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Matter-field interaction in atomic physics and quantum optics

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Almost forty years ago one of us (W.E.L.) noticed that within the analysis of experiments on the hydrogen fine structure the matter-field interaction was sensitive to the choice of gauge when decaying states were used. In the present paper this problem is resolved for the Bethe-Lamb equations in the context of the two-level model with Weisskopf-Wigner decay included.

I. INTRODUCTION

It is perhaps surprising to note that one of the outstanding problems of modern quantum optics is the choice between the two matter-field interaction Hamiltonians which are commonly used: $-e\mathbf{E}\cdot\mathbf{r}$ and $-(e/m)\mathbf{p}\cdot\mathbf{A}+(e^2/2m)\mathbf{A}^2$. These two different interactions correspond to two different gauges of the electromagnetic field. In 1952 calculations based on the two different interactions were, for the first time, compared to experimental results.[1] In particular, the line shape for the Lamb-shift transition $2S_{1/2}\rightarrow 2P_{1/2}$ in an H atom in the presence of a rf field[2] was compared to theoretical results. It was pointed out in Ref. 1 that the $\mathbf{E}\cdot\mathbf{r}$ interaction was more convenient in describing the experimental results.

Since that time there has been a widespread opinion that the two interactions would yield different results and that only the $\mathbf{E}\cdot\mathbf{r}$ interaction should be used for practical calculations. For example, Jaynes nicely summarized the problem in 1976 saying: "... a whole generation of physicists has stumbled on this problem and lived, not only under the shadow of the immediate difficulty: 'How can I ever know whether a practical calculation has been done right?,' but the deeper mystery: 'How is it possible that a theory, for which formal gauge invariance is proved easily once and for all, can lead to grossly noninvariant results as soon as we try to apply it to the simplest real problem?'" (cited in Ref. 3).

The $\mathbf{E}\cdot\mathbf{r}$ Hamiltonian was introduced for the first time by M. Göppert-Mayer in 1931.[4] Equations of motion for the amplitudes of a two-level atom in an external static electric field were given by Bethe.[5] The general unitary transformation connecting the minimal coupling Hamiltonian $-(e/m)\mathbf{p}\cdot\mathbf{A}+(e^2/2m)\mathbf{A}^2$ to the multipole expansion of the field was given by Power and Zienau.[6] In the electric dipole approximation the multipolar Hamiltonian reduces to the $-e\mathbf{E}\cdot\mathbf{r}$ form.[7] The fundamentals of gauge invariance and gauge transformations in quantum mechanics are explained in textbooks by Pauli[8] and by Cohen-Tannoudji *et al.*[9] Yang[10] and Kobe and Smirl[3] obtained gauge-invariant transition amplitudes by calculating transition matrix elements between eigenstates of the energy operator. A summary of these basic publications is given in Ref. 11. However, even though the subject is rather elementary, this is by no means a complete list of publications on the problem. During the last decade we have seen rather an inflation of—partly very controversial—papers[12] on the subject, many of which claim to be motivated by Ref. 1. However, few of these papers address the line-shape problem and none of them is concerned with the same experimental situation as Ref. 1. In particular, the key point of the finite lifetime of the states is not taken into account. Appendix B gives examples for different kinds of calculations in which the $\mathbf{E}\cdot\mathbf{r}$ versus $\mathbf{p}\cdot\mathbf{A}$ problem occurs and presents the different approaches for its resolution specific to the respective calculations.

The experiment described in Ref. 2 was set up to determine the fine structure of the hydrogen atom by a microwave method. The spacing between the levels of the L shell was measured with high precision. The experimental setup consisted of four major elements: a source, an excitation region, an interaction region, and a detector. A tungsten oven served as the source for the beam of atomic hydrogen. In the excitation region the hydrogen atoms were excited to the metastable $2S_{1/2}$ state by electron bombardment. In the interaction region the metastable atoms were exposed to a magnetic field of variable strength so that the spacing between the energy levels could be varied by the Zeeman effect. Furthermore, the metastable atoms were exposed to a rf field (or a static electric field). This electric field couples the metastable $2S_{1/2}$ state to $2P_{1/2}$ which rapidly decays to the ground state $1S_{1/2}$. This depopulation or quenching of the metastable $2S_{1/2}$ state is the largest when the frequency of the rf field equals the spacing between $2S_{1/2}$ and $2P_{1/2}$ (or, in the case of a dc field, when the two levels are degenerate). In the experiments the frequency of the rf field was kept constant and the levels were Zeeman shifted through the resonance. The detector was only sensitive to the metastable state, i.e., it was

possible to measure how many metastable atoms decayed in the interaction region for a fixed magnetic field strength. This is a very universal setup which is still used at present for fundamental investigations of the matter-field interaction.[13]

In order to compare the measured resonance curve with the theory, it was necessary to calculate the rate for the field-induced decay of the metastable $2S_{1/2}$ state via $2P_{1/2}$ to $1S_{1/2}$ as a function of the level spacing. The employed theory included phenomenological decay terms and derived the probability amplitudes for finite interaction times. It was in this context where the supposed discrepancy between $\mathbf{E}\cdot\mathbf{r}$ and $\mathbf{p}\cdot\mathbf{A}$ occurred.

It is the purpose of this paper to show (i) that the Bethe-Lamb equations used in Ref. 1 yield the transition amplitudes only for the $\mathbf{E}\cdot\mathbf{r}$ interaction in a straightforward way and (ii) how the correct answer can also be obtained via a $\mathbf{p}\cdot\mathbf{A}$ approach. We restrict the discussion to a two-level atom and we derive the $\mathbf{p}\cdot\mathbf{A}$ equivalent of the Bethe-Lamb equations. We stress the importance of introducing atomic decay into the physics as well as the fact that we are interested in the time evolution of the transition rate in the presence of the field. The decay is treated phenomenologically, and we consider only a uniform electric field, i.e., we apply the electric dipole approximation. A rigorous derivation of the field-induced decay rates would start from a three-level system, consisting of the two levels under consideration plus a lower-lying level, and would derive the decay terms from the Weisskopf-Wigner theory.[14] Such a calculation could be carried out along the same lines outlined in this paper.

In Sec. II we define the problem and recall the original calculation of Ref. 1. In Sec. III the equations of motion for the two different forms of the interaction are derived. Section IV makes contact between the solutions of these equations and the transition probabilities which are measured in an experiment. Section V presents simple examples (a two-level atom in a dc or an ac field, treated with first-order perturbation theory) to show the essential steps for the resolution of the $\mathbf{E}\cdot\mathbf{r}$ versus $\mathbf{p}\cdot\mathbf{A}$ problem on a textbook level. Section VI summarizes our results. Two appendixes complete the paper. One is intended to remind the reader of the energy operator formalism and the way in which the probability for transitions between different energy eigenstates is calculated in different gauges. The other one lists some of the arguments commonly used for the "resolution" of the $\mathbf{E}\cdot\mathbf{r}$ versus $\mathbf{p}\cdot\mathbf{A}$ problem and points out that these arguments always hold only for specific kinds of calculations and do not apply to the original calculation of Ref. 1.

