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Photon wave functions

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We argue that a photon wave function can be introduced if one is willing to redefine, in what we feel is a physically meaningful way, what one wishes to mean by such a wave function. The generation of a photon wave function by a spontaneously emitting atom is discussed.

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I. INTRODUCTION

An intrinsically relativistic particle, the photon fits uncomfortably within the framework of elementary, nonrelativistic quantum mechanics. With no rest mass it cannot be "stopped," except by an absorption process that destroys it; thus separate spin and orbital angular momentum are not physically meaningful and only a helicity can be introduced. Also associated with the absence of rest mass is the lack of photon localizability first discussed in detail by Newton and Wigner [1]: There is no probability density for the position of the photon and thus a position-representation wave function cannot be consistently introduced.

This latter property is a disappointment from the perspective of quantum optics, where thought and real experiments involving one and few photons abound. Although full calculations can of course always be made with quantum electrodynamics, one would like to obtain by introducing one- and few-photon wave functions the kind of insight achieved in atomic and molecular physics by introducing one- and few-electron wave functions.

In this paper we argue that a photon wave function *can* in fact be introduced, if one is willing to redefine, in what we feel is a physically meaningful way, exactly what one *wishes to mean* by such a wave function. In Sec. II we begin along the naive route one would take to introduce a photon wave function. After sketching diversions from this path that have been taken in the past, we introduce what we feel is a reasonable way to proceed and present our wave-function description of the photon as a kind of minimum modification of the naive route. On the basis of this we construct in Sec. III a second-quantized, many-photon theory. This reproduces, in the main, the usual field theory obtained by quantizing the free radiation field. The viewpoint, however, is quite different: the quantized electromagnetic field is achieved here through the approach of many-particle physics rather than through canonical quantization. The single-photon theory of Sec. II can then be recovered by looking at the manifold of one-photon states.

That such a photon wave-function perspective is reasonable and useful can only be confirmed by considering its description of simple quantum processes. In this paper we begin such a consideration. After an outline in Sec. IV of aspects of the Power-Healy transformation [2], which we wish to employ in treating the interaction of atoms with the radiation field, we turn in Sec. V to the calculation of the photon wave function generated in a single-photon spontaneous emission event. We find that the wave function generated is a causal field, propagating away from the atomic source at the speed of light. The result is discussed in Sec. VI, where we also summarize the approach we have taken, consider alternatives, and present our concluding remarks.

As this work was being completed, we became aware of a publication by Bialynicki-Birula [3] that also addresses the issue of photon wave functions. The initial perspectives of our two contributions are certainly at least formally different: We begin with the idea of photons as particles (see Sec. II), while Bialynicki-Birula [3] begins with the Maxwell equations. Much is similar: We both end up arguing for the same normalization condition (2.13), for example, although the definitions of $\Psi(\mathbf{r},t)$ we adopt are different. Despite similarities in spirit, however, there are issues addressed here that Bialynciki-Birula does not consider. He considers only the free radiation field, although in more detail than we do here, and does not go on to establish a connection between his wave functions and the usual second-quantized theory; that connection and the generation of a photon field by spontaneous emission are two of the foci of this work.

II. SINGLE-PHOTON WAVE FUNCTIONS

We begin from the simplest point of view, basing our formulation on two properties we assert for photons: they can be of positive and negative helicity and, being massless, the relation between their energy and momentum is $E=cp$, where $p=|\mathbf{p}|$. If we then introduce probability amplitudes for photons of momentum $\mathbf{p}$ and helicity $\pm$, $\gamma_{\pm}(\mathbf{p},t)$, we would expect these momentum-representation probability amplitudes to satisfy a Schrödinger-like equation

$$i\hbar\frac{\partial\gamma_{\pm}(\mathbf{p},t)}{\partial t}=cp\gamma_{\pm}(\mathbf{p},t)\ . \tag{2.1}$$

