Form of the Hamiltonian and the initial conditions in radiation problems

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The use of two of the most often employed forms of the Hamiltonian describing the interaction of atoms and molecules with an electromagnetic field is examined using the example of spontaneous emission. It is shown that formally the same initial state corresponds in the cases of different Hamiltonians to physically different initial conditions: a stationary Coulomb field exists in the initial state in one case and a nonstationary field, arising upon sudden excitation of the atom, exists in another. The differences in the initial conditions determine the differences in the photon spectra arising upon subsequent emission. The choice of initial conditions in real situations can be made by making a physical analysis of the excitation process. The Hamiltonian is transformed from one form to another. It is emphasized that the Hamiltonians are equivalent only if the states are correspondingly transformed. The Lamb-Retherford experiment is analyzed qualitatively.

CONTENTS

1. INTRODUCTION

Quantum electrodynamics developed primarily as a theory of scattering, i.e., the initial conditions in the theory were imposed in the limit $t \to -\infty$. There exists, however, a wide range of problems in which the initial condition must be imposed at some definite moment in time, for example, at $t = 0$. The role of initial conditions in the problems of emission from atoms and molecules or, more generally, in problems of quantum electrodynamics, has not been adequately studied. In this paper we call attention to one aspect of this problem, related to the choice of one of two different forms of the Hamiltonian describing the interaction between atoms and the electromagnetic field.

The first form of the Hamiltonian is as follows

$$H = \frac{1}{2m}(\mathbf{p} - e\mathbf{A}(\mathbf{r}))^2 + U(\mathbf{r}) + \frac{1}{8\pi}\int dV(\mathbf{E}^2 + \mathbf{H}^2); \quad (1)$$

the leading (linear with respect to e) term of the atom-field interaction in the Coulomb gauge is equal to

$$-\frac{e}{m}\mathbf{pA}(\mathbf{r}).$$

The second form of the Hamiltonian, which we shall not for the time being write out completely, is as follows

$$H' = \frac{1}{2m}\mathbf{p}^2 + U(\mathbf{r}) + \frac{1}{8\pi}\int dV(\mathbf{E}^2 + \mathbf{H}^2) - e\mathbf{r}\mathbf{E}^{\perp} + \ldots. \quad (2)$$

As we can see, the unperturbed part in the second form is the same as in the first form, but the term describing the interaction of the atom with the field is equal to

$$-e\mathbf{r}\mathbf{E}^{\perp}. \quad (3)$$

Already in 1931 Maria Goeppert-Meyer[1] examined the canonical transformation of the Hamiltonian (1) which leads to the interaction of atoms with a field in the form (3). This transformation was performed only in the dipole approximation and with an unquantized field. It was later examined in Ref. 2, where the advantages of the second form, involving the elimination of some low-frequency divergences, were pointed out. Then, in Ref. 3, based now on the quantum theory, a unitary transformation corresponding to the classical canonical transformation was established:

$$H' = S^{-1}HS, \quad (4)$$

where S is the transformation operator (see below). Based on the existence of the canonical transformation from one form to another and on the fact that both forms follow from Maxwell's equations and the equations of motion of the electron, there was complete confidence in the equivalence of the two forms of the Hamiltonian, when in 1947–1948 W. P. Lamb showed, in a well-known series of papers[4] on the measurement of the Lamb shift, that some of the spectral distributions which he measured are described better theoretically if the form (3) of the interaction Hamiltonian is used. This demonstrated for the first time that the two "theoretically

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equivalent" forms of the Hamiltonian used in ordinary quantum-mechanical calculations, for example, in calculations of the shape of a spectral line, lead to different results and that these results agree with experiments only for one of the forms, namely, for form (2). In essence, a paradox, which gave rise to a series of papers[5-8] expressing a wide spectrum of opinions about its nature, appeared.

The paradox is easily resolved, at least in the case when both the field and the atoms are described quantum-mechanically. Indeed, in quantum mechanics the Hamiltonian describes the variation of a state with time:

$$|\Delta\psi\rangle \approx \frac{\Delta t}{i\hbar} H|\psi_0\rangle, \tag{5}$$

where $|\psi_0\rangle$ is the initial state of the system. As long as spontaneous emission is studied, as in this paper, $|\psi_0\rangle = |b, 0\rangle$ refers to the excited state of the atom $|b\rangle$ and the vacuum state of the field, i.e., zero photons $|0\rangle$. In order that relation (5) be valid over long time intervals Δt, both the Hamiltonian and the state are usually described in the interaction representation. For our purposes, however, this circumstance is not important and we shall ignore it.

The probability amplitudes of the transitions are obtained if the relation (5) is multiplied on the left by the state $\langle n|$ belonging to some complete set of orthogonal states:

$$M = \langle n|\Delta\psi\rangle \approx \frac{\Delta t}{i\hbar}\langle n|H|\psi_0\rangle. \tag{6}$$

Evidently, the transition probability amplitudes M do not change if the entire equality (6) is subjected to a unitary transformation:

$$M = \langle n|\Delta\psi\rangle \approx \frac{\Delta t}{i\hbar}\langle n|SS^{-1}HSS^{-1}|\psi_0\rangle = \frac{\Delta t}{i\hbar}\langle n'|H'|\psi_0'\rangle.$$

As we can see, under a unitary transformation described by the operator S, both the Hamiltonian (4) and the states

$$|\psi_0'\rangle = S^{-1}|\psi_0\rangle, \quad \langle n'| = \langle n|S, \tag{7}$$

must be transformed. This resolves the paradox, since the states, and in particular the initial state $|\psi_0\rangle$, are not transformed according to (7) (see Ref. 4) and the untransformed states are used. Naturally, in this case, the unitary equivalence of the Hamiltonians breaks down and different computational results are obtained.

The resolution of the paradox does not however, exhaust all problems. Indeed, the reluctance to transform the states, and in particular the initial state, can be understood as follows. Since the operator S, as will be evident below, contains the photon creation and annihilation operators, the transformed states correspond to the presence of photons in the initial state but not in the vacuum state. Since we are studying spontaneous emission, i.e., the process of photon creation, the presence of photons in the initial state seems illogical. On the other hand, it seems natural to take as the initial state the vacuum state of the field, i.e., the untransformed initial state.

The use of untransformed states with the transformed Hamiltonian means that the quantity

$$M' = \frac{\Delta t}{i\hbar}\langle n \mid H' \mid \psi_0\rangle = \frac{\Delta t}{i\hbar}\langle n \mid S^{-1}HS \mid \psi_0\rangle = \frac{\Delta t}{i\hbar}\langle n'' \mid H \mid \psi_0''\rangle,$$

where

$$|\psi_0''\rangle = S|\psi_0\rangle, \quad \langle n''| = \langle n|S^{-1}, \tag{8}$$

is calculated, i.e., it may be regarded that the old Hamiltonian is used with the new initial conditions. The question of the representation of the Hamiltonians in two forms therefore reduces to a change in the initial conditions, and it is important to clarify the nature of the state $S|\psi_0\rangle$ and how it differs from $|\psi_0\rangle$.

A second question of interest is: how should the photons in the state $|\psi_0'\rangle$, which is equivalent to the state $|\psi_0\rangle$ with no photons, be interpreted? As we shall see, both these questions have essentially a single answer. In Sec. 2, we shall study the state $|\psi_0''\rangle$. for this, we will have to find the average value of the electric field in this state.

