where $\vec{H} \neq 0$, must intersect with V_e (otherwise (16) would be true for V_e and then $\vec{\nabla}\chi' = 0$). Such a field leads, of course, to the observable level splitting.

We call the quasigauge a transformation which looks like the usual gauge one but only in some (simple-connected) part V of the whole space. The region V must cover the physical system under consideration. Then the quasigauge transformation will not be accompanied by changes of observables which are measured inside V and will be indistinguishable inside V from the usual gauge transformation.

The gauge invariance of the momentum $\vec{P}'$ follows also from the fact that r.h.s. of eq. (3) is invariant under (13)–(15). Note that

$$\Lambda(\vec{q}) + \Lambda^{ex}(\vec{q},t) \to \Lambda(\vec{q}) + \Lambda^{ex}(\vec{q},t) - \chi(\vec{q}) + \chi(0) - \eta(\vec{q},t) + \eta(0,t).$$

Of course, one ought to speak more exactly that $\vec{p}'$ has no gauge freedom within the new gauge.

The operator $H_e' = p'^2/2m + W(q')$, its eigenfunctions (which describe atom states) and interaction Hamiltonian also are invariant under any (usual and quasi) gauge transformations.

5. Now of course one can rewrite H_e' in terms of the Coulomb-gauge operators and try to use it for the atom state description in the Coulomb gauge. But H_e' does not commute with $\int d^3x (\vec{E}_\perp^2 + \vec{H}^2)$ as well as with the photon number operator. The consequence is that one cannot describe even the simplest state "atom in the ground state, no photons". So, one will be forced to alter also the photon description. If we prooeed in a correct manner, we shall obtain the same results which new gauge gives in the standard consistent manner.

Other gauge invariant descriptions of the atom states were proposed in /3,4/ for the electron which interacts only with the external field A_μ^{ex}. In particular, Kuo Ho Yang used $(\vec{p} - e\vec{A}^{ex})^2/2m + W$ instead of $H_e' = [\vec{p} - e\vec{\nabla}\int d\vec{\xi}\cdot\vec{A}^{ex}]^2/2m + W$. This approach cannot be generalized, however, to the case of the eleotron which interacts with the quantized field (the reasons are similar to those presented at the beginning of this subsection).

6. Consider the Hamiltonian (1) in the dipole (long-wave) approximation, substituting $\vec{A}_\perp(0)$ and $\vec{A}^{ex}(0,t)$ for $\vec{A}_\perp(\vec{q})$ and $\vec{A}^{ex}(\vec{q},t)$. The equivalent replacement for $A_0^{ex}(\vec{q},t)$ is (see sect. IIIA in ref. /3/)

$$A_0^{ex}(\vec{q},t) \cong A_0^{ex}(0,t) + \sum_m q_m \left[\partial A_0^{ex}(\vec{x},t)/\partial x_m\right]_{\vec{x}=0} .$$

The c-number $A_0^{ex}(0,t)$ can be discarded in the Hamiltonian. We get

$$H_d = [\vec{p} - e\vec{A}_\perp(0) - e\vec{A}^{ex}(0,t)]^2/2m + W(\vec{q}) + e\vec{q}\cdot\vec{\nabla}A_0^{ex}(0,t) + \frac{1}{2}\int d^3x(\vec{E}_\perp^2 + \vec{H}^2) . \qquad (17)$$

Letting $\vec{q} = 0$ in eq. (7) and using $\vec{A}(0) = \vec{A}^{ex}(0,t) = 0$, see eq. (8), one obtains

$$\vec{p} - e\vec{A}_\perp(0) - e\vec{A}^{ex}(0,t) = \vec{p}' .$$

The term $-e\,\partial\Lambda^{ex}/\partial t$ in (12) can be treated in the same manner as $A_0^{ex}(q,t)$. Using (4) and then (8) at $x = 0$ one has

$$\Lambda^{ex}(\vec{q}',t) \cong \sum_m q_m' \left[\partial\Lambda^{ex}(\vec{x},t)/\partial x_m\right]_{\vec{x}=0} = -\vec{q}'\cdot\vec{A}^{ex}(0,t) .$$