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It is useful to introduce vector amplitudes associated with $\gamma_\pm(\mathbf{p},t)$, which identify the helicity in three-space. For each $\mathbf{p}$ introduce two unit vectors $\hat{\mathbf{e}}_1(\hat{\mathbf{p}})$ and $\hat{\mathbf{e}}_2(\hat{\mathbf{p}})$ such that the unit vectors $[\hat{\mathbf{e}}_1(\hat{\mathbf{p}}), \hat{\mathbf{e}}_2(\hat{\mathbf{p}}), \hat{\mathbf{p}} \equiv \mathbf{p}/|\mathbf{p}|]$ for a right-handed triad. We introduce helicity vectors associated with each $\hat{\mathbf{p}}$;

$$\mathbf{e}_\pm(\hat{\mathbf{p}}) \equiv \mp \frac{1}{\sqrt{2}} [\hat{\mathbf{e}}_1(\hat{\mathbf{p}}) \pm i \hat{\mathbf{e}}_2(\hat{\mathbf{p}})] \tag{2.2}$$

and define the vector amplitudes $\boldsymbol{\gamma}_\pm(\mathbf{p},t)$ according to

$$\boldsymbol{\gamma}_\pm(\mathbf{p},t) = \mathbf{e}_\pm(\hat{\mathbf{p}}) \gamma_\pm(\mathbf{p},t) \ . \tag{2.3}$$

Then we associate

$$\boldsymbol{\gamma}_+^*(\mathbf{p},t) \cdot \boldsymbol{\gamma}_+(\mathbf{p},t) d\mathbf{p} = \gamma_+^*(\mathbf{p},t) \gamma_+(\mathbf{p},t) d\mathbf{p} \tag{2.4}$$

with the probability of detecting a photon of positive helicity and momentum between $\mathbf{p}$ and $\mathbf{p}+d\mathbf{p}$ and likewise for photons of negative helicity. Note that

$$\boldsymbol{\gamma}_+^*(\mathbf{p},t) \cdot \boldsymbol{\gamma}_-(\mathbf{p},t) = 0 \ . \tag{2.5}$$

At this point it is natural to define Fourier transforms of these functions

$$\boldsymbol{\Phi}_\pm(\mathbf{r},t) \equiv \int \frac{d\mathbf{p}}{(2\pi\hbar)^{(3/2)}} \boldsymbol{\gamma}_\pm(\mathbf{p},t) e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \ . \tag{2.6}$$

It is then easy to verify that Eq. (2.1) is satisfied if the $\boldsymbol{\Phi}_\pm(\mathbf{r},t)$ satisfy

$$i\hbar \frac{\partial \boldsymbol{\Phi}_\pm(\mathbf{r},t)}{\partial t} = \pm c\hbar \nabla \times \boldsymbol{\Phi}_\pm(\mathbf{r},t) \ . \tag{2.7}$$

From the assumption that we are dealing with a single photon follows the normalization condition

$$\int [\boldsymbol{\gamma}_+^*(\mathbf{p},t) \cdot \boldsymbol{\gamma}_+(\mathbf{p},t) + \boldsymbol{\gamma}_-^*(\mathbf{p},t) \cdot \boldsymbol{\gamma}_-(\mathbf{p},t)] d\mathbf{p} = 1 \ , \tag{2.8}$$

which is equivalent to

$$\int [\boldsymbol{\Phi}_+^*(\mathbf{r},t) \cdot \boldsymbol{\Phi}_+(\mathbf{r},t) + \boldsymbol{\Phi}_-^*(\mathbf{r},t) \cdot \boldsymbol{\Phi}_-(\mathbf{r},t)] d\mathbf{r} = 1 \ . \tag{2.9}$$

Of course, the dynamical equations [(2.1) or (2.7)] guarantee that if Eqs. (2.8) and (2.9) are satisfied at one time, they are satisfied at all later times. In fact, it follows from the dynamical equations that

$$\boldsymbol{\Phi}_\pm(\mathbf{r},t) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^{(3/2)}} \boldsymbol{\gamma}_\pm(\mathbf{p},0) e^{-icpt/\hbar} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \ . \tag{2.10}$$

Now the natural temptation is to try and identify the $\boldsymbol{\Phi}_\pm(\mathbf{r},t)$ as the position-representation probability amplitudes of photons of positive and negative helicity or perhaps their sum $\boldsymbol{\Phi}(\mathbf{r},t) \equiv \boldsymbol{\Phi}_+(\mathbf{r},t) + \boldsymbol{\Phi}_-(\mathbf{r},t)$ as the position-representation wave function of a photon. But from very general principles Newton and Wigner [1] have shown (see also Wightman [4]) that the photon, being a particle of zero rest mass, is not localizable. In particular, there does not exist a probability density for the position of the photon; thus a probability amplitude, at least in the usual sense of a position-representation probability amplitude, cannot exist.