2. TRANSFORMATION OF THE ELECTRIC FIELD

We shall assume that the states $|\psi_0''\rangle$ and $|\psi_0\rangle$ are represented by the average values of some observables in these states. In particular, we will be interested in the average value of the electric field **E**. Naturally, the average values of observables by no means exhaust the states $|\psi_0''\rangle$. and $|\psi_0\rangle$. For example, a knowledge of the average value of the field says nothing about the average value of the square of the field, etc. As we shall see, however, the average values of the field will already clearly demonstrate the difference between the states $|\psi_0''\rangle$ and $|\psi_0\rangle$.

In the Coulomb gauge, as always, the electric field consists of transverse $\mathbf{E}^{\perp}(\mathbf{R})$ and longitudinal $\mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R})$ parts (the longitudinal part is a function of the coordinates as well as of the point of observation **R**). We shall first examine the transverse field in the state $|\psi_0''\rangle$. Its average value equals

$$\langle \mathbf{E}^{\perp}(\mathbf{R})\rangle = \langle \psi_0'' \mid \mathbf{E}^{\perp}(\mathbf{R}) \mid \psi_0''\rangle = \langle \psi_0 \mid S^{-1}\mathbf{E}^{\perp}(\mathbf{R})\, S \mid \psi_0\rangle.$$

We can therefore first transform the field

$$\mathbf{E}^{\perp\prime} = S^{-1}\mathbf{E}^{\perp}S$$

and then average it over the old state $|\psi_0\rangle$.

The unitary operator S has the form[1),3]

$$S = \exp\left[ie \int \mathrm{d}\mathbf{x}\mathbf{P}(\mathbf{r}, \mathbf{x})\, \mathbf{A}(\mathbf{x})\right], \tag{9}$$

where

$$\mathbf{P}(\mathbf{r}, \mathbf{x}) = \mathbf{r}\left[1 - \frac{1}{2!}(\mathbf{r}\nabla) + \frac{1}{3!}(\mathbf{r}\nabla)^2 - \ldots\right]\delta(\mathbf{x}) \tag{10}$$

(the operator ∇ refers to differentiation with respect to **x** and $\mathbf{A}(\mathbf{x})$ is the vector potential. The form of the operator S is obtained in Ref. 3 from the condition that the transformation (4) give the same result as in the canonical Goeppert-Meyer transformation.[1] The vector field $\mathbf{P}(\mathbf{r}, \mathbf{x})$,[2)] which depends on the position vector of the electron **r** as a parameter, can be represented in the form

[1)]The sign in the exponent of the operator S in the paper by Power and Zienau is not correct (Ref. 3, p. 450).

[2)]It is incorrectly stated in the paper by Power and Zienau that the field $\mathbf{P}(\mathbf{r}, \mathbf{x})$ satisfies the equality $\mathbf{j} = \dot{\mathbf{P}}(\mathbf{r}, \mathbf{x})$, where $\mathbf{j}(\mathbf{r}, \mathbf{x})$ is the current.

$$\mathbf{P}(\mathbf{r},\ \mathbf{x})=\hat{\mathbf{r}}\Big[1-\Big(1-(\mathbf{r}\nabla)+\frac{1}{2!}(\mathbf{r}\nabla)^2-\frac{1}{3!}(\mathbf{r}\nabla)^3+\ldots\Big)\Big]$$

$$\times V(\mathbf{r},\ \mathbf{x})=\hat{\mathbf{r}}\,[V(\mathbf{r},\ \mathbf{x})-V(\mathbf{r},\ \mathbf{x}-\mathbf{r})], \qquad (11)$$

where $\hat{\mathbf{r}}$ is the unit vector corresponding to the direction of $\mathbf{r}$ and $V(\mathbf{r}, \mathbf{x})$ is determined by the condition

$$(\mathbf{r}\nabla)\ V(\mathbf{r},\ \mathbf{x})=\delta(\mathbf{x}).$$

The function $V(\mathbf{r}, \mathbf{x})$ can also be represented as

$$V(\mathbf{r},\ \mathbf{x})=\frac{i\mathbf{r}}{(2\pi)^3}\int d\mathbf{k}\,\frac{e^{-i\mathbf{k}\mathbf{x}}}{(\mathbf{u}\mathbf{k})+i\varepsilon}, \qquad \varepsilon>0,$$

and

$$V(\mathbf{r},\ \mathbf{x})=\theta(\mathbf{x}^{\parallel})\,\delta(\mathbf{x}^{\perp}),$$

where

$$\mathbf{x}=\mathbf{x}^{\parallel}+\mathbf{x}^{\perp}, \quad \mathbf{x}^{\parallel}\parallel\mathbf{r}, \quad \mathbf{x}^{\perp}\perp\mathbf{r}.$$

The last expression for $V(\mathbf{r}, \mathbf{x})$ permits giving a simple physical description of the field $\mathbf{P}(\mathbf{r}, \mathbf{x})$ which we have not encountered in the literature, making it possible to perform calculations without using multipole expansions. The field $\mathbf{P}(\mathbf{r}, \mathbf{x})$ is nonzero (equal to infinity) in a narrow (infinitely narrow) tube, which is oriented away from the origin of coordinates toward the point at which the electron is located, and is oriented along the tube (Fig. 1). This field must be viewed as a generalized function of $\mathbf{x}$; it can enter into the final expressions only as an integrand in an integral over $\mathbf{x}$.

The field $\mathbf{P}(\mathbf{r}, \mathbf{x})$, just as, in general, any field, can be decomposed into rotational and irrotational parts. An important property of the field $\mathbf{P}(\mathbf{r}, \mathbf{x})$ is that its irrotational part coincides to within a factor of $-4\pi e$ with the total Coulomb field of the nucleus and of the electron, when the former is located at the origin of coordinates and the latter is located at the point $\mathbf{r}$:

$$\mathbf{E}^{\parallel}(\mathbf{r},|\ \mathbf{R})=-4\pi e\mathbf{P}^{\parallel}(\mathbf{r},\ \mathbf{R}). \qquad (12)$$

To separate out the longitudinal part of the field $\mathbf{P}(\mathbf{r}, \mathbf{x})$, we shall use the well-known relation

$$P_{\lambda}^{\parallel}(\mathbf{r},\ \mathbf{R})=\int d\mathbf{x}\delta_{\lambda\mu}^{\parallel}(\mathbf{x}-\mathbf{R})\,P_{\mu}(\mathbf{r},\ \mathbf{x}),$$

where

$$\delta_{\lambda\mu}^{\parallel}(\mathbf{x}-\mathbf{R})=\frac{1}{4\pi}\frac{\partial^2}{\partial x_{\lambda R}\,\partial x_{\mu x}}\frac{1}{|\mathbf{x}-\mathbf{R}|}$$

is the so-called longitudinal δ function. Substituting here

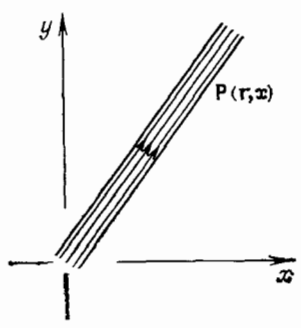


FIG. 1. The field $\mathbf{P}(\mathbf{r}, \mathbf{x})$.