So, the Hamiltonian (12) in the dipole approximation turns into

$$H_d' = \vec{p}'^2/2m + W(\vec{q}') + e\vec{q}'\vec{\nabla}A_0^{ex}(0,t) + e\vec{q}'\frac{\partial}{\partial t}\vec{A}^{ex}(0,t) - e\int_0^{\vec{q}'} d\vec{\xi}\cdot\vec{E}_\perp'(\vec{\xi}) + \frac{1}{2}\int d^3x(\vec{E}_\perp'^2 + \vec{H}'^2) + \frac{e^2}{2}\sum_{n,m}\int_0^{q_n'} d\xi_n \int_0^{q_m'} d\xi_m' \,\delta_{nm}^{tr}(\xi - \xi') . \qquad (18)$$

A similar operator can be obtained from H_d by means of a canonical transformation which is simpler than (2)

$$S = \exp\left\{(-ie)\left[\vec{q}\cdot\vec{A}_\perp(0) + \vec{q}\cdot\vec{A}^{ex}(0,t)\right]\right\} .$$

Denoting S^+qS, S^+pS, ... by primed operators q', p'... as before we get

$$H_{ds}' = \vec{p}'^2/2m + W(q') - e\vec{q}'\cdot\vec{E}^{ex}(0,t) - e\vec{q}'\cdot\vec{E}_\perp'(0) + \frac{1}{2}\int d^3x(\vec{E}_\perp'^2 + \vec{H}'^2) + \frac{e^2}{2}\sum_{n,m} q_n q_m \,\delta_{nm}^{tr}(0) , \qquad (19)$$

$$\vec{E}^{ex} \equiv -\partial\vec{A}^{ex}/\partial t - \vec{\nabla}A_0^{ex} .$$

7. Let us comment the oitation from /1/ quoted in the Introduotion. The miorowave radiation will be approximated by a plane wave having the eleotric field

$$E_x^{ex} = E_y^{ex} = 0 \quad , \quad E_z^{ex}(x,y,z,t) = E_0\cos\left[\kappa(x-t) + \beta\right] . \qquad (20)$$

The field can be described by two sets of potentials

$$A_x^{ex} = 0 = A_y^{ex} \quad , \quad A_z^{ex}(x,y,z,t) = E_0\kappa^{-1}\sin\left[\kappa(x-t) + \beta\right] \quad , \quad A_0^{ex} = 0 , \qquad (21)$$

$$\tilde{A}_x^{ex} = \tilde{A}_y^{ex} = 0 \quad , \quad \tilde{A}_z^{ex}(x,y,z,t) = E_0\kappa^{-1}\left\{\sin\left[\kappa(x-t) + \beta\right] + \sin\left[\kappa t - \beta\right]\right\} ,$$
$$\tilde{A}_0^{ex}(x,y,z,t) = -E_0 z\cos(\kappa t - \beta) . \qquad (22)$$

The sets are connected by the gauge transformation

$$\tilde{A}_\mu = A_\mu + \partial_\mu\eta \quad , \quad \eta = E_0\kappa^{-1} z\sin(\kappa t - \beta) .$$

The electron interaction with the external field is represented in the Hamiltonian H_d by the term $-e p_z A_z^{ex}(0,t)/m$ in the case (21) and by $e A_0^{ex} = -e q_z' E_z^{ex}(0,t)$ in the case (22) (note that $\tilde{A}_z^{ex}(0,t) = 0$). The interaction term is equal to $-e\bar{q}'\cdot\bar{E}^{ex}(0,t)$ in H_d' and does not depend upon choosing (21) or (22). It coincides with the interaction term of H_d when (22) is used. So, standard calculations using H_d will give the correct (gauge invariant) answer only if just the potentials (22) are used in H_d (cf. Sect. IIIC in ref. [3]).