II. REVIEW OF THE PROBLEM

The first systematic theory of the effect of a static uniform electric field on the fine structure of hydrogen is due to Bethe.[5] He considered two degenerate levels $|a\rangle$ $(2S_{1/2})$ and $|b\rangle$ $(2P_{1/2})$ with different decay constants $\gamma_b \gg \gamma_a$ under the influence of a static field $\mathbf{E}_0$. The Bethe equations for the probability amplitudes a and b have the form

$$\begin{aligned}\dot{a} &= -\frac{\gamma_a}{2}a - \frac{i}{\hbar}V_{ab}b \ , \\ \dot{b} &= -\frac{\gamma_b}{2}b - \frac{i}{\hbar}V_{ba}a \ ,\end{aligned} \tag{2.1}$$

where V_{ba} is the matrix element for the transition $a \rightarrow b$ of the interaction

$$V = -e\mathbf{E}_0\cdot\mathbf{r} \ . \tag{2.2}$$

In order to take the removal of the degeneracy of $2S_{1/2}$ and $2P_{1/2}$ into account, Eqs. (2.1) have to be generalized to allow for a spacing $E_a - E_b = \hbar\omega$ between levels $|a\rangle$ and $|b\rangle$. The Bethe equations can furthermore be generalized to allow for an ac field $\mathbf{E}(t) = \mathbf{E}_0\sin(\nu t)$ with frequency ν. This leads to the Bethe-Lamb equations for a two-level atom with radiation damping:

$$\begin{aligned}\dot{a} &= -\frac{\gamma_a}{2}a + \frac{i}{\hbar}e\mathbf{E}_0\cdot\mathbf{r}_{ab}\sin(\nu t)e^{i\omega t}b \ , \\ \dot{b} &= -\frac{\gamma_b}{2}b + \frac{i}{\hbar}e\mathbf{E}_0\cdot\mathbf{r}_{ba}\sin(\nu t)e^{-i\omega t}a \ .\end{aligned} \tag{2.3}$$

In the rotating-wave approximation these equations reduce to

$$\begin{aligned}\dot{a} &= -\frac{\gamma_a}{2}a - \frac{e}{2\hbar}\mathbf{E}_0\cdot\mathbf{r}_{ab}e^{i\Delta t}b \ , \\ \dot{b} &= -\frac{\gamma_b}{2}b + \frac{e}{2\hbar}\mathbf{E}_0\cdot\mathbf{r}_{ba}e^{-i\Delta t}a \ ,\end{aligned} \tag{2.4}$$

where Δ denotes the detuning $\Delta = \omega - \nu$. Since in the experiment only the probability of finding the atom in the $2S_{1/2}$ state was measured, Eqs. (2.4) can be replaced by a second-order equation for a:

$$\ddot{a} + \left[\frac{\gamma_a}{2} + \frac{\gamma_b}{2} - i\Delta\right]\dot{a} + \left[\frac{\gamma_a}{2}\left[\frac{\gamma_b}{2} - i\Delta\right] + \left[\frac{e}{2\hbar}\right]^2 |\,\mathbf{E}_0\cdot\mathbf{r}_{ab}\,|^2\right]a = 0 \ . \tag{2.5}$$

Since we are particularly interested in exponentially decaying solutions, we can make an ansatz for a of the form

$$a(t) = e^{\mu t} \ . \tag{2.6}$$

By inserting this ansatz into Eq. (2.5) we obtain a quadratic equation for μ. Together with the initial condition $a(0) = 1$, $\dot{a}(0) = -\gamma_a/2$, the two roots of this equation give the following expression for the probability amplitude of state $|a\rangle$:

$$a(t) = \frac{1}{4\Omega}[(2\Omega - \Delta + i\delta)e^{-(1/2)(\gamma - i\Delta - 2i\Omega)t} + (2\Omega + \Delta - i\delta)e^{-(1/2)(\gamma - i\Delta + 2i\Omega)t}] \ . \tag{2.7}$$

The symbols γ and δ denote the sum and the difference of the decay constants

$$\gamma = \frac{\gamma_a + \gamma_b}{2}, \quad \delta = \frac{\gamma_a - \gamma_b}{2} \tag{2.8}$$

and Ω stands for the generalized Rabi frequency

$$\Omega=\left[\tfrac{1}{4}(\Delta-i\delta)^2+\left[\frac{e}{2\hbar}\right]^2|\,\mathbf{E}_0\cdot\mathbf{r}_{ab}\,|^2\right]^{1/2}. \tag{2.9}$$

In order to describe the experiment it is sufficient to take the limit of small electric fields and $\gamma_a \ll \gamma_b$. The first term of Eq. (2.7) decays already in the interaction region and the field-induced depopulation of the metastable $2S_{1/2}$ state as measured at the detector is given by

$$|\,a(t)\,|^2\sim e^{-\gamma_s t},$$
$$\gamma_s=\left[\frac{e}{2\hbar}\right]^2|\,\mathbf{E}_0\cdot\mathbf{r}_{ab}\,|^2\frac{\gamma_b}{\Delta^2+\left[\frac{\gamma_b}{2}\right]^2}. \tag{2.10}$$

Clearly the quenching of the $2S_{1/2}$ state depends on the detuning between level spacing and rf frequency and is the largest at resonance for $\omega=\nu$.

So far we followed Bethe's approach to the dc problem and described the interaction between the atom and the external field in terms of $\mathbf{E}\cdot\mathbf{r}$. The alternative approach for the calculation of the time evolution of the system starts from the minimal coupling Hamiltonian and uses

$$V'=-\frac{e}{m}\mathbf{p}\cdot\mathbf{A}+\frac{e^2}{2m}\mathbf{A}^2 \tag{2.11}$$

for the interaction. If one were to simply replace the interaction $-e\mathbf{E}_0\cdot\mathbf{r}\sin(\nu t)$ in the Bethe-Lamb equations (2.3) by the $\mathbf{p}\cdot\mathbf{A}$ interaction (2.11), one would end up with a quenching of the $2S_{1/2}$ state which is different from Eq. (2.10). This can be seen from the following argument. For a plane wave of frequency ν the vector potential $\mathbf{A}_0\cos(\nu t)$ is related to the electric field $\mathbf{E}_0\sin(\nu t)$ via

$$\mathbf{A}_0=\frac{1}{\nu}\mathbf{E}_0, \tag{2.12}$$

whereas the momentum operator $\mathbf{p}$ can be expressed in terms of $\mathbf{r}$ as

$$\mathbf{p}=\frac{i}{\hbar}m[H_0,\mathbf{r}], \tag{2.13}$$

where H_0 denotes the unperturbed Hamiltonian including the binding potential U,

$$H_0=\frac{\mathbf{p}^2}{2m}+U(\mathbf{r}). \tag{2.14}$$

By combining Eqs. (2.12) and (2.13) we see that the matrix elements of the interactions $\mathbf{E}\cdot\mathbf{r}$ and $\mathbf{p}\cdot\mathbf{A}$ differ essentially by a factor ω/ν,

$$\left\langle b\left|-\frac{e}{m}\mathbf{p}\cdot\mathbf{A}_0\right|a\right\rangle=-i\frac{\omega}{\nu}\langle\, b\,|\,-e\mathbf{E}_0\cdot\mathbf{r}\,|\,a\,\rangle. \tag{2.15}$$

The use of the $\mathbf{p}\cdot\mathbf{A}$ interaction (2.11) in the Bethe-Lamb equations (2.4) would therefore lead to a field-induced quenching rate

$$\left[\frac{e}{2\hbar}\right]^2|\,\mathbf{E}_0\cdot\mathbf{r}_{ab}\,|^2\left[\frac{\omega}{\nu}\right]^2\frac{\gamma_b}{\Delta^2+\left[\frac{\gamma_b}{2}\right]^2}, \tag{2.16}$$

which differs from Eq. (2.10) by a factor $(\omega/\nu)^2$. Since this factor is frequency dependent, it would give rise to a significant distortion of the resonance curve (Fig. 1). For lower rf frequencies the distortion would be even stronger.