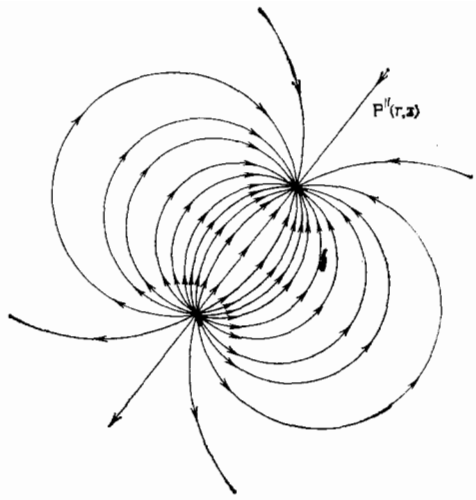


FIG. 2. The field $\mathbf{P}^{\parallel}(\mathbf{r}, \mathbf{x})$.

(10) and integrating by parts, we obtain

$$\mathbf{P}^{\parallel}(\mathbf{r},\ \mathbf{R})=-\frac{1}{4\pi}\operatorname{grad}_R\frac{1}{R}+\frac{1}{4\pi}\operatorname{grad}_R\frac{1}{|\mathbf{r}-\mathbf{R}|},$$

which coincides to within a factor of $-4\pi e$ with the Coulomb potential of a nucleus located at the origin and of an electron located at the point $\mathbf{r}$ (Fig. 2). We now have enough information to carry out the transformation of the field:

$$\mathbf{E}^{\perp\prime}=S^{-1}\mathbf{E}^{\perp}S.$$

For this, we shall use the well-known operator relation

$$e^{A}Be^{-A}=B+[A;\ B]+\frac{1}{2!}[A;\ [A;\ B]]+\frac{1}{3!}[A;\ [A;\ [A;\ B]]]+\ldots \qquad (13)$$

and we shall calculate the first commutator in this expression for the case under study:

$$\Big[-ie\int d\mathbf{x}\mathbf{P}(\mathbf{r},\ \mathbf{x})\,\mathbf{A}(\mathbf{x});\ \mathbf{E}^{\perp}(\mathbf{R})\Big]$$

$$=ie\sum_{\lambda\mu}\mathbf{e}_{\mu}\int d\mathbf{x}P_{\lambda}(\mathbf{r},\ \mathbf{x})\Big[A_{\lambda}(\mathbf{x});\ \frac{\partial A_{\mu}(\mathbf{R})}{\partial t}\Big].$$

Since the commutator in the last expression is equal, to within a factor of $4\pi i$ to the so-called transverse δ function $\delta_{\lambda\mu}^{\perp}(\mathbf{x}-\mathbf{R})$ we have

$$-4\pi e\sum_{\lambda\mu}\int d\mathbf{x}P_{\lambda}(\mathbf{r},\ \mathbf{x})\,\delta_{\lambda\mu}^{\perp}(\mathbf{x}-\mathbf{R})$$

$$=-4\pi e\mathbf{P}^{\perp}(\mathbf{r},\ \mathbf{R})=-4\pi e\,[\mathbf{P}(\mathbf{r},\ \mathbf{R})-\mathbf{P}^{\parallel}(\mathbf{r},\ \mathbf{R})];$$

the field $\mathbf{P}^{\perp}(\mathbf{r}, \mathbf{R})$ is shown in Fig. 3. It is evident from here that all higher-order commutators in (13) vanish, and the transformed field therefore has the form

$$\mathbf{E}^{\perp\prime}=\mathbf{E}^{\perp}(\mathbf{R})-4\pi e\,[\mathbf{P}(\mathbf{r},\ \mathbf{R})-\mathbf{P}^{\parallel}(\mathbf{r},\ \mathbf{R})]. \qquad (14)$$

We shall now examine the Coulomb field. The Coulomb field is not described by a Hamiltonian. Under quantization it is eliminated in the transformation from the Lagrangian description to the Hamiltonian description,[9] since it is not a real Hamiltonian variable (the momentum conjugate to the

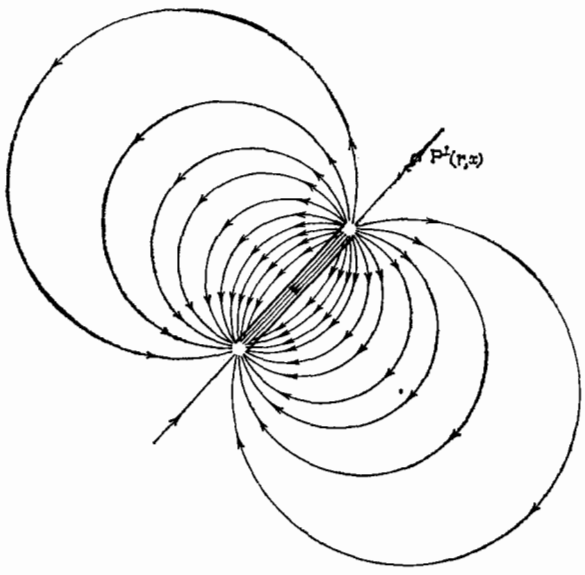


FIG. 3. The field $\mathbf{P}^{\perp}(\mathbf{r}, \mathbf{x})$.

Coulomb potential equals zero). However, the elimination of the Coulomb field from the Hamiltonian apparatus by no means indicates that this field does not exist physically. Actually, the equations following from the Hamiltonian must be supplemented by an independent equation for the scalar potential

$$\Delta\varphi = 4\pi\rho \tag{15}$$

or, if the electron is assumed to be a point particle,

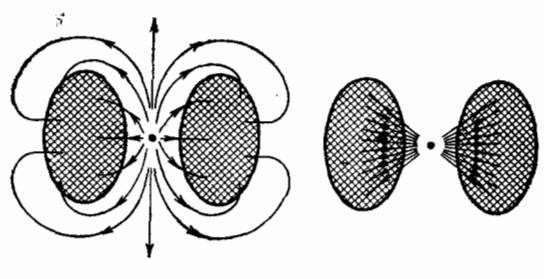
$$\mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R}) = -\operatorname{grad}\varphi = e\operatorname{grad}_R \frac{1}{|\mathbf{r}-\mathbf{R}|} - e\operatorname{grad}\frac{1}{|\mathbf{R}|},$$

where the first term represents the Coulomb field of the electron and the second term represents the Coulomb field of the nucleus. The Coulomb field of an atom (it is also the average total field in the transformed state) in the p state is shown in Fig. 4a. Since this field depends only on the coordinates of the electron and therefore commutes with the exponent in (9), under the transformation

$$\mathbf{E}^{\parallel\prime}(\mathbf{r}, \mathbf{R}) = S^{-1}\mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R})\, S = \mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R}) \tag{16}$$

it remains unchanged. According to (12),

$$\mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R}) = -4\pi e\mathbf{P}^{\parallel}(\mathbf{r}, \mathbf{R});$$



a b

FIG. 4. The electric field in the states $|b, 0\rangle$ (a) and $S|b, o\rangle$ (b). $|b\rangle$ is the p-state of the excited atom.

adding (14) and (16), we obtain the transformation of the total field

$$\mathbf{E}'(\mathbf{r}, \mathbf{R}) = S^{-1}\mathbf{E}(\mathbf{r}, \mathbf{R})\, S = \mathbf{E}^{\perp}(\mathbf{R}) - 4\pi e\mathbf{P}(\mathbf{r}, \mathbf{R}). \tag{17}$$

Averaging this field over the vacuum state and over the excited state of the atom (for example, over the p state), we obtain the field pattern shown in Fig. 4b. The average field in the transformed state, as already mentioned, equals the Coulomb field (Fig. 4a), since due to the nonlinearity with respect to the creation and annihilation operators we have $\langle\overline{\mathbf{E}}^{\perp}\rangle = 0$.