4. Probability of Electromagnetic Excitation of the Atom.

1. Suppose that at t=0 the atom is in the ground state and there is one photon with the energy κ (the state ϕ_κ). Then $A_{n\kappa} = \langle \phi_n | U(t,0) | \phi_\kappa \rangle$ is the probability amplitude to find at the moment t the state ϕ_n : atom is an excited state n, no photons. The atom excitation probability is defined usually as $|A_{n\kappa}|^2$. But $|A_{n\kappa}|^2$ is only a part of the total probability to find an atom in the state n

$$P_{n\kappa} = \sum_\nu |\langle \phi_{n\nu} | U(t,0) | \phi_\kappa \rangle|^2 . \qquad (23)$$

Here summation runs over all states of the kind "atom is in n , there are arbitrary number ν of photons with arbitrary momenta and polarizations ε . Just the $P_{n\kappa}$ corresponds to the experiment in which one detects only the atom excitation and does not measure any accompanying photons. Of course, in the majority of the transitions $\phi_\kappa \to \phi_{n\nu}$ in (23) the energy is not conserved, if "energy" means an eigenvalue of the free part of the total Hamiltonian. The probabilities of such "virtual transitions" are known to be nonzero for finite t . In particular, an atom can go to the state n and, moreover, emit a photon with any momentum κ' . Note that the described process proceeds independently of the presence of the initial photon. The r.h.s. of (23) is not equal to zero even if the initial state is not ϕ_κ but ϕ_0 : atom is in the ground state, no photons. Therefore, the measured total probability of the atom excitation must correspond only to the part of $P_{n\kappa}$, which is due to the presence of the photon κ in the initial state (it is the physical cause of the atom excitation). That part will be defined as

$$W_{n\kappa}(t) = \sum_\nu |\langle \phi_{n\nu} | U(t,0) | \phi_\kappa \rangle|^2 - \sum_\nu |\langle \psi_{n\nu} | U(t,0) | \phi_0 \rangle|^2 . \qquad (24)$$

We subtract from $P_{n\kappa}$ the "theoretical background", i.e., the probability of the "causeless transitions". It should be stressed that ϕ_κ in (24) must be normalized to unity, as the state ϕ_0 is.

Similar definitions for other cases were proposed, e.g., in refs. [14-17] .

Note that the Weisskopf-Wigner approximation does not take into account the virtual transitions in any way. They can be absent if atom and photon states are described in a special way, see, e.g., ref. [6] . In such a case (24) will be equal to $|\langle \phi_n | U(t,0) | \phi_\kappa \rangle|^2$.

2. I shall represent (23) as an expectation value of the Heisenberg operator $\hat{N}_n(t) = U^+(t,0)\,\hat{N}_n\,U(t,0)$ of the number of electrons in the state n (taken in the state ϕ_κ). The operator can be found by solving the equations for Heisenberg operators (without using $U(t,0)$ which may not exist [18]).

The second-quantized description of the nonrelativistic electron is needed. The Hamiltonian (1) corresponds to the one-electron sector of the Hamiltonian $\int d^3x\, H(x)$

$$H(\vec{x}) = \psi^*(\vec{x})\left\{[-i\vec{\nabla} - e\vec{A}_\perp - e\vec{A}^{ex}]^2/2m + W(\vec{x}) + e A_0^{ex}(\vec{x})\right\}\psi(\vec{x}) + \frac{1}{2}\left[\vec{E}_\perp^2(x) + \vec{H}^2(x)\right]$$

(see, e.g., [19]). The operator $\psi(x)$ is expanded over eigenfunctions φ_n of $H_e = p^2/2m + W(x)$

$$\psi(x) = \sum_n \varphi_n(x)\,\alpha_n , \qquad (25)$$

$\sum_n$ denotes summation and integration over H_e spectrum. Using electron and photon creation operators α_n^+ and $a^+(\kappa,\varepsilon)$ the states ϕ_κ , ϕ_n and ϕ_0 can be written as

$$\phi_\kappa = \alpha_0^+ a^+(\kappa,\varepsilon)\Omega_0 \quad , \quad \phi_n = \alpha_n^+\Omega_0 \quad , \quad \phi_0 = \alpha_0^+\Omega_0 , \qquad (26)$$

where Ω_0 is the no-particle state and α_0^+ creates the electron in the ground state.