Of course the discrepancy by a factor $(\omega/\nu)^2$ is not restricted to the particular example considered here. It occurs in any calculation which uses the same equations of motion with the two different interactions $\mathbf{E}\cdot\mathbf{r}$ (2.2) and $\mathbf{p}\cdot\mathbf{A}$ (2.11). This even holds for the simplest example of a two-level atom in a weak field whose impact on the atom can be calculated in first-order perturbation theory. In Sec. V we will use this example to demonstrate the resolution of the problem. It should furthermore be mentioned that the Bethe-Lamb equations play not only an important role in quantum optics and atomic physics, but also in other fields such as, for example, nuclear physics.[15]

In Ref. 1 the appearance of the additional factor $(\omega/\nu)^2$ was commented on as follows: "Of course, the difference between the perturbations $\mathbf{E}\cdot\mathbf{r}$ and $-(\mathbf{A}\cdot\mathbf{p})/m$ just corresponds to a gauge transformation under which the theory is known to be invariant, so that 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, and no additional factor $(\omega/\nu)^2$ actually occurs." It is the purpose of the following two sections to outline this "closer examination" in order to show that (i) equations of motion with the $\mathbf{p}\cdot\mathbf{A}$ interaction have a form different from the Bethe-Lamb equations (2.3) and (ii) that the quantities a and b cannot be interpreted as probability amplitudes if $\mathbf{p}\cdot\mathbf{A}$ is used.

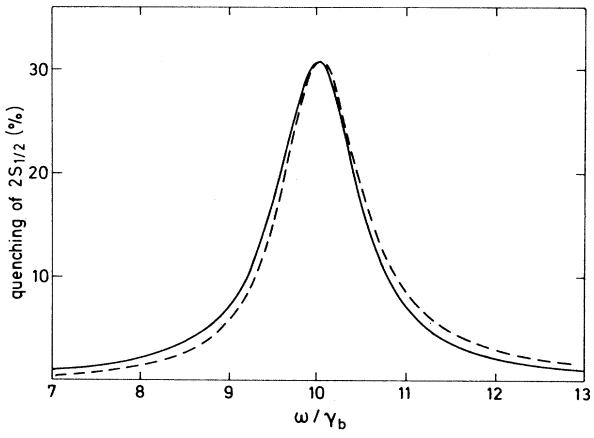

FIG. 1. Quenching of the $2S_{1/2}$ state as a function of the level spacing ω for a rf frequency $\nu/2\pi=1000$ MHz and a lifetime of $2P_{1/2}$ $\gamma_b^{-1}=1.6\times10^{-9}$ sec. Solid curve, decay according to Eq. (2.10); dashed curve, decay rate given by Eq. (2.16).

III. EQUATIONS OF MOTION

Throughout this paper we only consider two-level atoms. A system with only two levels can be described in a mathematically consistent way by representing all the operators by 2×2 matrices and the states by two-component vectors.[7] In particular, the operators $\mathbf{r}$ and $\mathbf{p}$ are then represented essentially by the Pauli spin matrices σ_1 and σ_2, respectively. However, in order to clarify our calculations we stick to the notation $\mathbf{r}$ and $\mathbf{p}$ and keep in mind that these operators are represented by σ_1 and σ_2 in our particular model.

Before deriving equations of motion with the $\mathbf{p}\cdot\mathbf{A}$ interaction, it might be useful to recall the derivation of the Bethe-Lamb equations (2.3). For this purpose we start from the Schrödinger equation with the $\mathbf{E}\cdot\mathbf{r}$ interaction

$$i\hbar\frac{\partial}{\partial t}\Psi=[H_0-\tfrac{1}{2}i\hbar\Gamma-e\mathbf{E}(t)\cdot\mathbf{r}]\Psi\ . \tag{3.1}$$

H_0 denotes the unperturbed Hamiltonian (2.14) with eigenstates ψ_a and ψ_b

$$H_0\psi_a=\hbar\omega_a\psi_a,\quad H_0\psi_b=\hbar\omega_b\psi_b\ . \tag{3.2}$$

The spontaneous decay of these levels is included phenomenologically by adding a Weisskopf-Wigner type decay operator Γ (Ref. 14) to the Hamiltonian in Eq. (3.1). The eigenvalues of Γ are given by the natural decay constants γ_a and γ_b:

$$\Gamma\psi_a=\gamma_a\psi_a,\quad \Gamma\psi_b=\gamma_b\psi_b\ . \tag{3.3}$$

The wave function of the two-level system $\{|a\rangle,|b\rangle\}$ can then be written as

$$\Psi(\mathbf{r},t)=a(t)e^{-i\omega_a t}\psi_a(\mathbf{r})+b(t)e^{-i\omega_b t}\psi_b(\mathbf{r})\ . \tag{3.4}$$

By inserting this expansion into the Schrödinger equation (3.1), one obtains the Bethe-Lamb equations (2.3) for the amplitudes a and b.

In order to replace the $\mathbf{E}\cdot\mathbf{r}$ interaction in the Schrödinger equation (3.1) by the $\mathbf{p}\cdot\mathbf{A}$ interaction, the wave function Ψ has to be transformed according to

$$\Psi(\mathbf{r},t)=T^{\dagger}(\mathbf{r},t)\Psi'(\mathbf{r},t),\quad T(\mathbf{r},t)=e^{ie\,\mathbf{A}(t)\cdot\mathbf{r}/\hbar}\ . \tag{3.5}$$

Ψ' satisfies the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi'=\left[H_0-\tfrac{1}{2}i\hbar\Gamma'(\mathbf{r},t)-\frac{e}{m}\mathbf{p}\cdot\mathbf{A}(t)+\frac{e^2}{2m}\mathbf{A}^2(t)\right]\Psi'\ . \tag{3.6}$$

The important new feature is that the damping operators in Eqs. (3.1) and (3.6) are different:

$$\Gamma'=T\Gamma T^{\dagger}\ . \tag{3.7}$$

Γ' depends on $\mathbf{r}$ and t and is not diagonal with respect to the eigenstates ψ_a and ψ_b of H_0, in contrast to Γ (3.3). For the two-level atom which we exclusively consider, the damping matrices have the form

$$\Gamma=\begin{bmatrix}\gamma_a & 0\\ 0 & \gamma_b\end{bmatrix},$$

$$\Gamma'=\begin{bmatrix}\gamma_a\cos^2\phi+\gamma_b\sin^2\phi & -i(\gamma_a-\gamma_b)\sin\phi\cos\phi\\ i(\gamma_a-\gamma_b)\sin\phi\cos\phi & \gamma_a\sin^2\phi+\gamma_b\cos^2\phi\end{bmatrix} \tag{3.8}$$

with $\phi=e\,\mathbf{A}(t)\cdot\mathbf{r}_{ba}/\hbar$.

By expanding Ψ' in terms of ψ_a and ψ_b

$$\Psi'(\mathbf{r},t)=\alpha(t)e^{-i\omega_a t}\psi_a(\mathbf{r})+\beta(t)e^{-i\omega_b t}\psi_b(\mathbf{r}) \tag{3.9}$$

and inserting this expression into the Schrödinger equation (3.6), one obtains the equations of motion for the amplitudes α and β:

$$\begin{aligned}\frac{\partial}{\partial t}\alpha=&-\left[\tfrac{1}{2}\Gamma'_{aa}(t)+\frac{i}{\hbar}\frac{e^2}{2m}\mathbf{A}^2(t)\right]\alpha\\ &-\left[\tfrac{1}{2}\Gamma'_{ab}(t)-\frac{i}{\hbar}\frac{e}{m}\mathbf{p}_{ab}\cdot\mathbf{A}(t)\right]e^{i\omega t}\beta\ ,\\ \frac{\partial}{\partial t}\beta=&-\left[\tfrac{1}{2}\Gamma'_{bb}(t)+\frac{i}{\hbar}\frac{e^2}{2m}\mathbf{A}^2(t)\right]\beta\\ &-\left[\tfrac{1}{2}\Gamma'_{ba}(t)-\frac{i}{\hbar}\frac{e}{m}\mathbf{p}_{ba}\cdot\mathbf{A}(t)\right]e^{-i\omega t}\alpha\ .\end{aligned} \tag{3.10}$$

These are the required equations which include the $\mathbf{p}\cdot\mathbf{A}$ interaction and are equivalent to the Bethe-Lamb equations (2.3). Obviously, it is not correct simply to replace the $\mathbf{E}\cdot\mathbf{r}$ interaction by the $\mathbf{p}\cdot\mathbf{A}$ form. Simultaneously, also the damping matrix has to be changed. In particular, the off-diagonal elements of Γ' contribute to the coupling between ψ_a and ψ_b. Provided that the two levels $|a\rangle$ and $|b\rangle$ are degenerate so that $\omega=0$ and $\mathbf{p}_{ab}=\mathbf{p}_{ba}=0$, then only the off-diagonal damping matrix elements Γ'_{ab} and Γ'_{ba} cause a coupling between α and β. Off-diagonal decay terms were first used by Breit in 1933[16] in connection with the scattering of radiation by an atom with degenerate lower and upper levels. However, his off-diagonal Γ's were due to matrix elements between different degenerate magnetic sublevels, whereas our Γ' comes from the transformation (3.7) and is time dependent.