To illustrate the consequent difficulties that would ensue in practice if one nonetheless insisted on using the $\boldsymbol{\Phi}_\pm(\mathbf{r},t)$ as position-representation probability amplitudes, it is useful to compare the photon problem with that of a (nonrelativistic, spinless) electron. There one certainly can define a position-representation probability amplitude, the usual wave function $\Psi(\mathbf{r},t)$ of Schrödinger's equation for an electron. Here it is common to think of "introducing" an electron in a small region of space at, say, $t=0$ and following the subsequent evolution of the wave function. Indeed, this kind of picture is the basis of Feynman's path-integral formulation of nonrelativistic quantum mechanics [5]. And of course one can even contemplate injecting a free electron in such a manner by, for example, ionizing an atomic bound state with a very short laser pulse, producing a wave packet of continuum states initially located in the neighborhood of the nucleus, but which will then subsequently spread away from it.

The corresponding "introduction" of a photon into a system is even easier to imagine: simply start with an atom in an excited state and let it spontaneously emit. If one had a reasonable description of a (position-representation) photon wave function, one would certainly want it to be confined to within $c\tau$ of the atom at a time τ after the atom was placed in the excited state. Yet, if $\boldsymbol{\Phi}(\mathbf{r},t)$ or something like it is adopted as such a wave function, this property does not hold, as we discuss in Sec. V. This provides a rather striking illustration of the problem of nonlocalizability discussed in a more formal sense by Newton, Wigner, and Wightman [1,4]. Note that this problem occurs despite the fact that Eqs. (2.7), which hold the absence of any photon generation, are clearly local and lead to propagation at the speed of light.

One way around these difficulties was pointed out by Jauch and Piron [6], who showed that an operator representing the number of photons in an arbitrary volume V can be rigorously defined, but not as the integral over V of a photon density operator. Earlier, Mandel [7] had defined an operator representing the number of photons in a volume V as the integral over V of a so-called "detection operator" and showed that when the linear dimensions of V are large compared to the photon wavelengths this led to a simple formula for the probability that n photons are present in V. It was later shown [8] that Mandel's operator agrees with the rigorous theory of Jauch and Piron in the stated limit. Cook [9,10] extended the work to show the existence of a photon current density operator in such a limit, leading to a full theory of photon dynamics that he demonstrated was Lorentz covariant. The vector fields he uses to describe the photon in fact satisfy Eqs. (2.7) above, although their physical interpretation is somewhat different.

This school of thought then leads to a focus on what Cook [10] has called "coarse-grained" photon density and current density operators. The approach we take here is different, in that we aim for more "microscopic" operators. We do this, despite the constraints indicated by the work of Newton, Wigner, and Wightman [1,4], by redefining what we wish to mean by the position-representation wave function. Our motivation for this is massless nature of the photon and is thus related to the

source of the localizability difficulty pointed out by Newton, Wigner, and Wightman [1,4].

Return for a moment to the description of an electron by a wave function $\Psi(\mathbf{r},t)$. We argue that it is physically meaningful to talk about the measurement of the position of the electron because there are rest quantities of the electron, such as its charge e and mass m, which signal such a detection. Indeed, we can interpret

$$m\Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t)d\mathbf{r} \tag{2.11}$$

as the expected value of the mass to be detected about $d\mathbf{r}$ of $\mathbf{r}$. But for a photon there is no such rest quantity that can be used to signal detection. What can be used to signal detection at a certain position is the energy detected. This suggests that, in attempting to write down a position-representation wave function, we should be seeking a probability amplitude $\Psi(\mathbf{r},t)$ for the photon energy to be detected about $d\mathbf{r}$ of $\mathbf{r}$. The expected value of the energy to be detected there would then be given by

$$\Psi^*(\mathbf{r},t)\cdot\Psi(\mathbf{r},t)d\mathbf{r} \tag{2.12}$$

and its integral over all space would give, or in any case be proportional to, the expected photon energy. Now that will be different for different photon states $\boldsymbol{\gamma}_\pm(\mathbf{p},t)$, so we must give up the idea of a position-representation wave function $\Psi(\mathbf{r},t)$ normalized in the usual sense. Rather, we should seek wave functions normalized in the sense that

$$\int \Psi^*(\mathbf{r},t)\cdot\Psi(\mathbf{r},t)d\mathbf{r}=\int cp[\boldsymbol{\gamma}_+^*(\mathbf{p},t)\cdot\boldsymbol{\gamma}_+(\mathbf{p},t)+\boldsymbol{\gamma}_-^*(\mathbf{p},t)\cdot\boldsymbol{\gamma}_-(\mathbf{p},t)]d\mathbf{p} \tag{2.13}$$

and that still respect the momentum representation dynamics (2.1).