We thus see that the average field in the states $|\psi_0\rangle = |b, 0\rangle$ (Fig. 4a) and $|\psi_0''\rangle = S\,|b, 0\rangle$ (Fig. 4b) differ in an essential way. The transformation under study actually eliminates the external part of the Coulomb field, and the remaining part of the field transforms in such a manner that Gauss's theorem would be satisfied. It should be noted that with respect to the operators $a_{k\lambda}^{+}$ and $a_{k\lambda}$ the operator S has the form

$$e^{i(za_{k\lambda}^{+} + z^{*}a_{k\lambda})},$$

i.e., it creates a coherent state of the field from the vacuum state. This is entirely natural, since the created field must compensate the unquantized longitudinal field. Therefore, emission when the initial state is $|\psi_0^{\parallel}\rangle = S\,|b, 0\rangle$ begins with a nonstationary Coulomb field, in contrast to the case when the initial state is $|\psi_0\rangle = |b, 0\rangle$, in which the Coulomb field is stationary. The situation here is the same as in the case of the free motion of an electron. V. S. Ginzburg[10] showed that if the equilibrium field is chosen as the initial state for the free electron, then the electron does not radiate; with a nonstationary field, however, the electron does radiate at the initial moment, as if it were enveloped by a stationary field. In the case under study the electron radiates in both cases, but, as will be shown in Sec. 5, it does so differently.

Thus the main difference between the states $|\psi_0\rangle$ and $|\psi_0''\rangle = S\,|\psi_0\rangle$ has been clarified and the answer to the first question posed at the end of Sec. 1 is clear. The answer to the second question is also clear. Indeed, the state $|\psi_0'\rangle = S^{-1}|\psi_0\rangle$, which is equivalent to the state $|\psi_0\rangle$, must contain a packet of photons forming a rotational field, which together with the field $-4\pi e\mathbf{P}$ leads to the same stationary Coulomb field as in the state $|\psi_0\rangle$ with the untransformed operators.

3. INSTANTANEOUS EXCITATION OF AN ATOM. NATURE OF THE FIELD P(r, x)

We shall examine the problem of the instantaneous excitation of the atom. This analysis will clarify the nature of the field $\mathbf{P}(\mathbf{r}, \mathbf{x})$. Let the atom, which is in the ground state $|a\rangle$ at time $t = 0$, experience a strong sudden perturbation, as a result of which it is excited and subsequently radiates, returning to the state $|a\rangle$. The Hamiltonian of the system atom + field + source-of-instantaneous-action depends on the time:

$$\mathcal{H} = H + K(t),$$

where H is the time-independent part of the Hamiltonian

and describes the atom, electromagnetic field, and their interaction (1) and $K(r, t)$ is the part of the Hamiltonian that describes the action of the external field on the atomic electron. We transform to the representation

$$W(t) = e^{iHt} K(t) e^{-tHt}.$$

Then the evolution operator has the form[11]

$$G(t) = e^{-i(Y_1+Y_2+\dots)},$$

where

$$Y_1(t) = \int_{t'}^{t} dt_1 W_1, \quad Y_2(t)$$

$$= \frac{-i}{2!} \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 [W_1; W_2]; \dots W_\alpha = W(t_\alpha).$$

We choose the following specific form of the operator $K(t)$:

$$K(t) = -m(\mathbf{ur}) \frac{d\delta(t)}{dt}, \quad \operatorname{grad}_r K(t) = -m\mathbf{u} \frac{d\delta(r)}{dt},$$

$$\mathbf{u} = \text{const}.$$

The field created by the external perturbation in the vicinity of the atom is spatially uniform and its time-dependence follows that of the derivative of the $\delta(t)$ function with respect to time (Fig. 5). The quantity $Y_1(t)$ is easily calculated:

$$Y_1(t) = \int_{t'}^{t} dt_1 W_1 = -m \int_{t'}^{t} dt_1 \frac{d\delta(t_1)}{dt_1} e^{iHt_1} (\mathbf{ur}) e^{-iHt_1}$$

$$= im[H; \mathbf{ur}] = \mathbf{u}(\mathbf{p} - e\mathbf{A}(\mathbf{r})).$$

Calculating Y_2, we obtain an infinite quantity, which, however, is a C-number, and not an operator, and makes a contribution only to the unimportant phase of the state. Neglecting higher order terms, we find that the evolution operator, arising due to the "instantaneous" action, has the following form:

$$G = e^{-i\mathbf{u}(\mathbf{p} - e\mathbf{A}(\mathbf{r}))}. \tag{18}$$

We shall examine the state of the system after the instantaneous action, but before the onset of emission. As before, we shall describe it by the average values of some quantities in this state. In particular, we shall calculate the average value of the electric field. To calculate the average value of the quantity $\hat{O}$ in the state

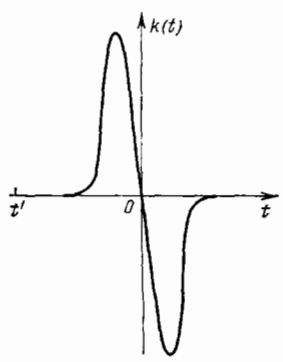


FIG. 5. The perturbing potential as a function of time.

$$|\psi\rangle = G|a, 0\rangle$$

the quantity $\hat{O}$ must be transformed according to the rule

$$\hat{O}_G = G^{-1}\hat{O}G$$

and the resulting expression must be averaged over the initial state

$$\langle \hat{O}_G \rangle = \langle a, O | G^{-1}OG | a, 0 \rangle.$$

We shall examine the transformation of different operators under the action of the unitary operator G. We shall first examine the transformation of the coordinates of the electron:

$$\mathbf{r}_G = e^{i\mathbf{u}(\mathbf{p}-e\mathbf{A}(\mathbf{r}))} \mathbf{r} e^{-i\cdot \mathbf{p}-e\mathbf{A}(\mathbf{r}))} = \mathbf{r} + \mathbf{u}.$$