Consider the operator $N_n = \alpha_n^+\alpha_n$ of the number of electrons in the state n . Expand $\alpha_n^+\alpha_n$ in the operators Π_N which project on the states with N electrons on the level n . The states may have electrons on other levels along with an arbitrary number of photons

$$\alpha_n^+\alpha_n = 0\cdot\Pi_0 + 1\cdot\Pi_1 + 2\cdot\Pi_2 + \ldots \qquad (27)$$

$$\Pi_1 = \sum_{\nu=0}^{\infty} \int d\kappa_1 \dots \int d\kappa_\nu \sum_{\varepsilon_1,\dots\varepsilon_\nu} |\phi_{n\nu}\rangle\langle\phi_{n\nu}| + \dots \qquad (28)$$

$$\phi_{n\nu} \equiv \alpha_n^+ a^+(\kappa_1,\varepsilon_1)\dots a^+(\kappa_\nu,\varepsilon_\nu)\Omega_0$$

Only the one-electron part of Π_1 is written. Of course, if our nonrelativistic electrons obey Fermi statistics, there cannot be two electrons in the same state and $\Pi_2 = 0$. Because of (27) and (28) we have

$$\langle U(t,0)\phi_\kappa | \alpha_n^+ \alpha_n | U(t,0)\phi_\kappa\rangle = \qquad (29)$$

$$= \sum_\nu \langle U(t,0)\phi_\kappa | \phi_{n\nu}\rangle\langle\phi_{n\nu} | U(t,0)\phi_\kappa\rangle = P_{n\kappa} .$$

As $U(t,0)\phi_\kappa$ is a one-electron state, only Π_1 contributes to (29), moreover, only the part of Π_1 contributes to (29), which is written in (27).

Introducing the Heisenberg operators $\alpha_n(t) = U^+(t,0)\alpha_n U(t,0)$ one can rewrite (24) as

$$W_{n\kappa}(t) = \langle\phi_\kappa | \alpha_n^+(t)\alpha_n(t) | \phi_\kappa\rangle - \langle\phi_0 | \alpha_n^+(t)\alpha_n(t) | \phi_0\rangle . \qquad (30)$$

Here α_n^+, α_n can be considered as creation-destruction operators of a second-quantized Dirac electron.

3. The atom states are described by eigenfunctions $\varphi_n(\vec{x})$ and $\varphi_n'(\vec{x})$ of $H_e = \vec{P}^2/2m + W(\vec{x})$ and $H_e' = \vec{P}'^2/2m + W(\vec{x})$ in the Coulomb and new gauge, respectively. If one uses, in the framework of each gauge, the same canonical representation $-i\vec{\nabla}$ for $\vec{p}$ and $\vec{p}'$, then $\varphi_n(\vec{x})$ and $\varphi_n(\vec{x}')$ are the same functions of $\vec{x}$. In the same manner the same canonical Fock representation can be used for the photon operators $a(\kappa,\varepsilon)$ and $a'(\kappa,\varepsilon)$ inside each gauge. So, one can use the same analytical description of ϕ_κ and ϕ_0 in both gauges. But interaction terms in (1) or (17) differ from those in (12) or (18). Therefore, the probability $W_{n\kappa}'$ calculated in the new gauge may differ from $W_{n\kappa}$ calculated in the Coulomb one. We shall calculate $W_{n\kappa}$ and $W_{n\kappa}'$ in the following solvable model.

If one assumes $W(q) = m\varkappa^2 q^2/2$ in (17), then one gets a solvable theory. It is possible to show that its Hamiltonian is not bounded from below (see Appendix A in [16]).