Perhaps the simplest way to do that is to set

$$\Psi(\mathbf{r},t)\equiv\Psi_+(\mathbf{r},t)+\Psi_-(\mathbf{r},t) \tag{2.14}$$

and take the $\Psi_\pm(\mathbf{r},t)$ to be given by

$$\Psi_\pm(\mathbf{r},t)\equiv\int\frac{\sqrt{cp}\,d\mathbf{p}}{(2\pi\hbar)^{(3/2)}}\boldsymbol{\gamma}_\pm(\mathbf{p},t)e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}\,. \tag{2.15}$$

Note that like the $\Phi_\pm(\mathbf{r},t)$ the $\Psi_\pm(\mathbf{r},t)$ satisfy

$$i\hbar\frac{\partial\Psi_\pm(\mathbf{r},t)}{\partial t}=\pm c\hbar\nabla\times\Psi_\pm(\mathbf{r},t) \tag{2.16}$$

[cf. Eqs. (2.7)]. However, they must be chosen to satisfy an initial condition given by the $t=0$ case of

$$\Psi_\pm(\mathbf{r},t)=\int\frac{\sqrt{cp}\,d\mathbf{p}}{(2\pi\hbar)^{(3/2)}}\boldsymbol{\gamma}_\pm(\mathbf{p},0)e^{-icpt/\hbar}e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \tag{2.17}$$

[cf. Eq. (2.10)].

This then completes our description of the quantum mechanics of a single free photon. In the momentum representation we have probability amplitudes (2.3) satisfying Eqs. (2.1). The moduli squared of these amplitudes give the probabilities of detecting the photon with specified helicity and momentum. They are normalized in the usual way [Eq. (2.8)]. In the position representation we argue that it is only meaningful to introduce a wave function describing the probability amplitude for measuring the expected energy of the photon in a given region of space. It is given by Eq. (2.14) and satisfies the dynamical equation (2.16), subject only to the initial condition given by the $t=0$ case of Eq. (2.17). Since $\boldsymbol{\gamma}_\pm(\mathbf{p},t)$ and $\Psi_\pm(\mathbf{r},t)$ are not Fourier transform pairs the arguments $\mathbf{p}$ (the usual photon momentum) and $\mathbf{r}$ (the "photon position," more precisely the position associated with the photon energy) are not conjugate variables. Nonetheless, we argue in the following section that the wave function $\Psi(\mathbf{r},t)$ is a useful quantity to use to describe the dynamics of a photon. In particular, we show in Sec. V that it leads to a photon wave function propagating at the speed of light away from a spontaneously emitting atom.

III. MANY-PHOTON STATES AND SECOND QUANTIZATION

In nonrelativistic many-particle physics [11] one usually begins with the description of a single particle, be it a fermion such as an electron or a (composite) boson such as ^{4}He. One can then write down many-particle wave functions to describe a number of such particles, by taking antisymmetrized or symmetrized forms of product wave functions, as appropriate. Such many-particle wave functions then form the foundation for introducing a Fock space and second quantizing the system.

Since we now have wave functions to describe a single photon, we can move along this route and introduce many-photon wave functions. We plan to turn to the interpretation and use of such many-photon wave functions in a future paper. In this paper, however, our main interest is in single-photon wave functions and how they evolve in, say, a spontaneous emission process. Since a photon is created in such a process, we will need to derive the wave-function equations from a second-quantized theory. For use in Secs. IV and V we therefore here build up a quantum field theory of the free radiation field from the single-particle description of the results. But the approach is rather different, since a canonical formulation of the electromagnetic field [12] is not the basis of the quantization and is not even required; the route, rather, is that of many-particle physics.