This transformation is easily obtained, if one makes use of the expansion (13) and takes into account the fact that it is truncated at the second term, since a C-number vector $\mathbf{u}$ is already obtained in this order:

$$[i\mathbf{u}(\mathbf{p} - e\mathbf{A}(\mathbf{r})); \mathbf{r}] = i \sum_{\lambda\mu} \mathbf{e}_\mu u_\lambda [p_\lambda; r_\mu] = \sum_{\lambda\mu} \mathbf{e}_\mu u_\lambda \delta_{\lambda\mu} = \mathbf{u},$$

which makes all subsequent commutators vanish. Thus the instantaneous action leads to a displacement of the charge distribution by the vector $\mathbf{u}$. This reveals the physical meaning of the vector $\mathbf{u}$. The vector potential at the point of observation $\mathbf{R}$ remains unchanged under the transformation being studied, since it does not depend on the coordinates of the electron and, therefore, commutes both with $\mathbf{p}$ and with $\mathbf{A}(\mathbf{r})$. The transformation of the transverse field $\mathbf{E}^\perp(\mathbf{R})$ is more interesting. We again use the expansion (13) and examine its second term:

$$i[\mathbf{u}(\mathbf{p} - e\mathbf{A}(\mathbf{r})); \mathbf{E}^\perp(\mathbf{R})] = -ie[\mathbf{uA}(\mathbf{r});$$

$$\mathbf{E}^\perp(\mathbf{R})] = ie \sum_{\lambda\mu} e_\mu u_\lambda \left[A_\lambda; \frac{\partial A_\mu}{\partial t}\right].$$

The commutator of the components of the vector potential and its time derivative is known and equals the so-called transverse $\delta^\perp(\mathbf{r} - \mathbf{R})$ function, multiplied by $4\pi i$. Therefore,

$$i[\mathbf{u}(\mathbf{p} - e\mathbf{A}(\mathbf{r})); \mathbf{E}^\perp(\mathbf{R})] = -4\pi e \sum_{\lambda\mu} \mathbf{e}_\mu u_\lambda \delta^\perp_{\lambda\mu}(\mathbf{r} - \mathbf{R})$$

$$= -4\pi e[\mathbf{u}\delta(\mathbf{r} - \mathbf{R}) - \sum_{\lambda\mu} \mathbf{e}_\mu u_\lambda \delta^{\parallel}_{\lambda\mu}(\mathbf{r} - \mathbf{R})]. \tag{19}$$

All subsequent commutators in the expansion (13) are now easily calculated with the help of the relation

$$i[\mathbf{u}(\mathbf{p} - e\mathbf{A}(\mathbf{r})); F(\mathbf{r})] = i[\mathbf{up}; F(\mathbf{r})]$$

$$= i \sum_\lambda u_\lambda [p_\lambda; F(\mathbf{r})] = \sum_\lambda u_\lambda \frac{\partial F}{\partial r_\lambda} = (\mathbf{u}\nabla) F.$$

For the first term from (19) all commutators of the expansion (13) can be put into the form

$$-4\pi e\mathbf{u}\left[1 + \frac{1}{2!}(\mathbf{u}\nabla_r) + \frac{1}{3!}(\mathbf{u}\nabla_r)^2 + \dots\right]\delta(\mathbf{r} - \mathbf{R}).$$

Replacing differentiation with respect to $\mathbf{r}$ by differentiation with respect to $\mathbf{R}$, we obtain

$$-4\pi e\mathbf{u}\left[1 - \frac{1}{2!}(\mathbf{u}\nabla_R) + \frac{1}{3!}(\mathbf{u}\nabla_R)^2 - \dots\right]\delta(\mathbf{R} - \mathbf{r})$$

$$= -4\pi e\mathbf{P}(\mathbf{u}, \mathbf{R} - \mathbf{r})$$

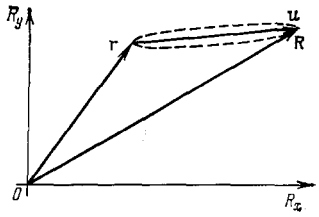


FIG. 6. The region where the field $\mathbf{P}(\mathbf{u}, \mathbf{R}-\mathbf{r})$ differs from zero.

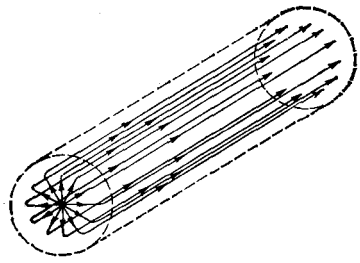


FIG. 7. The electric field in the excited state $G|a, 0\rangle$. $|a\rangle$ is the ground s-state of the atom.

which is the field $\mathbf{P}$ with which we are already familiar. Representing this expression in the form

$$-4\pi e\mathbf{P}(\mathbf{u}, \mathbf{R}-\mathbf{r}) = -4\pi e\hat{\mathbf{u}}[V(\mathbf{u}, \mathbf{R}-\mathbf{r}) - V(\mathbf{u}, \mathbf{R}-\mathbf{r}-\mathbf{u})],$$

where $\hat{\mathbf{u}}$ is the unit vector oriented along $\mathbf{u}$, it is easy to verify that the field $\mathbf{P}(\mathbf{u}, \mathbf{R}-\mathbf{r})$ differs from zero in the region marked by the dashed line in Fig. 6.

The second term in (19) can be expressed in terms of the Coulomb field of the electron

$$\mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R}) = -\nabla_R\varphi = -e\nabla_r\frac{1}{|\mathbf{r}-\mathbf{R}|},$$

if we take into account the fact that

$$(\mathbf{u}\nabla_r)\mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R}) = \frac{-e}{2\pi^2}\sum_{\lambda\mu}\mathbf{e}_\lambda u_\mu\int\frac{\mathbf{dk}k_\lambda k_\mu}{k^2}e^{i\mathbf{kQ}} = -4\pi e\sum_{\lambda\mu}e_\lambda u_\mu\delta^{\parallel}_{\lambda\mu}(\mathbf{R}-\mathbf{r}).$$

Then the sum of the commutators of the expansion (13) for the second term from (19) has the form

$$\left[1-\left(1+(\mathbf{u}\nabla_r)+\frac{1}{2!}(\mathbf{u}\nabla_r)^2+\frac{1}{3!}(\mathbf{u}\nabla_r)^3+\ldots\right)\right]\mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R}) = \mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R}) - \mathbf{E}^{\parallel}(\mathbf{r}+\mathbf{u}, \mathbf{R}).$$

Therefore, the transverse field transforms as follows:

$$\mathbf{E}^{\perp}_G = \mathbf{E}^{\perp}(\mathbf{R}) - 4\pi e\mathbf{P}(\mathbf{u}, \mathbf{R}-\mathbf{r}) - \mathbf{E}^{\parallel}(\mathbf{r}+\mathbf{u}, \mathbf{R}) + \mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R}).$$

The longitudinal field evidently transforms as

$$(\mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R}) + \mathbf{E}^{\parallel}_{\text{nucl}}(\mathbf{R}))_G = \mathbf{E}^{\parallel}(\mathbf{r}+\mathbf{u}, \mathbf{R}) + \mathbf{E}^{\parallel}_{\text{nucl}}(\mathbf{R}).$$

Thus the total field after transformation assumes the form

$$\mathbf{E}_G(\mathbf{r}, \mathbf{R}) = \mathbf{E}^{\parallel}_{\text{nucl}}(\mathbf{R}) + \mathbf{E}^{\parallel}(\mathbf{r}, \mathbf{R}) + \mathbf{E}^{\perp}(\mathbf{r}, \mathbf{R}) - 4\pi e\mathbf{P}(\mathbf{u}, \mathbf{r}-\mathbf{R}).$$

Averaging this expression over the state $|a, 0\rangle$ we verify that the average field in the state $G|a, 0\rangle$, obtained from $|a, 0\rangle$ as a result of the instantaneous perturbation, consists of the Coulomb field corresponding to the initial state $|a, 0\rangle$ and some additional field differing from zero only along the trajectory of motion of the charge. It is physically completely obvious that the changes in the field occurred only along the *trajectory* of the charge, since the changes at a point outside the trajectory arrive from points along the trajectory with a finite velocity, whereas the trajectory itself arises instantaneously.[3)] On the whole, the average of the field with respect to the state $G|a, 0\rangle$ has the form shown in Fig. 7.