For this and other reasons (see Sec. 1 in [16]) one should spread beforehand the local interaction of the electron with photons in (1). This is realized by replacing

$$\vec{A}_1(q) \to \hat{\vec{A}}(q) = \int d^3y\ G(|\vec{q}-\vec{y}|)\vec{A}_1(y) , \qquad (31)$$

$$G(\vec{x}) = (2\pi)^{-3}\int d^3k\ e^{i\vec{k}\vec{x}} \frac{\mu^2}{k^2+\mu^2} , \qquad \varkappa \ll \mu \ll \sqrt{m\varkappa} . \qquad (32)$$

After the replacement we substitute $\hat{\vec{A}}(0)$ and $\vec{A}^{ex}(0,t)$ for $\hat{\vec{A}}(q)$ and $\vec{A}^{ex}(q,t)$ in (1). Expanding further $\hat{\vec{A}}$ in multipoles we get that the electron interacts only with dipole photons. Retaining in the Hamiltonian only their creation-destruction operators we get the Hamiltonian h_d. It turns our to be a sum $h_x + h_y + h_z$ of three mutually commuting operators h_x, h_y, h_z where, e.g., h_z contains electron operators p_z, q_z and dipole photon operators $a_z(\kappa)$, $a_z^+(\kappa)$ of the "z-species" (the subscript z of $a_z(\kappa)$ stems from the z-projection of the photon total angular momentum). If the initial vector ϕ_κ is $a_z^+(\kappa)\Omega_0$, then the subsequent evolution is determined only by h_z. It is written explicitly (without A_μ^{ex}) in [16,20]. The model is exactly solvable because h_z is a quadratic form of p_z, q_z, $a_z(\kappa)$, $a_z^+(\kappa)$.

The eigenstates of the operator $p_z^2/2m + m\varkappa^2 q_z^2/2$ can be represented as $(\alpha_z^+)^n\Omega_0$, $n = 0,1,2,\dots$ using the operator

$$\alpha_z^+ = \left[p_z/\sqrt{m\varkappa} + i\,q_z\sqrt{m\varkappa}\right]/\sqrt{2} . \qquad (33)$$

The corresponding Hamiltonian h_z' of the new gauge is obtained using the simplified canonical transformation (see Sec. 3.6). If the replacement (31) is introduced, the transformation operator must be of the form

$$\hat{S} = \exp\left\{(-ie)\left[\vec{q}\cdot\hat{\vec{A}}(0) + \vec{q}\cdot\vec{A}^{ex}(0,t)\right]\right\} . \qquad (34)$$

4. Let the exciting electromagnetic field be described by an initial photon (as is the case in the preceding subsections 4.1 – 4.2) and not by an external potential. Let then $A_\mu^{ex} = 0$ in this subsection. It is possible to calculate exactly the probability

$$W_K(t) = \langle \phi_K \mid \alpha_2^+(t)\alpha_2(t) \mid \phi_K \rangle - \langle \Omega_0 \mid \alpha_2^+(t)\alpha_2(t) \mid \Omega_0 \rangle . \qquad (35)$$

For α_2^+ see (33); ϕ_K describes one dipole photon having the mean frequenoy K with dispersion $\Delta K \ll K$

$$\phi_K = \int_0^\infty dk' f_K(k') a_2^+(k') \Omega_0 , \qquad \int_0^\infty dk' |f_K(k')|^2 = 1 .$$

I present only the result of calculations with the Hamiltonian h_2 (for similar calculations see /16/). Note first that the difference (35) (unlike its first or second term) tends to zero as $t \to \infty$. This is natural because excited states are unstable. Further, $W_K(t)$ has the resonance term which is large for $K \cong \varkappa$. Retaining only this term and making some other neglects, we have for $1/\varkappa < t < 1/\Delta K$ and $\varkappa - 2\gamma < K < \varkappa + 2\gamma$

$$W_K(t) \cong C e^2 |d|^2 K \frac{\varkappa^2}{(K-\varkappa')^2+\gamma^2} \left[1 + e^{-2\gamma t} - 2e^{-\gamma t}\cos(K-\varkappa')t\right]. \qquad (36)$$

Here $|d|^2 = 1/2m\varkappa$ is the square of the dipole moment $d = \langle \alpha_2^+ \Omega_0 \mid q_2 \mid \Omega_0 \rangle$; $\varkappa'$ differs only slightly from $\varkappa$, if the cut-off parameter μ is chosen as in (32); $\gamma \cong e^2\varkappa^2/3m$ C does not depend upon K , $\varkappa \cong \varkappa'$, t.