To do this and be able easily to compare our results with well-known expressions, it is convenient to normalize our functions in a cubic box of volume $V=L^3$. We introduce

$$\mathbf{u}_\pm(\mathbf{k};\mathbf{r})\equiv\frac{\mathbf{e}_\pm(\hat{\mathbf{k}})}{\sqrt{V}}e^{i\mathbf{k}\cdot\mathbf{r}}\,, \tag{3.1}$$

where as usual $\mathbf{k}=(k_x,k_y,k_z)=2\pi(n_x,n_y,n_z)/L$, where n_x,n_y,n_z, are integers, not all zero. These are box normalized eigenfunctions for $\Phi_\pm(\mathbf{r},t)$, respectively, in Eqs. (2.7), with eigenvalues $\hbar\omega_k\equiv\hbar c|\mathbf{k}|$. The orthogonality conditions are

$$\int\mathbf{u}_s^*(\mathbf{k};\mathbf{r})\cdot\mathbf{u}_{s'}(\mathbf{k}';\mathbf{r})d\mathbf{r}=\delta_{\mathbf{k}\mathbf{k}'}\delta_{ss'}\,, \tag{3.2}$$

where the subscripts s and s' can be $+$ or $-$. Instead of Eq. (2.6) we now have

$$\mathbf{\Phi}_{\pm}(\mathbf{r},t)=\sum_{\mathbf{k}} ic_{\pm}(\mathbf{k};t)\mathbf{u}_{\pm}(\mathbf{k};\mathbf{r}) , \tag{3.3}$$

where the $c_{\pm}(\mathbf{k};t)$ are expansion coefficients and the factor of i is introduced for later convenience. The normalization condition (2.8) and (2.9) then becomes simply

$$\sum_{\mathbf{k},s}|c_s(\mathbf{k};t)|^2=1 , \tag{3.4}$$

the expected value of the energy is

$$E=\sum_{\mathbf{k},s}\hbar\omega_k|c_s(\mathbf{k};t)|^2 , \tag{3.5}$$

and the evolution of the $\mathbf{\Phi}_{\pm}(\mathbf{r},t)$ is given by

$$\mathbf{\Phi}_{\pm}(\mathbf{r},t)=\sum_{\mathbf{k}} ic_{\pm}(\mathbf{k};0)e^{-i\omega_k t}\mathbf{u}_{\pm}(\mathbf{k};\mathbf{r}) . \tag{3.6}$$

The initial condition (2.17) for a photon wave function then becomes

$$\Psi(\mathbf{r})=\sum_{\mathbf{k},s} ic_s(\mathbf{k};0)\sqrt{\hbar\omega_k}\,\mathbf{u}_s(\mathbf{k};\mathbf{r}) . \tag{3.7}$$

Second quantization now follows from the usual approach in many-particle physics [11]; since photons are bosons the $c_s(\mathbf{k};0)$ become operators $a_s(\mathbf{k})$, which satisfy the commutation relations

$$\begin{aligned}&[a_s(\mathbf{k}),a_{s'}(\mathbf{k}')]=0 ,\\ &[a_s(\mathbf{k}),a_{s'}^{\dagger}(\mathbf{k}')]=\delta_{ss'}\delta_{\mathbf{k}\mathbf{k}'} ,\end{aligned} \tag{3.8}$$

where [ ] indicates the usual commutator and the Hamiltonian generating the dynamics is then

$$H=\sum_{\mathbf{k},s}\hbar\omega_k a_s^{\dagger}(\mathbf{k})a_s(\mathbf{k}) . \tag{3.9}$$

In terms of the field operator

$$\boldsymbol{\psi}(\mathbf{r})\equiv\sum_{\mathbf{k},s} ia_s(\mathbf{k})\sqrt{\hbar\omega_k}\,\mathbf{u}_s(\mathbf{k};\mathbf{r}) \tag{3.10}$$

this can be written as

$$H=\int\boldsymbol{\psi}^{\dagger}(r)\cdot\boldsymbol{\psi}(r)d\mathbf{r} . \tag{3.11}$$

Note that there is no "zero-point" energy appearing in the state expansion Eq. (3.9) of the Hamiltonian, just as there is none that appears when one second quantizes, for example, the motion of a collection of ^{4}He atoms; we are beginning here from the viewpoint of a collection of single photons. What is unusual from the viewpoint of many-particle physics, of course, is the form (3.10) of the fundamental field operator $\boldsymbol{\psi}(\mathbf{r})$ [and thus of the commutator of $\boldsymbol{\psi}(\mathbf{r})$ and $\boldsymbol{\psi}^{\dagger}(\mathbf{r}')$] and of the Hamiltonian (3.11) in terms of it. The latter, in particular, indicates that the "existence of the photons" *is* the energy, a perspective in accord with the discussion leading to Eq. (2.13).