The examined problem permits interpreting the field $-4\pi e\mathbf{P}(\mathbf{u}, \mathbf{R}, -\mathbf{r})$ as an electric field which arises when the charge is instantaneously displaced from the point $\mathbf{r}$ to the point $\mathbf{r}+\mathbf{u}$.

Returning now to the state $|\psi_0''\rangle = S|b, 0\rangle$, examined in Sec. 2, it can be shown that the field in this state (17), illustrated in Fig. 4b, may be assumed to arise as a result of the instantaneous (occurring with infinite velocity) displacement of the charge from the nucleus into a distribution corresponding to $|b\rangle$, since the rectilinear lines of force of this field are determined precisely by the field P. Naturally, this process cannot occur in reality, if for no other reason than that the electron cannot be concentrated at the nucleus by virtue of the uncertainty principle, For this reason, the initial state $|\psi_0''\rangle = S|b, 0\rangle$ can reflect practically realizable states only with some degree of uncertainty. In addition, such an instantaneous displacement of the electron from the nucleus into the distribution $|b\rangle$ is not the only way that the state $|\psi_0''\rangle$ can arise.

4. CANONICAL POWER-ZIENAU TRANSFORMATION

We shall now find the complete second form of the Hamiltonian.[4)] For this, aside from transforming the electric field, it is also necessary to transform the magnetic field and the electron velocity operator:

$$\mathbf{v} = \frac{1}{m}[\mathbf{p} - e\mathbf{A}(\mathbf{r})].$$

As far as the magnetic field is concerned, it should be noted that because it commutes with the exponent in (9) the vector potential does not change under the transformation being examined; all its spatial derivatives also remain unchanged at the same time, in particular, the magnetic field

$$\mathbf{H} = \text{rot}\,\mathbf{A}$$

does not change. In order to transform the electron velocity operator, we shall once again use the expansion (13) and we shall calculate in it the first commutator, keeping in mind that vector potentials evaluated at the same moment in time commute:

$$-\frac{ie}{m}\left[\int\mathbf{dx}\mathbf{P}(\mathbf{r}, \mathbf{x})\mathbf{A}(\mathbf{x}); \mathbf{p}\right] = \frac{e}{m}\nabla_r\int\mathbf{dx}\mathbf{P}(\mathbf{r}, \mathbf{x})\mathbf{A}(\mathbf{x}).$$

[3)]The displacement of the charge with a velocity exceeding the velocity of light in vacuum, in particular, with an infinitely large velocity, does not conflict with the theory of relativity. Such a displacement can occur, for example, with the creation of a set of electron-positron pairs along the trajectory with subsequent annihilation of the electrons and positrons with neighboring positrons and electrons, respectively.

[4)]In the paper by Power and Zienau, the canonical transformation is not correctly performed. The electric field in the Hamiltonian was replaced by the operator $S^{-1}\mathbf{E}S - 4\pi e\mathbf{P}^{\perp} = S^{-1}\mathbf{E}^{\perp}S - 4\pi e\mathbf{P}$. The correct substitution is $S^{-1}\mathbf{E}(\mathbf{r}, \mathbf{p})S = \mathbf{E}^{\perp}(\mathbf{R}) - 4\pi e\mathbf{P}(\mathbf{r}, \mathbf{R})$.

Since this expression depends only on the vector potential and the coordinates of the electron, all subsequent commutators in the expansion (13) vanish. Therefore,

$$\mathbf{v}' = \frac{1}{m} S^{-1}(\mathbf{p} - e\mathbf{A}(\mathbf{r}))S = \frac{1}{m}\left[\mathbf{p} - e\mathbf{A}(\mathbf{r}) + e\nabla_r \int d\mathbf{x}\mathbf{P}(\mathbf{r}, \mathbf{x})\mathbf{A}(\mathbf{x})\right]. \quad (20)$$

Averaging both the transformed and untransformed velocity operator over the state $|b, 0\rangle$ gives zero. Analogously, we can verify that the average values of the transformed and untransformed current operators in this state are identical. As pointed out above, however, the average value of the operator does not exhaust all characteristics of the state, since the average values of powers of these operators can differ. These differences can also reveal the difference between the states $|\psi_0''\rangle$ and $|\psi_0\rangle$.

Using the first terms of the multipole expansion of $\mathbf{P}(\mathbf{r}, \mathbf{x})$ (10) and $\mathbf{A}(\mathbf{r})$,

$$\mathbf{A}(\mathbf{r}) = \mathbf{A}(0) + (\mathbf{r}\nabla)\mathbf{A}(0) + \ldots,$$

we obtain the following approximate expression for the velocity operator:

$$\mathbf{v}' = \frac{\mathbf{p}}{m} + \frac{e}{2m}[\mathbf{r}, [\nabla_x, \mathbf{A}(\mathbf{x})]_{x=0}] = \frac{\mathbf{p}}{m} + \frac{e}{2m}[\mathbf{r}, \mathbf{H}(0)].$$

We now perform the canonical Power–Zienau transformation (4). We first transform the atomic part of the Hamiltonian. For this, we note that the potential energy of the electron $U(\mathbf{r})$ does not change under the transformation (4), while in order to transform the part containing the momentum, it is sufficient to square the expression (2) and multiply by $m/2$:

$$\frac{1}{2m}\left[\mathbf{p} - e\mathbf{A}(\mathbf{r}) + e\nabla_r \int d\mathbf{x}\mathbf{P}(\mathbf{r}, \mathbf{x})\mathbf{A}(\mathbf{x})\right]^2.$$

To transform the field part of the Hamiltonian, it is sufficient to replace the field $\mathbf{E}(\mathbf{r}, \mathbf{R})$ in the integrand in the Hamiltonian by the expression (17). As a result, we obtain

$$S^{-1}\left[\frac{1}{8\pi}\int d\mathbf{R}(\mathbf{E}^2(\mathbf{r}, \mathbf{R}) + \mathbf{H}^2(\mathbf{R}))\right]S = \frac{1}{8\pi}\int d\mathbf{R}(\mathbf{E}^{\perp 2}(\mathbf{R}) + \mathbf{H}^2(\mathbf{R})) - e\int d\mathbf{R}\mathbf{E}^{\perp}(\mathbf{R})\mathbf{P}(\mathbf{r}, \mathbf{R}) + 2\pi e^2 \int d\mathbf{R}\mathbf{P}^2(\mathbf{r}, \mathbf{R}).$$

The term in the middle gives precisely the interaction of the atomic electron with the electric field in the form (3). Indeed, retaining the first two terms in (10), we obtain

$$-e\int d\mathbf{R}\mathbf{E}^{\perp}(\mathbf{R})\mathbf{P}(\mathbf{r}, \mathbf{R}) \cong -e\mathbf{r}\mathbf{E}^{\perp}(0) - \frac{1}{2}e(\mathbf{r}\nabla_R)(\mathbf{r}\mathbf{E}^{\perp}(\mathbf{R}))_{\mathbf{R}=0} + \ldots$$