It should be noted that Eqs. (3.10) hold only for a two-level atom. In the case of an n-level atom they would have to be replaced by a set of n coupled equations since the wave function Ψ' has to be expanded in terms of a complete set of eigenfunctions ψ_n of H_0.

IV. PROBABILITY AMPLITUDES

The quantities of physical interest are the probabilities P_a and P_b of finding the atom in the energy eigenstates $|a\rangle$ or $|b\rangle$, respectively. In the $\mathbf{E}\cdot\mathbf{r}$ formalism we follow Bethe's approach for a static uniform electric field and take the projection of the wave function Ψ onto the eigenstates ψ_a or ψ_b (3.2) of the unperturbed Hamiltonian H_0 in order to calculate P_a or P_b:

$$P_n(t)=|\langle\psi_n|\Psi\rangle|^2,\quad n=a,b\ . \tag{4.1}$$

It is shown in Appendix A that this is the correct form of the transition probability at arbitrary time t.

In the $\mathbf{p}\cdot\mathbf{A}$ formalism we cannot apply the "textbook wave functions" ψ_a and ψ_b anymore. After all, the transformation (3.5) describes a gauge transformation from the Hamiltonian in the electric field gauge (3.1) to the Hamiltonian in the radiation gauge (3.6). Correspondingly, all the wave functions are subject to the transformation operator T. We therefore should project the wave function Ψ' onto the transformed wave functions

$$\psi'_n = T\psi_n, \quad n=a,b \tag{4.2}$$

in order to obtain the transition probability

$$P'_n(t) = |\langle \psi'_n | \Psi' \rangle|^2 = |\langle \psi_n | T^\dagger | \Psi' \rangle|^2 . \tag{4.3}$$

In Appendix A we summarize from another point of view why the textbook wave functions can, in general, only be applied in the $\mathbf{E}\cdot\mathbf{r}$ formalism and why the wave functions representing the states $|a\rangle$ and $|b\rangle$ have to be transformed when going from one gauge of the electromagnetic field to another.

Let us now define the physical probability amplitudes

$$p_n(t) = \langle \psi_n | \Psi \rangle, \quad p'_n(t) = \langle \psi_n | T^\dagger | \Psi' \rangle \tag{4.4}$$

so that

$$P_n = |p_n|^2, \quad P'_n = |p'_n|^2 . \tag{4.5}$$

Using for Ψ and Ψ' the expansions (3.4) and (3.9), we obtain a relation between the probability amplitudes p_a and p_b (p'_a and p'_b) and the expansion amplitudes a and b (α and β). In the electric field gauge the probability amplitudes coincide with the expansion amplitudes

$$p_a(t) = a(t)e^{-i\omega_a t}, \quad p_b(t) = b(t)e^{-i\omega_b t} . \tag{4.6}$$

In the radiation gauge the probability amplitudes p'_a and p'_b and the expansion amplitudes α and β are different:[17]

$$\begin{aligned} p'_a(t) &= T^\dagger_{aa}\alpha e^{-i\omega_a t} + T^\dagger_{ab}\beta e^{-i\omega_b t} , \\ p'_b(t) &= T^\dagger_{ba}\alpha e^{-i\omega_a t} + T^\dagger_{bb}\beta e^{-i\omega_b t} . \end{aligned} \tag{4.7}$$

Finally it should be mentioned that also the radiation gauge wave function Ψ' can be expanded in such a way that the expansion amplitudes coincide with the probability amplitudes. Instead of choosing the basis ψ_a and ψ_b one also can write Ψ' in terms of the transformed wave functions ψ'_a and ψ'_b (4.2):

$$\Psi'(\mathbf{r},t) = \alpha'(t)e^{-i\omega_a t}\psi'_a(\mathbf{r},t) + \beta'(t)e^{-i\omega_b t}\psi'_b(\mathbf{r},t) . \tag{4.8}$$

Obviously α' and β' satisfy the Bethe-Lamb equations (2.3) and are identical with the probability amplitudes

$$p'_a(t) = \alpha'(t)e^{-i\omega_a t}, \quad p'_b(t) = \beta'(t)e^{-i\omega_b t} . \tag{4.9}$$

This allows inversion of the relation (4.7):

$$\begin{aligned} \alpha(t) &= T_{aa}p'_a e^{i\omega_a t} + T_{ab}p'_b e^{i\omega_a t} , \\ \beta(t) &= T_{ba}p'_a e^{i\omega_b t} + T_{bb}p'_b e^{i\omega_b t} . \end{aligned} \tag{4.10}$$

Since $p'_a(t)$ and $p'_b(t)$ are the physical quantities, they determine the initial condition of the system. Therefore, the initial conditions for the $\mathbf{p}\cdot\mathbf{A}$ equations of motion (3.10) have to be derived from Eq. (4.10) and are in general different from the initial conditions of the Bethe-Lamb equations.

V. EXAMPLES

In this section we demonstrate the points made in the previous sections with two simple examples: In order to make contact with Bethe's calculation we first consider a two-level atom $\{|a\rangle, |b\rangle\}$ in a uniform and static electric field

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0 . \tag{5.1}$$

We are interested in the field-induced transitions $|a\rangle \rightarrow |b\rangle$ and we assume that the field is weak so that the transition can be calculated in first-order perturbation theory. In this limit the Bethe-Lamb equations yield for an atom which is initially in state $|a\rangle$, the following probability amplitude for state $|b\rangle$:

$$\begin{aligned} p_b(t) &= b(t)e^{-i\omega_b t} \\ &= -\frac{e}{\hbar}\mathbf{E}_0\cdot\mathbf{r}_{ba}\frac{e^{-(\gamma_a/2+i\omega_a)t} - e^{-(\gamma_b/2+i\omega_b)t}}{\omega - i\delta} . \end{aligned} \tag{5.2}$$

The vector potential for the static electric field (5.1) has the form

$$\mathbf{A}(t) = -t\mathbf{E}_0 . \tag{5.3}$$

The use of the $\mathbf{p}\cdot\mathbf{A}$ interaction with this vector potential in the Bethe-Lamb equations would lead in first order to

$$-\frac{e}{\hbar}\mathbf{E}_0\cdot\mathbf{r}_{ba}\frac{\omega}{\omega-i\delta} \times \frac{[1+(i\omega+\delta)t]e^{-(\gamma_a/2+i\omega_a)t} - e^{-(\gamma_b/2+i\omega_b)t}}{\omega - i\delta} . \tag{5.4}$$

This differs from Eq. (5.2) not only by a prefactor $\omega/(\omega-i\delta)$ but also by a term which linearly increases with time.