Equations (3.10) and (3.11), with the fundamental commutation relations (3.8), define the field theory of the many-photon system. To establish the connection with the classical radiation theory we note that the dynamical equations for $\Psi(\mathbf{r},t)$ in the Heisenberg picture are found, using the Hamiltonian (3.9) and (3.11) to be

$$i\hbar\frac{\partial\boldsymbol{\psi}_{\pm}(\mathbf{r},t)}{\partial t}=\pm c\hbar\nabla\times\boldsymbol{\psi}_{\pm}(\mathbf{r},t) \tag{3.12}$$

[cf. Eq. (2.16)], where

$$\boldsymbol{\psi}_{\pm}(\mathbf{r})=\sum_{\mathbf{k}} ia_{\pm}(\mathbf{k})\sqrt{\hbar\omega_k}\,\mathbf{u}_{\pm}(\mathbf{k};\mathbf{r}) \tag{3.13}$$

are the positive and the negative helicity parts of $\boldsymbol{\psi}(\mathbf{r})$. From the form (3.13) and Eqs. (3.12) we see that

$$\begin{aligned}&c\nabla\times[\boldsymbol{\psi}_{+}(\mathbf{r},t)+\boldsymbol{\psi}_{-}^{\dagger}(\mathbf{r},t)]=i\frac{\partial}{\partial t}[\boldsymbol{\psi}_{+}(\mathbf{r},t)+\boldsymbol{\psi}_{-}^{\dagger}(\mathbf{r},t)] ,\\ &\nabla\cdot[\boldsymbol{\psi}_{+}(\mathbf{r},t)+\boldsymbol{\psi}_{-}^{\dagger}(\mathbf{r},t)]=0 .\end{aligned} \tag{3.14}$$

Maxwell's equations for the free space radiation field satisfy

$$\begin{aligned}&c\nabla\times[\mathbf{E}_T(\mathbf{r},t)+i\mathbf{B}(\mathbf{r},t)]=i\frac{\partial}{\partial t}[\mathbf{E}_T(\mathbf{r},t)+i\mathbf{B}(\mathbf{r},t)] ,\\ &\nabla\cdot[\mathbf{E}_T(\mathbf{r},t)+i\mathbf{B}(\mathbf{r},t)]=0 ,\end{aligned} \tag{3.15}$$

where the subscript on $\mathbf{E}_T(\mathbf{r},t)$ indicates the transverse nature of the free-space electric field. Comparing Eqs. (3.14) with Eqs. (3.15), we are led to identify the operator for the field combination $\mathbf{E}_T(\mathbf{r})+i\mathbf{B}(\mathbf{r})$ as proportional to $\boldsymbol{\psi}_{+}(\mathbf{r})+\boldsymbol{\psi}_{-}^{\dagger}(\mathbf{r})$. If we choose that proportionality constant to be $2\sqrt{2\pi}$, we find that

$$\sum_{\mathbf{k},s}\hbar\omega_k a_s^{\dagger}(\mathbf{k})a_s(\mathbf{k})=\frac{1}{8\pi}\int[E_T^2(\mathbf{r})+B^2(\mathbf{r})]d\mathbf{r}-\frac{1}{2}\sum_{\mathbf{k},s}\hbar\omega_k . \tag{3.16}$$

Since the right-hand side of Eq. (3.16) is, apart from a constant, the classical energy of the transverse electromagnetic field and the left-hand side of Eq. (3.16) is our Hamiltonian, we adopt this identification. This leads to the correspondence

$$\begin{aligned}\mathbf{E}_T(\mathbf{r})&=\sqrt{2\pi}[\boldsymbol{\psi}_{+}(\mathbf{r})+\boldsymbol{\psi}_{+}^{\dagger}(\mathbf{r})+\boldsymbol{\psi}_{-}(\mathbf{r})+\boldsymbol{\psi}_{-}^{\dagger}(\mathbf{r})]\\ &=\sqrt{2\pi}[\boldsymbol{\psi}(\mathbf{r})+\boldsymbol{\psi}^{\dagger}(\mathbf{r})] ,\\ \mathbf{B}(\mathbf{r})&=-i\sqrt{2\pi}[\boldsymbol{\psi}_{+}(\mathbf{r})-\boldsymbol{\psi}_{+}^{\dagger}(\mathbf{r})-\boldsymbol{\psi}_{-}(\mathbf{r})+\boldsymbol{\psi}_{-}^{\dagger}(\mathbf{r})]\end{aligned} \tag{3.17}$$

and the resulting expressions

$$\begin{aligned}\mathbf{E}_T(\mathbf{r})&=i\sum_{\mathbf{k},j}\left[\frac{2\pi\hbar\omega_k}{V}\right]^{(1/2)}\hat{e}_j(\hat{k})\\ &\quad\times[a_j(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}-a_j^{\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{r}}] ,\\ \mathbf{B}(\mathbf{r})&=i\sum_{\mathbf{k},j}\left[\frac{2\pi\hbar\omega_k}{V}\right]^{(1/2)}[\hat{k}\times\hat{e}_j(\hat{k})]\\ &\quad\times[a_j(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}-a_j^{\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{r}}] .\end{aligned} \tag{3.18}$$