On the whole, the Hamiltonian assumes the following form:

$$H' = S^{-1}HS = \frac{1}{2m}\left[\mathbf{p} - e\mathbf{A}(\mathbf{r}) + e\nabla_r \int d\mathbf{x}\mathbf{P}(\mathbf{r}, \mathbf{x})\mathbf{A}(\mathbf{x})\right]^2 + U(\mathbf{r}) + \frac{1}{8\pi}\int d\mathbf{R}[\mathbf{E}^{\perp 2}(\mathbf{R}) + \mathbf{H}^2(\mathbf{R})] - e\int d\mathbf{R}\mathbf{E}^{\perp}(\mathbf{R})\mathbf{P}(\mathbf{r}, \mathbf{R}) + 2\pi e^2 \int d\mathbf{R}\mathbf{P}^2(\mathbf{r}, \mathbf{R}). \quad (21)$$

Using the multipole expansions indicated above, the Hamiltonian approximately equals

$$H' = S^{-1}HS = \frac{1}{2m}\mathbf{p}^2 + U(\mathbf{r}) + \frac{1}{8\pi}\int d\mathbf{R}(\mathbf{E}^{\perp 2}(\mathbf{R}) + \mathbf{H}^2(\mathbf{R})) - e\mathbf{r}\mathbf{E}^{\perp}(0) - e\sum_{\lambda\mu} Q_{\lambda\mu}\nabla_{\lambda R}E_{\mu}^{\perp}|_{\mathbf{R}=0} - \frac{e}{2m}\mathbf{H}\mathbf{L} + \frac{e^2}{8m}[\mathbf{r}, \mathbf{H}]^2 + 2\pi e^2\int d\mathbf{R}\mathbf{P}^2(\mathbf{r}, \mathbf{R}), \quad (22)$$

where

$$eQ_{\lambda\mu} = \frac{1}{2}er_{\lambda}r_{\mu}$$

is the nondiagonalized quadrupole moment of the electron and $\mathbf{L} = [\mathbf{r}, \mathbf{p}]$ is the orbital angular momentum of the electron. This form of the Hamiltonian is interesting in that the total interaction of the atom with the field is split into the interaction with the field of elementary moments: electric dipole, electric quadrupole, magnetic dipole, etc.

We emphasize once again that the Hamiltonians (1) and (21) are equivalent only in the case when all states are transformed as in (7).

5. PHOTON SPECTRA IN CALCULATIONS WITH DIFFERENT HAMILTONIANS. THE LAMB-RETHERFORD RESULT

We shall examine the spontaneous emission of an excited atom, using the different forms of the Hamiltonian. As is obvious from the preceding text, the physical difference between the Hamiltonians reduces to the difference in the initial conditions. We shall now be interested in the consequences of these differences.

Thus we shall examine a system described by the Hamiltonian

$$H = H_0 + V,$$

where H_0 is the unperturbed part of the Hamiltonian and V is the perturbation. The evolution operator of the system can be represented in the form

$$U(t) = \frac{-1}{2\pi i}\int_C dz\frac{e^{-izt}}{z - H},$$

where $R(z) = (z - H)^{-1}$ is the resolvent operator[12] and the contour lies some distance above the real axis. We shall take the initial condition in the form $|b, 0\rangle$ and we shall be interested in the probability that a photon with wave vector k and polarization λ appears and the atom drops down into the ground state $|a\rangle$. This probability is characterized by the amplitude

$$M(t) = \langle a, 1_{k\lambda}|U(t)|b, 0\rangle = \frac{-1}{2\pi i}\int_C dz e^{-izt}\langle a, 1_{k\lambda}|R(z)|b, 0\rangle. \quad (23)$$

The matrix element of $R(z)$ can be approximately represented in the form

$$\frac{-V_{a, k\lambda; b, 0}}{(z - \hbar\omega)\left(z - \hbar\omega_0 - \sum_{\lambda k}\frac{|V_{a, k\lambda; b, 0}|^2}{z - \hbar\omega}\right)}.$$

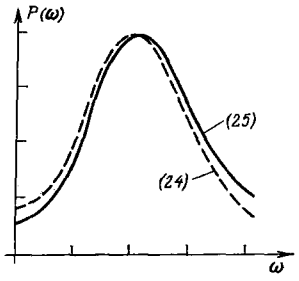


FIG. 8. The frequency distribution of photons emitted under different initial conditions, described by relations (24) and (25).

The expression in the second pair of parentheses in the denominator of this expression is approximately equal to $z - \hbar\omega_0 + i\hbar\gamma/2$, where

$$\gamma = \frac{4}{3}\frac{e^2\omega_0^3}{c^3} |\langle \mathbf{r} \rangle|^2,$$

and thus has a pole in the lower half-plane (we ignore the Lamb shift in this case, making the assumption that it is small). In calculating the integral in (23) only the residue at $z = \hbar\omega$ need be included, since the residue of the second pole decays with time. As a result, we obtain

$$|M_{t\to\infty}|^2 = \frac{|V_{a,k\lambda;b,0}|^2/\hbar^2}{(\omega-\omega_0)^2+(1/4)\gamma^2}.$$

The square of the modulus of the matrix element of V assumes different values for the Hamiltonians in the forms (1) and (2). In the first case, it is equal to

$$|V_{a,k\lambda;b,0}|^2 = \frac{2\pi e^2\omega_0^2}{\omega c} |\langle \mathbf{r}_{ba}\mathbf{e}_{k\lambda}\rangle|^2,$$

whereas in the second case it is given by

$$|V_{a,k\lambda;b,0}|^2 = \frac{2\pi e^2\omega}{c} |\langle \mathbf{r}_{ba}\mathbf{e}_{k\lambda}\rangle|^2.$$

The second expression is obtained from the first one if it is multiplied by the ratio $(\omega/\omega_0)^2$. In fact, the difference in the frequency distributions of the photons reduces to this factor; there is also a negligibly small difference in the damping constants (or transition probabilities), which we shall not take the time to discuss here. The photon frequency distributions finally assume the following forms (Fig. 8):

$$P(\omega)\,d\omega = \frac{2}{3\pi}\frac{e^2}{c^4}\frac{\omega_0^2\omega\,|\langle \mathbf{r}\rangle|^2}{(\omega-\omega_0)^2+(1/4)\gamma^2}\,d\omega, \qquad (24)$$

for Hamiltonian (1) and

$$P(\omega)\,d\omega = \frac{2}{3\pi}\frac{e^2}{c^4}\frac{\omega^3\,|\langle \mathbf{r}\rangle|^2}{(\omega-\omega_0)^2+(1/4)\gamma^2}\,d\omega \qquad (25)$$

for Hamiltonian (2). It is easy to see that the last expression (25) does not decrease as $\omega\to\infty$. This should not surprise us; after all, the initial state in this case corresponds to the unlikely process of an instantaneous (with infinitely high velocity) appearance of the distribution $|b\rangle$ from the nucleus. Any real physical process can correspond only approximately to such an initial state. For this reason, the distribution (25) must be cut off for frequencies somewhat greater than ω_0 and an appropriate normalization factor must be introduced.