In deriving the probability amplitude from the equations (3.10) we can use the transformation operator T in the form

$$T(\mathbf{r},t) = 1 + \frac{i}{\hbar}e\,\mathbf{A}(t)\cdot\mathbf{r} . \tag{5.5}$$

Since in our special example $T(\mathbf{r},t=0)=1$ the initial conditions for Eqs. (3.10) are the same as for the Bethe-Lamb equations:

$$\alpha(0) = p'_a(0) = 1, \quad \beta(0) = p'_b(0) = 0 . \tag{5.6}$$

The matrix elements of the damping operator Γ' have the form

$$\begin{aligned} &\Gamma'_{aa} = \gamma_a, \quad \Gamma'_{bb} = \gamma_b , \\ &\Gamma'_{ab} = 2\frac{i}{\hbar}e\,\delta t\,\mathbf{E}_0\cdot\mathbf{r}_{ab}, \quad \Gamma'_{ba} = -2\frac{i}{\hbar}e\,\delta t\,\mathbf{E}_0\cdot\mathbf{r}_{ba} . \end{aligned} \tag{5.7}$$

The quantity δ denotes again the difference of the decay constants (2.8). With the help of Eq. (2.13) the first-order solution of Eqs. (3.10) reads

$$\alpha(t)=e^{-(\gamma_a/2)t},$$
$$\beta(t)=-\frac{e}{\hbar}\mathbf{E}_0\cdot\mathbf{r}_{ba}\times\frac{[1+(i\omega+\delta)t]e^{-(\gamma_a/2+i\omega)t}-e^{-(\gamma_b/2)t}}{\omega-i\delta}. \tag{5.8}$$

A comparison with expression (5.4) shows that the prefactor $\omega/(\omega-i\delta)$ in (5.4) disappears when the off-diagonal elements of the damping operator (5.7) are taken into account.

In order to obtain the probability amplitude p_b' (4.15) the two solutions α and β have to be combined according to

$$p_b'(t)=\beta(t)e^{-i\omega_b t}+\frac{i}{\hbar}e\mathbf{E}_0\cdot\mathbf{r}_{ba}t\alpha(t)e^{-i\omega_a t}. \tag{5.9}$$

The second term in p_b' just cancels the term proportional to $(i\omega+\delta)t$ in $\beta(t)$ (5.8) and we obtain for p_b'

$$p_b'(t)=-\frac{e}{\hbar}\mathbf{E}_0\cdot\mathbf{r}_{ba}\frac{e^{-(\gamma_a/2+i\omega_a)t}-e^{-(\gamma_b/2+i\omega_b)t}}{\omega-i\delta} \tag{5.10}$$

in agreement with the $\mathbf{E}\cdot\mathbf{r}$ result (5.2).

We now proceed to a two-level atom $\{|a\rangle,|b\rangle\}$ in a rf field

$$\mathbf{E}(t)=\mathbf{E}_0\sin(\nu t). \tag{5.11}$$

The Bethe-Lamb equations with the rotating-wave approximation (2.4) then give in first-order perturbation theory

$$p_b(t)=b(t)e^{-i\omega_b t}=\frac{ie}{2\hbar}\mathbf{E}_0\cdot\mathbf{r}_{ba}\frac{e^{-[\gamma_a/2+i(\omega_a-\nu)]t}-e^{-(\gamma_b/2+i\omega_b)t}}{\Delta-i\delta}. \tag{5.12}$$

Using the Bethe-Lamb equations with the $\mathbf{p}\cdot\mathbf{A}$ interaction and the corresponding vector potential

$$\mathbf{A}(t)=\mathbf{A}_0\cos(\nu t),\quad \mathbf{A}_0=\frac{1}{\nu}\mathbf{E}_0 \tag{5.13}$$

would result in first-order perturbation theory in

$$\frac{ie}{2\hbar}\mathbf{E}_0\cdot\mathbf{r}_{ba}\left[\frac{\omega}{\nu}\right]\frac{e^{-[\gamma_a/2+i(\omega_a-\nu)]t}-e^{-(\gamma_b/2+i\omega_b)t}}{\Delta-i\delta}. \tag{5.14}$$

This differs from Eq. (5.12) just by the factor (ω/ν) which was discussed in Sec. II.

In deriving the result (5.12) from $\mathbf{p}\cdot\mathbf{A}$ we can again use the transformation operator T in the form (5.5) and the damping matrix elements in the form

$$\Gamma_{aa}'=\gamma_a,\quad \Gamma_{bb}'=\gamma_b,$$
$$\Gamma_{ab}'=-2\frac{i}{\hbar}e\delta\,\mathbf{A}(t)\cdot\mathbf{r}_{ba},\quad \Gamma_{ba}'=2\frac{i}{\hbar}e\delta\,\mathbf{A}(t)\cdot\mathbf{r}_{ba}. \tag{5.15}$$

The initial conditions for Eqs. (3.10) are now given by

$$\alpha(0)=1,\quad \beta(0)=\frac{i}{\hbar}e\,\mathbf{A}(0)\cdot\mathbf{r}_{ba}. \tag{5.16}$$

The first-order solution of Eqs. (3.10) with the rotating-wave approximation then reads

$$\alpha(t)=e^{-(\gamma_a/2)t},$$
$$\beta(t)=\frac{ie}{2\hbar}\mathbf{E}_0\cdot\mathbf{r}_{ba}\left[\frac{\omega-i\delta}{\nu}\frac{e^{-(\delta+i\Delta)t}-1}{\Delta-i\delta}+\frac{1}{\nu}\right]e^{-(\gamma_b/2)t}. \tag{5.17}$$

In the expression for β the second term proportional to $1/\nu$ in the bracket is due to the modified initial condition (5.16) and the portion proportional to $-i\delta/\nu$ of the first term originates from the off-diagonal matrix element Γ_{ba}' (5.15). Without these two contributions β would just equal $b(t)$ (5.12) multiplied by the factor ω/ν. Combining the two solutions α and β to the probability amplitude

$$p_b'(t)=\beta e^{-i\omega_b t}-\frac{i}{\hbar}e\,\mathbf{A}(t)\cdot\mathbf{r}_{ba}\alpha e^{-i\omega_a t} \tag{5.18}$$

gives

$$p_b'(t)=\frac{ie}{2\hbar}\mathbf{E}_0\cdot\mathbf{r}_{ba}\frac{e^{-[\gamma_a/2+i(\omega_a-\nu)]t}-e^{-(\gamma_b/2+i\omega_b)t}}{\Delta-i\delta}. \tag{5.19}$$

The α admixture to p_b' in effect cancels all the crucial terms in β (5.17) and the result (5.19) agrees with Eq. (5.12).

For higher-order processes in a two-level atom our formalism can be applied in a similar fashion. However, to solve the $\mathbf{p}\cdot\mathbf{A}$ equations (3.10) in higher orders becomes more and more cumbersome due to the transformed damping matrix elements so that for practical calculations the use of the Bethe-Lamb equations is much more convenient.

VI. CONCLUSIONS

In this paper we reviewed the original problem which led to the Bethe-Lamb equations, we demonstrated why these equations (which use the $\mathbf{E}\cdot\mathbf{r}$ interaction) yield the correct answer and why they fail if one simply replaces $\mathbf{E}\cdot\mathbf{r}$ by $\mathbf{p}\cdot\mathbf{A}$, and we showed for the simple two-level model how to derive some equations which are the $\mathbf{p}\cdot\mathbf{A}$ equivalent of the Bethe-Lamb equations.

It has long been known that the two interactions $\mathbf{E}\cdot\mathbf{r}$ and $\mathbf{p}\cdot\mathbf{A}$ correspond to two different gauges of the Hamiltonian. It is, however, sometimes overlooked that the transformation from one form of the interaction to the other has two consequences which are crucial for the kind of calculations considered in this paper.

(1) First, the wave functions have to be transformed when going from $\mathbf{E}\cdot\mathbf{r}$ to $\mathbf{p}\cdot\mathbf{A}$. For the $\mathbf{p}\cdot\mathbf{A}$ interaction the initial and final state wave functions are not given by the textbook wavefunctions, i.e., by the eigenstates of H_0, but by the transformed wave functions (4.2). The transformation of the wave functions leads to modified initial conditions for the expansion amplitudes α and β in Eq. (3.10) and to the relation (4.7) between the experi-

mentally accessible transition amplitudes p_a' and p_b' and the amplitudes α and β.