Here the $\hat{e}_j(\hat{k})$ $(j=1,2)$ label the linear polarizations [cf. Eqs. (2.2)] and the $a_j(\mathbf{k})$

$$\begin{aligned}a_1(\mathbf{k})&=-(\tfrac{1}{2})^{1/2}[a_{+}(\mathbf{k})-a_{-}(\mathbf{k})] ,\\ a_2(\mathbf{k})&=-i(\tfrac{1}{2})^{1/2}[a_{+}(\mathbf{k})+a_{-}(\mathbf{k})]\end{aligned} \tag{3.19}$$

are the lowering operators for the linearly polarized

modes. Equations (3.18) are identical to the expressions obtained in the usual canonical quantization [12] of the free radiation field. So we have recovered the usual result and in the process obtained the relations (3.17) between the electromagnetic field and the fundamental photon operators $\psi_{\pm}(\mathbf{r})$ we have defined here. The result (3.16) is also found in the usual canonical quantization procedure, but in a different form with a different physical interpretation:

$$\frac{1}{8\pi}\int [E_T^2(\mathbf{r})+B^2(\mathbf{r})]d\mathbf{r}=\sum_{\mathbf{k},s}\hbar\omega_k[a_s^{\dagger}(\mathbf{k})a_s(\mathbf{k})+\tfrac{1}{2}] . \tag{3.20}$$

In the usual canonical quantization procedure the left-hand side of Eq. (3.20) is, through analogy with classical electrodynamics, identified as the Hamiltonian of the system. This results in a zero-point energy associated with the vacuum state, which is divergent. Here, where we begin with single particles and build up the many-photon system, the Hamiltonian is taken to be the left-hand side of Eq. (3.16); its expectation value in the state with no photons is zero and energy exists in the system only insofar as there are photons present. The relation (3.16) is used only to relate the electromagnetic fields to the photon fields, establishing the connection to classical electromagnetic theory; although the integral over the volume of $E_T^2(\mathbf{r})+B^2(\mathbf{r})$ is divergent, it is not associated here with the energy of the photon field.

In fact, the expectation value of the operator $\psi^{\dagger}(\mathbf{r})\cdot\psi(\mathbf{r})$ gives the expected photon energy about $d\mathbf{r}$ of $\mathbf{r}$; that operator can be written as

$$\psi^{\dagger}(\mathbf{r})\cdot\psi(\mathbf{r})=\frac{1}{2\pi}[\mathbf{E}_T^{(c)}(\mathbf{r})\cdot\mathbf{E}_T^{(a)}(\mathbf{r})] , \tag{3.21}$$

where $\mathbf{E}_T^{(c)}(\mathbf{r})$ and $\mathbf{E}_T^{(a)})(\mathbf{r})$ are, respectively, the parts of $\mathbf{E}_T(\mathbf{r})$ containing creation and annihilation operators. The quantity (3.21) is often introduced as an appropriate measure of the "intensity" to which an idealized detector is sensitive [13]. Whether or not a given detector is sensitive to (3.21) is of course not of immediate relevance here; what is of more significance is that it is a reasonable quantity to come out of a second-quantized theory for the "field intensity," given the perspective [see the discussion of Eq. (2.13)] adopted for the corresponding one-photon theory.

Having constructed the second-quantized many-photon theory from the description of a single photon, we may now extract that single-photon theory out of the second-quantized description in the special instance when only one photon is present. If indeed only one photon is present the ket describing the state is of the form

$$|\Xi(t)\rangle=\sum_{\mathbf{k},s}f_{\mathbf{k}s}(t)|1_{\mathbf{k}s}\rangle , \tag{3.22}$$

where

$$|1_{\mathbf{k}s}\rangle=a_s^{\dagger}(\mathbf{k})|\Gamma\rangle \tag{3.23}$$

is the state with one photon in mode $\mathbf{k}$ and helicity s and no other photons present; $|\Gamma\rangle$ is the ground state with no photons. The state (3.22) evolves according to