Analogous probability W_K' was calculated in the new gauge (all operators in (35) are replaced by the primed ones). It turns out to be exaotly equal to $K^2/\varkappa^2 \cdot W_K(t)$, so that for $1/\varkappa < t < 1/\Delta K$ and $\varkappa - 2\gamma < K < \varkappa + 2\gamma$ one has

$$W_K'(t) \cong C e^2 |d|^2 K \frac{K^2}{(K-\varkappa')^2+\gamma^2} \left[1 + e^{-2\gamma t} - 2e^{-\gamma t}\cos(K-\varkappa')t\right]. \qquad (37)$$

I stress that here $\varkappa'$ and γ are the same quantities as in (36): the line shift and its width are the same in either gauges.

Note that the average number of the photon of the frequency K which are emitted by the exoited oscillator

$$\langle \alpha_2^+ \Omega_0 \mid a_2^+(K,t) a_2(K,t) \mid \alpha_2^+ \Omega_0 \rangle - \langle \Omega_0 \mid a_2^+(K) a_2(K) \mid \Omega_0 \rangle$$

is represented approximately by the r.h.s. of (36) at $1/\varkappa < t < \infty$. The expression coincides with eq. (124) from Ch.8 of ref. /21/ (eq. (124) is also approximate). At large t the r.h.s. of (36) and of (37) coinoide also with eqs. (50) and (53) of ref. /2/, respeotively.

The importance of the discrepancy between (36) and (37) for the Lamb shift determination has been discussed in ref. /2,5/.

Note that both gauges of the model have the same S-matrix (i.e., photon-electron soattering). For its calculation see Appendix B in ref. /16/ and also ref. /22/.

5. The external-field approximation seems to provide a better description of the microwave radiation of the Lamb-shift experiments than the one-photon description. The microwave field is strong and has a complicated structure.

Consider the simple external field (20). The reason for writing the phase β is the following. The metastable atoms enter into the microwave field region at unknown accidental moments of time. They are initial moments (t=0) of the field action on atoms and $\vec{E}^{ex}(0,t)$ must not be maximum at t=0. The final result must be averaged over all β , $0 \le \beta < 2\pi$, cf. /11/, Sec. 4.2. The averaging corresponds also to the completely uncertain phase of the one-photon wave.

The difference

$$\langle \mathcal{U}(t,0)\Omega \mid \alpha_2^+ \alpha_2 \mid \mathcal{U}(t,0)\Omega \rangle - \langle \mathcal{U}_0(t,0)\Omega \mid \alpha_2^+ \alpha_2 \mid \mathcal{U}_0(t,0)\Omega \rangle \qquad (38)$$

was calculated in the model described in subsection 4.3. Here $\mathcal{U}(t,0)$ satisfies the eq. $i\partial\mathcal{U}/\partial t = h_2(t)\mathcal{U}$ where $h_2(t)$ contains the external potential (21). $\mathcal{U}_0(t,0)$ is the evolution operator in the case the external field (the cause of atom excitation) is absent: $\mathcal{U}_0(t,0) = exp(-it\,h_2^0)$, where h_2^0 does not contain A_μ^{ex} (as in subsection 4.4). For Ω one can take, e.g., the "bare" or "physical" vaouum. Let $W_K^{ex}(t)$ denote the difference (38) averaged over β . The result of its calculation (for similar calculation see /23/) can be approximately represented at $t < 1/\varkappa$ by the r.h.s. of (36) if the amplitude E_0 in (20) is chosen so that the energy of the dipole part of the external field is equal to the energy K of the one-dipole-photon state ϕ_K in (35).

The analogous quantity $W_K'^{ex}(t)$ of the new gauge turns out to be exactly equal to $K^2/\varkappa^2 \cdot W_K^{ex}(t)$.

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