(2) Second, the damping operator has to be transformed, too. The damping matrix has off-diagonal elements for the $\mathbf{p}\cdot\mathbf{A}$ interaction and the correct $\mathbf{p}\cdot\mathbf{A}$ equations of motion are given by Eqs. (3.10). This is a key point in the present analysis and has not been properly appreciated heretofore.

The calculations in Sec. V show how one obtains identical results with the two different interactions. The advantage of the $\mathbf{E}\cdot\mathbf{r}$ interaction derives from the fact that the energy operator equals H_0 since it corresponds to a gauge with vanishing vector potential. In this case the expansion amplitudes a and b in Eq. (3.4) coincide with the probability amplitudes.

APPENDIX A

In the example of the Lamb shift experiment the initial and final states are energy eigenstates. An atom in an external field represents a nonconservative system so that we have to distinguish between the energy and the Hamiltonian of the system. In the absence of any field-atom interaction the energy is the sum of the kinetic and potential energy of the electron as it moves in the atomic orbit

$$\mathcal{E}=\frac{\pi^2}{2m}+U(\mathbf{r})\ , \tag{A1}$$

where $\pi=m\mathbf{v}$ denotes the kinetic momentum (v is the electron velocity). In the presence of a field the kinetic momentum π can be expressed in terms of the canonical momentum $\mathbf{p}$ and the vector potential $\mathbf{A}$ as $\pi=\mathbf{p}-e\,\mathbf{A}$.

The atomic states $|a\rangle$ and $|b\rangle$ are characterized by the energy operator (A1) and are in general not eigenstates of H_0.[3,10,18] This can be illustrated by gauge arguments based on the concept of gauge-invariant quantities as introduced in Ref. 9. Gauge-invariant quantities are represented by operators whose eigenvalues are invariant under gauge transformations. Examples are the position operator $\mathbf{r}$ and the kinetic momentum $\pi=\mathbf{p}-e\,\mathbf{A}$ as well as any combination of these two quantities. On the other hand, the canonical momentum $\mathbf{p}$ or the vector potential $\mathbf{A}$ have gauge-dependent eigenvalues and are therefore nonphysical quantities. The same statement holds for the unperturbed Hamiltonian H_0 (2.14). A physical system can only be prepared in an eigenstate of a gauge-invariant (physical) quantity, not in an eigenstate of a nonphysical quantity. In the case of a hydrogen atom the states $|a\rangle$ and $|b\rangle$ are therefore in general not eigenstates of H_0 whose eigenvalues are gauge dependent. Instead they are eigenstates of the energy operator $\mathcal{E}$ which is given by Eq. (A1).

The $\mathbf{E}\cdot\mathbf{r}$ interaction corresponds to a gauge in which the vector potential vanishes $\mathbf{A}=0$. Therefore, the kinetic momentum π and the canonical momentum $\mathbf{p}$ are the same:

$$\pi=\mathbf{p}=\frac{\hbar}{i}\nabla \tag{A2}$$

and the energy operator equals the unperturbed Hamiltonian H_0

$$\mathcal{E}=\frac{\mathbf{p}^2}{2m}+U(\mathbf{r})=H_0\ . \tag{A3}$$

Hence, the wave functions representing the states $|a\rangle$ and $|b\rangle$ in the electric field gauge follow directly from Eq. (3.2):

$$\mathcal{E}\psi_a=\hbar\omega_a\psi_a,\quad \mathcal{E}\psi_b=\hbar\omega_b\psi_b\ . \tag{A4}$$

In the $\mathbf{p}\cdot\mathbf{A}$ formulation, on the other hand, kinetic and canonical momentum are different:

$$\pi=\mathbf{p}-e\,\mathbf{A} \tag{A5}$$

and therefore also energy operator and unperturbed Hamiltonian,

$$\mathcal{E}=\frac{1}{2m}(\mathbf{p}-e\,\mathbf{A})^2+U(\mathbf{r})\neq H_0\ . \tag{A6}$$

The energy eigenstates in the radiation gauge

$$\left[\frac{1}{2m}(\mathbf{p}-e\,\mathbf{A})^2+U(\mathbf{r})\right]\psi_n'=\hbar\omega_n\psi_n',\quad n=a,b \tag{A7}$$

are then also different from the eigenstates ψ_n in Eq. (A4). The relation between ψ_n' and ψ_n is the same as the relation between the wave functions Ψ' and Ψ in Eq. (3.5)

$$\begin{aligned}&\psi_n'=T\psi_n,\quad n=a,b\\ &T=e^{ie\,\mathbf{A}(t)\cdot\mathbf{r}/\hbar}\ .\end{aligned} \tag{A8}$$

Since in the experiment the probability of finding the atom in a particular energy eigenstate is measured the wave function Ψ' in the $\mathbf{p}\cdot\mathbf{A}$ formalism has to be projected onto the transformed wave functions ψ_a' or ψ_b' (A8) in order to obtain the probability (4.3).

APPENDIX B

In this Appendix we will distinguish between different classes of calculations in which the $\mathbf{E}\cdot\mathbf{r}$ versus $\mathbf{p}\cdot\mathbf{A}$ question arises and we will list some of the arguments commonly put forward for the resolution of this question. It will be shown that there are classes of calculations where one can obtain the same result with both forms of the interaction without using the whose machinery developed in this paper, in particular without transforming the eigenstates when going from one gauge to the other. On the other hand, there are classes of calculations where commonly used arguments (such as the completeness of the intermediate states) are not sufficient to resolve the problem and where the transformation of the damping operator and the distinction between expansion amplitudes and probability amplitudes is essential.

We restrict the calculations to simple examples and refer the reader to the original literature for more detailed calculations. For our purpose it is convenient to distinguish between five different classes of calculations.

(i) Plane-wave field, solution at $t\to\infty$, no radiation damping. For this class of calculations both forms of the interaction give the same result even if the textbook wave functions are used for the $\mathbf{p}\cdot\mathbf{A}$ approach. The proof of this statement relies on (1) energy conservation and (2) the completeness of the intermediate states. In

order to demonstrate this we first consider the simplest example of a first-order transition from a state $|a\rangle$ to a state $|b\rangle$ with spacing $E_a - E_b = \hbar\omega$, induced by a plane wave of frequency ν. The calculation can start from Eqs. (2.4) which is already written for a plane-wave field. After dropping the decay terms the first-order solution of Eqs. (2.4) yields in the limit $t \to \infty$

$$\lim_{t\to\infty} \frac{|b(t)|^2}{t} = 2\pi \left[\frac{e}{2\hbar}\right]^2 |\mathbf{E}_0\cdot\mathbf{r}_{ba}|^2 \delta(\omega-\nu) . \quad \text{(B1)}$$

This is Fermi's golden rule for the transition rate. If the $\mathbf{E}\cdot\mathbf{r}$ interaction in Eqs. (2.4) is replaced by the $\mathbf{p}\cdot\mathbf{A}$ form and if Eq. (2.15) is employed, one obtains

$$2\pi \left[\frac{e}{2\hbar}\right]^2 \left[\frac{\omega}{\nu}\right]^2 |\mathbf{E}_0\cdot\mathbf{r}_{ba}|^2 \delta(\omega-\nu) . \quad \text{(B2)}$$

The expressions (B1) and (B2) differ by the usual factor $(\omega/\nu)^2$, but the δ function takes care that this factor equals unity so that both expressions are actually identical.