It should be noted that the distributions (24) and (25) were presented in the paper by Power and Zienau[3]; in addition, the first of these distributions was described as being incorrect and the second was described as being correct. As is evident from the above presentation, these assertions of Power and Zienau are not correct. Both distributions are correct, but they correspond to different initial states. We can say that the first distribution corresponds to emission from a state with a stationary Coulomb field, whereas the second one corresponds to emission from the state with a nonstationary Coulomb field.

The choice of Hamiltonian or of the corresponding initial condition in a specific physical situation can be made only by analyzing the process of atomic excitation. If the initial condition must be known exactly, then the excitation process must be included in the quantum-mechanical problem under study; of course, this will return us to scattering theory. In many experimental situations this is quite difficult to do.

It should be noted that for narrow spectral lines the question of the form of the Hamiltonian is entirely unimportant. Indeed, for narrow lines (in most cases the true widths of the lines in relative units is less than 10^{-7}–10^{-8}) the factor $(\omega/\omega_0)^2$ equals unity with a high degree of accuracy. However, there are exceptions. In this content, it is interesting to examine the Lamb-Retherford experiment.[4]

Unfortunately, our investigation is not directly applicable to the analysis of the Lamb-Retherford experiment. Indeed, the analysis above referred only to a two-level system, while a three-level system was used in the Lamb-Retherford experiment. They worked with stimulated and spontaneous emission. Finally, spin played an important role in the scheme that they investigated. Our investigation can therefore only hint at the reasons that the Hamiltonian in the form (2) must be used to obtain a theoretical explanation of their results.

First of all, why was their experiment sensitive to the form of the Hamiltonian at all? This is easily understood if we take into account the fact that they investigated the low-frequency transition 3→2 (Fig. 9), whose width is determined by the short lifetime of the level 2, since the transition 2→1 is allowed. It turns out that the relative width of the transition 3→2 is of the order of 0.1 (Fig. 8). Naturally, the factor $(\omega/\omega_0)^2$ can give in this case corrections of up to 20%, which in the precision experiment of Lamb-Retherford was already an appreciable quantity.

Second, it would appear that under electron-impact excitation of the state 3 it is possible that in their experiment there was not enough time for the Coulomb field to be established. Indeed, the electron impact time is of the order of 10^{-15}–10^{-16} s, which is much shorter than the period 10^{-9} s

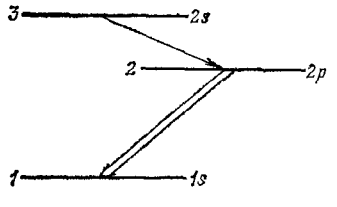


FIG. 9. Diagram of the levels in the Lamb-Retherford experiment.

of interest to us (correspondingly, in the Coulomb field the components tens of centimeter long are important). Third, the state 3 is excited from the ground 1*s* state, lying close to the nucleus. When the distribution corresponding to the excited state 3 is formed, the atomic electron appears to be knocked out of the nucleus by the external electron. These circumstances indicate the advantage of the second form (2) of the Hamiltonian in interpreting the Lamb-Retherford experiment. We recall that they observed that the Hamiltonian (2) gives a better description of the experimental results. This is all that we can in fact say about the Lamb-Retherford experiment. Of course, it would be desirable to investigate this experiment in greater detail. Perhaps it will be possible to do so in the future.

6. CONCLUSIONS

In this paper we investigated the role of the initial conditions in radiation problems, when both the atom and the electromagnetic field are described quantum-mechanically. In addition, we investigated the aspect of the problem related to the two forms of the Hamiltonian describing the interaction of atoms with an electromagnetic field that are most often used in theoretical calculations.

We showed that the transformation from one form of the Hamiltonian to the other leaves the character of the physical process unchanged only when such a transformation is accompanied by a corresponding change in the states, in particular, of the initial state. It is worth emphasizing that only the form of the initial state changes; the physical content of the state remains unchanged. Using different forms of the Hamiltonian with the same form of the initial condition is equivalent to analyzing the emission process with physically different initial conditions.

We showed that in the initial state $|b, 0\rangle$ the Hamiltonian (1) describes the emission from a state with a stationary Coulomb field; with the initial state of the same form the Hamiltonian (2) describes emission from the state with a nonstationary Coulomb field. The situation here is completely equivalent to that of the free motion of an electron, first analyzed by V. L. Ginzburg.[10] Generally speaking, both states can be realized in practice to some degree of accuracy. The selection between these states can be made only as a result of a physical analysis of the conditions of excitation. For narrow emission lines, the differences in the form of the Hamiltonian have virtually no effect on their line shapes.

It should not be thought that the state with the stationary Coulomb field is in any way distinguished. The excited state of the atom is itself not stationary and the requirement that it be accompanied by a stationary Coulomb field has no logical foundations.

It should be noted that there exists an infinite number of unitary operators which transform the Hamiltonian from one form to an other. Amongst these operators, the Power-Zienau operator is distinguished only by the simplicity of the interpretation of the corresponding initial state.

Generally speaking, cases are possible when the results of the calculations with different Hamiltonians do not depend on whether or not the states used are changed. This occurs for those quantities for which the width of the level is not important or which refer to the center of the line. For these quantities the photon frequency entering into them can be replaced by the transition frequency of the atom or molecule. An example of such a quantity also occurs in this paper: the probability of the transition from the excited state into the unexcited state or the damping constant of the upper level. The existence of quantities that are insensitive to the change in the states is not accidental: it arises due to the fact that the matrix elements of both Hamiltonians coincide if the frequency of the photon equals the transition frequency. One of these important particular cases is examined by F. V. Bunkin.[13] He showed that the probability of two-quantum decay of the excited state can be calculated in the dipole approximation with the help of either of the Hamiltonians without a change in the states (the use of the Hamiltonian (2), in this case, has only computational advantages). To identify such particular cases, it is important that the system of unperturbed states be complete in a number of cases, the quadratic term $e^2\mathbf{A}^2$ be included in the Hamiltonian (1). There are also papers on analogous particular cases, but their discussion falls outside the scope of this paper. These are particular cases; in the general case, the use of the unchanged states with different Hamiltonians will lead to different results—which is what this paper points out.

The difference in the forms of the Hamiltonian can also lead to different physical results in the classical theory, if the transformation of the form of the Hamiltonian is not accompanied by a transformation of the form of the initial condition. For example, assume that the initial momentum of the system equals zero in one form of the Hamiltonian. Under a canonical transformation the momenta also change and the new momentum does not necessarily equal zero in the same state. Therefore, the form of the initial condition must change under the canonical transformation.

Of course, the same considerations concerning the initial state of the system also apply to the analysis of stimulated emission, i.e., a change in the Hamiltonian without a change of the initial state, which, in this case, is equivalent to a physical change of the initial conditions. In this case, however, there arises a question which we did not consider and which deserves special attention. This is the question of the representation of the interaction of atoms with an unquantized and, correspondingly, macroscopic electromagnetic field. This question is discussed in a number of recently published papers.[6–8] In our opinion, this question can be resolved by passing to the limit from a quantized field to an unquantized field, while artificial recipes or conjectures will hardly lead to the solution.

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