For a second-order process the equivalence of the two approaches is not so obvious. Let us go for the moment beyond the two-level model which we exclusively considered in this paper so that the second-order transition rate involves a sum over many intermediate states. For the emission of two photons with frequencies ν_1 and ν_2 the $\mathbf{E}\cdot\mathbf{r}$ calculation gives

$$\lim_{t\to\infty} \frac{|b(t)|^2}{t} = 2\pi \left[\frac{e}{2\hbar}\right]^4 \left|\sum_n \frac{(\mathbf{E}_2\cdot\mathbf{r}_{bn})(\mathbf{E}_1\cdot\mathbf{r}_{na})}{\omega_a-\omega_n-\nu_1} + \frac{(\mathbf{E}_1\cdot\mathbf{r}_{bn})(\mathbf{E}_2\cdot\mathbf{r}_{na})}{\omega_a-\omega_n-\nu_2}\right|^2 \delta(\omega-\nu_1-\nu_2) , \quad \text{(B3)}$$

whereas simply replacing the $\mathbf{E}\cdot\mathbf{r}$ matrix elements by the $\mathbf{p}\cdot\mathbf{A}$ matrix elements according to Eq. (2.15) results in

$$2\pi \left[\frac{e}{2\hbar}\right]^4 \left|\sum_n \frac{(E_a-E_n)(E_n-E_b)}{\hbar^2\nu_1\nu_2} \left[\frac{(\mathbf{E}_2\cdot\mathbf{r}_{bn})(\mathbf{E}_1\cdot\mathbf{r}_{na})}{\omega_a-\omega_n-\nu_1} + \frac{(\mathbf{E}_1\cdot\mathbf{r}_{bn})(\mathbf{E}_2\cdot\mathbf{r}_{na})}{\omega_a-\omega_n-\nu_2}\right]\right|^2 \delta(\omega-\nu_1-\nu_2) . \quad \text{(B4)}$$

In order to show that the expressions (B3) and (B4) are the same, one has to exploit not only the energy conservation as expressed by the δ function but also the completeness of the intermediate states $|n\rangle$.[19,20] In a similar fashion the equivalence of both approaches can also be shown for a three-photon interaction[21] as well as for multiphoton processes of arbitrary order.[22]

The importance of the closure relation has also been numerically demonstrated by an exactly solvable example, the $1S \to 2S$ transition in hydrogen via two-photon absorption.[23] In the case that all the intermediate states including the continuum are taken into account both expressions (B3) and (B4) give exactly the same numerical result for the two-photon transition rate, but the respective contributions of the individual intermediate states are very different. The intermediate wave function ψ_{2P} (3.2), for example, gives the dominant contribution to the sum (B3) in the $\mathbf{E}\cdot\mathbf{r}$ formalism, whereas it does not contribute at all to the sum (B4) in the $\mathbf{p}\cdot\mathbf{A}$ formalism, since $\langle 2S_{1/2}|\mathbf{p}|2P_{1/2}\rangle = 0$ for degenerated states $2S_{1/2}$ and $2P_{1/2}$. The contribution of the continuum, on the other hand, is negligible in the $\mathbf{E}\cdot\mathbf{r}$ formalism, but it plays a very important role in the $\mathbf{p}\cdot\mathbf{A}$ approach. In the examples given in Ref. 23 the continuum contributes by more than 50% to the sum (B4).

This situation is unsatisfactory from a physics point of view. The two forms of the interaction lead to the same result due only to the reason that one works with a complete set of eigenstates, but in the $\mathbf{p}\cdot\mathbf{A}$ formalism these textbook eigenstates (3.2) do not describe the physical (energy) eigenstates of the system anymore. When going from the electric field gauge to the radiation gauge, the physical eigenstates become a superposition of the eigenstates ψ_n (3.2) of the unperturbed Hamiltonian H_0 with a major admixture of continuum states of H_0. The reason why one has to sum over so many states in the $\mathbf{p}\cdot\mathbf{A}$ formalism in order to obtain an accurate result is therefore due to the fact that one "forgot" to use the transformed eigenstates for $\mathbf{p}\cdot\mathbf{A}$.

(ii) Adiabatically turned-off field, no radiation damping. In an experiment the system is usually prepared before the field is turned on and the measurement takes place after the field is turned off. The strictly monochromatic field in (*i*) should therefore be replaced by a wave packet with finite frequency bandwidth. The electric field $\mathbf{E}(t)$ and the vector potential $\mathbf{A}(t)$ in the radiation gauge then have the form

$$\mathbf{E}(t) = \int d\omega\, \mathbf{E}(\omega)\cos(\omega t) ,$$
$$\mathbf{A}(t) = -\int d\omega\, \mathbf{E}(\omega)\frac{\sin(\omega t)}{\omega} . \quad \text{(B5)}$$

In this case energy conservation arguments cannot be applied as in (*i*). Nevertheless, in the limit of long interaction times both forms of the interaction lead again to the same transition rates, even if the transformation of the eigenstates for $\mathbf{p}\cdot\mathbf{A}$ is not taken into account. This can be proven by showing[18,24] that for a field (B5) which is adiabatically turned on and off the transformation operator T (3.5) approaches unity in the limit $t \to \pm\infty$:

$$\lim_{t\to\pm\infty} T(\mathbf{r},t) = \lim_{t\to\pm\infty} e^{ie\,\mathbf{A}(t)\cdot\mathbf{r}/\hbar} = 1 . \quad \text{(B6)}$$

According to Eq. (4.7) the expansion amplitudes α and β in the $\mathbf{p}\cdot\mathbf{A}$ formalism then coincide in the limit $t \to \infty$ with the probability amplitudes p_a' and p_b' so that the $\mathbf{p}\cdot\mathbf{A}$ approach with the textbook wave functions in Eq. (4.3) gives the correct result for this class of calculations.

(iii) Suddenly turned-off field, no radiation damping.

We now come to transient effects which depend on the duration of the interaction. In an experiment typical for this class of calculations the electromagnetic field is suddenly turned on for a finite time or the atom passes through a locally well-restricted field with a finite velocity, and one looks for the transition probability as a function of the interaction time. This is now a situation where the $\mathbf{p}\cdot\mathbf{A}$ approach with the textbook wave functions does not give the correct answer. The reason for this is that even if the electric field is (suddenly) switched off there may very well be a (time-independent) vector potential remaining. In contrast to Eq. (B6) the transformation operator T then still has nonvanishing off-diagonal matrix elements even when the field is switched off. According to Eq. (4.7) probability amplitudes and $\mathbf{p}\cdot\mathbf{A}$ expansion amplitudes are then different.

We can illustrate this point by the simple example of a first-order transition in an arbitrary field $\mathbf{E}(t)$. The equations of motion for this example look similar to the Bethe-Lamb equations (2.3), but without the decay terms and with an arbitrary $\mathbf{E}(t)$. If the initial state is prepared at some time t_0 before the field is switched on and if the measurement is taken at some time t_1 when the field is switched off again, the first-order solution in the $\mathbf{E}\cdot\mathbf{r}$ approach reads

$$b(t_1)=\frac{ie}{\hbar}\int_{t_0}^{t_1} dt\ \mathbf{E}(t)\cdot\mathbf{r}_{ba}e^{-i\omega t}\ . \tag{B7}$$

Simply replacing the $\mathbf{E}\cdot\mathbf{r}$ interaction by the $\mathbf{p}\cdot\mathbf{A}$ form and integrating by parts gives

$$\frac{i}{\hbar}\frac{e}{m}\int_{t_0}^{t_1} dt\ \mathbf{A}(t)\cdot\mathbf{p}_{ba}e^{-i\omega t}=\frac{ie}{\hbar}\int_{t_0}^{t_1} dt\ \mathbf{E}(t)\cdot\mathbf{r}_{ba}e^{-i\omega t} + \frac{ie}{\hbar}[\,\mathbf{A}(t_1)\cdot\mathbf{r}_{ba}e^{-i\omega t_1} - \mathbf{A}(t_0)\cdot\mathbf{r}_{ba}e^{-i\omega t_0}]\ . \tag{B8}$$

The two expressions (B7) and (B8) obviously only coincide if the vector potential vanishes simultaneously with the electric field

$$\mathbf{A}(t_0)=\mathbf{A}(t_1)=\mathbf{0}\ . \tag{B9}$$

Since this is in general not the case the transformation (4.2) of the eigenstates has to be taken into account in order to obtain the correct result with the $\mathbf{p}\cdot\mathbf{A}$ approach for this class of calculations.

(iv) Plane-wave field, solution at finite time, no radiation damping. Even for experiments which measure transition probabilities as a function of the interaction time, the calculations are usually done with plane-wave fields. This requires the knowledge of the probability amplitudes in the presence of the field.

In contrast to (*i*) energy conservation arguments can no longer be applied in this case. The conclusion for this class of calculations is therefore the same as in (*iii*): if the textbook wave functions would be used for both forms of the interaction, one would obtain different results for finite interaction times and only the $\mathbf{E}\cdot\mathbf{r}$ result is the correct one. For probability amplitudes in the presence of the field it is essential to use the transformed eigenstates in the $\mathbf{p}\cdot\mathbf{A}$ calculation. Examples of current interest for this class of calculations are the temporal evolution of multiphonon ionization rates[17,25] and the detection of Rabi-type oscillations of the atomic population,[13] as well as all kinds of coherent transient effects.[7]

(v) Radiation damping. So far in this Appendix we have only discussed calculations without radiation damping. Calculations with radiation damping are the subject of the main body of this paper. It is shown there that it is crucial for this class of calculations to use the transformed decay matrix for the Schrödinger equation (3.6) in the radiation gauge and to employ the transformed eigenstates (4.2) for the transition probabilities (4.3) in the $\mathbf{p}\cdot\mathbf{A}$ approach. If these transformations are not taken into account the $\mathbf{p}\cdot\mathbf{A}$ formalism gives an incorrect result for finite interaction times[1] as well as in the limit $t\rightarrow\infty$.[26]

A typical example for this class of calculations are the Bethe-Lamb equations (2.3). For the Lamb shift experiment these equations yield the evolution of the $2S_{1/2}$ population as a function of the interaction time. For a given interaction time they give the $2S_{1/2}$ population as a function of the rf frequency or the level spacing, i.e., the line shape. There have been alternative approaches for calculating the line shape.[6,20,27,28] For instance, if one assumes a linear (and subsequently exponential) decay of the $2S_{1/2}$ population inside the rf field, the rate of this field-induced decay can be calculated in lowest-order perturbation theory in the limit $t\rightarrow\infty$. Compared to this approach the Bethe-Lamb equations are more powerful in the sense that they give a nonperturbative solution (2.7) for the $2S_{1/2}$ population for arbitrary interaction time, for arbitrary strength of the rf field, and for arbitrary decay constants of the two levels $|a\rangle$ and $|b\rangle$.

The calculation of the linewidth in Ref. 20 follows the procedure described in (*i*). For the $\mathbf{p}\cdot\mathbf{A}$ approach it uses the textbook wave functions as well as the same decay constants as in the $\mathbf{E}\cdot\mathbf{r}$ approach, and the transition rate for the two-step process $2S_{1/2}\rightarrow 2P_{1/2}\rightarrow 1S_{1/2}$ is derived in the limit $t\rightarrow\infty$. Just as in Eqs. (2.10) and (2.16) both forms of the interaction then lead to transition rates which differ by the ratio $(\omega/\nu)^2$. If in analogy to the discussion in (*i*) all the other intermediate states besides $2P_{1/2}$ are taken into account in the $\mathbf{p}\cdot\mathbf{A}$ calculation and if energy conservation is exploited, part of the discrepancy is removed.

Similar conclusions were reached in Ref. 28 where the line-shape problem was treated from a fully quantum-electrodynamical point of view rather than by a semiclassical theory with phenomenological decay terms. By generalizing the Weisskopf-Wigner theory to a multilevel system it was found that in the $\mathbf{p}\cdot\mathbf{A}$ approach the background contribution due to virtual transitions to all nonresonant levels has to be taken into account in order to resolve the discrepancy with the experimental results.

[1]W. E. Lamb, Jr., Phys. Rev. **85**, 259 (1952).
[2]W. E. Lamb, Jr. and R. C. Retherford, Phys. Rev. **79**, 549 (1950).
[3]D. H. Kobe and A. L. Smirl, Am. J. Phys. **46**, 624 (1978).
[4]M. Göppert-Mayer, Ann. Phys. (Leipzig) **9**, 273 (1931).
[5]H. A. Bethe, in *Quantentheorie,* Vol. 24/1 of *Handbuch der Physik,* 2nd ed. (Springer, Berlin, 1933), p. 273.
[6]E. A. Power and S. Zienau, Philos. Trans. R. Soc. London **251**, 427 (1959).
[7]M. Sargent III, M. O. Scully, and W. E. Lamb, Jr., *Laser Physics* (Addison-Wesley, Reading, MA, 1974).
[8]W. Pauli, in *Quantentheorie,* Vol. 24/1 of *Handbuch der Physik,* 2nd ed. (Springer, Berlin, 1933), p. 83.
[9]C. Cohen-Tannoudji, B. Diu, and F. Laloe, *Quantum Mechanics* (Hermann/Wiley, Paris, 1977).
[10]K.-H. Yang, Ann. Phys. (N.Y.) **101**, 62 (1976).
[11]R. R. Schlicher, W. Becker, J. Bergou, and M. O. Scully, *Quantum Electrodynamics and Quantum Optics,* edited by A. O. Barut (Plenum, New York, 1984), p. 405.
[12]Reference 11 contains a list of some 50 examples.
[13]D. Meschede, H. Walther, and G. Müller, Phys. Rev. Lett. **54**, 551 (1985).
[14]V. F. Weisskopf and E. Wigner, Z. Phys. **63**, 54 (1930).
[15]W. Becker, R. R. Schlicher, M. O. Scully, M. S. Zubairy, and M. Goldhaber, Phys. Lett. **131B**, 16 (1983); W. Becker, R. R. Schlicher, and M. O. Scully, *ibid.* **106A**, 441 (1984).
[16]G. Breit, Rev. Mod. Phys. **5**, 91 (1933).
[17]C. Leubner and P. Zoller, J. Phys. B **13**, 3613 (1980).
[18]J. J. Forney, A. Quattropani, and F. Bassani, Nuovo Cimento B **37**, 78 (1977).
[19]W. L. Peticolas, R. Norris, and K. E. Rieckhoff, J. Chem. Phys. **42**, 4164 (1965); F. V. Bunkin, Zh. Eksp. Teor. Fiz. **50**, 1685 (1966) [Sov. Phys.—JETP **23**, 1121 (1966)].
[20]Z. Fried, Phys. Rev. A **8**, 2835 (1973).
[21]G. Grynberg and E. Giacobino, J. Phys. B **12**, L93 (1979).
[22]K. Haller and R. B. Sohn, Phys. Rev. A **20**, 1541 (1979); Y. Aharonov and C. K. Au, *ibid.* **20**, 1553 (1979); S. Olariu, I. Popescu, and C. B. Collins, Phys. Rev. D **20**, 3095 (1979); E. Kazes, T. E. Feuchtwang, P. H. Cutler, and H. Grotch, Ann. Phys. (N.Y.) **142**, 80 (1982).
[23]F. Bassani, J. J. Forney, and A. Quattropani, Phys. Rev. Lett. **39**, 1070 (1977).
[24]J. Bergou, J. Phys. B **16**, L647 (1983).
[25]S. Geltman, J. Phys. B **10**, 831 (1977); H. S. Antunes Neto and L. Davidovich, Phys. Rev. Lett. **53**, 2238 (1984); W. Elberfeld and M. Kleber, *Physics of Strong Fields,* edited by W. Greiner (Plenum, New York, in press).
[26]D. H. Kobe, Phys. Rev. Lett. **40**, 538 (1978).
[27]F. E. Low, Phys. Rev. A **20**, 1567 (1979).
[28]L. Davidovich and H. M. Nussenzveig, *Foundations of Radiation Theory and Quantum Electrodynamics,* edited by A. O. Barut (Plenum, New York, 1980), p. 83.