$$|\Xi(t)\rangle=U(t)|\Xi(0)\rangle\equiv U(t)|\Xi\rangle , \tag{3.24}$$

where the evolution operator $U(t)$ satisfies

$$i\hbar\frac{\partial U(t)}{\partial t}=HU(t) , \tag{3.25}$$

with H given by Eqs. (3.9) and (3.11). In such a state (3.22) we obviously have

$$\langle\Xi(t)|\psi_{\pm}(\mathbf{r})|\Xi(t)\rangle=\langle\Xi|\psi_{\pm}(\mathbf{r},t)|\Xi\rangle=0 ; \tag{3.26}$$

the one-photon amplitudes $\Psi_{\pm}(\mathbf{r},t)$ can be extracted as

$$\begin{aligned}\Psi_{\pm}(\mathbf{r},t)&\equiv\langle\Gamma|\psi_{\pm}(\mathbf{r})|\Xi(t)\rangle\\&=\langle\Gamma|\psi_{\pm}(\mathbf{r},t)|\Xi\rangle\\&=\sum_{\mathbf{k}}if_{\mathbf{k}\pm}(t)\sqrt{\hbar\omega_k}\,\mathbf{u}_{\pm}(\mathbf{k};\mathbf{r}) .\end{aligned} \tag{3.27}$$

This obviously leads to a form (3.7) for $\Psi(\mathbf{r},t)$ at $t=0$ and bracketing Eqs. (3.12) between $\langle\Gamma|$ and $|\Xi\rangle$ leads to Eqs. (2.16). Further,

$$\begin{aligned}\Psi^*(\mathbf{r},t)\cdot\Psi(\mathbf{r},t)&=\langle\Xi(t)|\psi^{\dagger}(\mathbf{r})\cdot\psi(\mathbf{r})|\Xi(t)\rangle\\&=\langle\Xi|\psi^{\dagger}(\mathbf{r},t)\cdot\psi(\mathbf{r},t)|\Xi\rangle\end{aligned} \tag{3.28}$$

so, as expected, the single photon theory of Sec. II is completely recovered.

IV. ATOM-FIELD INTERACTION

We are now in a position to address the problem of calculating the wave function of a photon emitted during a spontaneous emission process. For simplicity we consider an atom consisting of a single, spinless electron bound to a fixed nucleus; generalizations are straightforward. As the total Hamiltonian we then take

$$\begin{aligned}H&=\int\psi^{\dagger}(\mathbf{r})\cdot\psi(\mathbf{r})d\mathbf{r}+\frac{1}{2m}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{q})\right]^2+V_c(\mathbf{q})\\&=\frac{1}{8\pi}\int[E_T^2(\mathbf{r})+B^2(\mathbf{r})]d\mathbf{r}-\frac{1}{2}\sum_{\mathbf{k},s}\hbar\omega_k\\&\quad+\frac{1}{2m}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{q})\right]^2+V_c(\mathbf{q}) ,\end{aligned} \tag{4.1}$$

where henceforth $\mathbf{q}$ and $\mathbf{p}$ refer to the position and canonical momentum of the electron, with charge e and mass m; $V_c(\mathbf{q})$ describes the Coulomb potential binding it to the origin. If as usual we take

$$\begin{aligned}\mathbf{A}(\mathbf{r})=\sum_{\mathbf{k},j}&\left[\frac{2\pi\hbar c^2}{V\omega_k}\right]^{(1/2)}\\&\times\hat{e}_j(\hat{k})[a_j(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}+a_j^{\dagger}(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{r}}]\end{aligned} \tag{4.2}$$

for the vector potential $\mathbf{A}(\mathbf{r})$, we find that the Hamiltonian (4.1) leads to the correct Heisenberg equations for both the electron and the electromagnetic field. The Hamiltonian (4.1) is (except for the lack of the usual divergent zero-point energy) the conventional one; thus we can expect the conventional results in the description of a spontaneous emission process.

Before beginning to describe the photon wave function associated with such a process, however, there is a technical matter with which we deal. Implicit in Eq. (4.1) is the use of the Coulomb gauge, in which the electric field is decomposed into a longitudinal and transverse part

$$\mathbf{E}=\mathbf{E}_L+\mathbf{E}_T \ , \tag{4.3}$$

where $\mathbf{E}_L$, describing the Coulomb field, depends on the variables of the electron and $\mathbf{E}_T$, the transverse field, is described by the photons. Since it is only the total $\mathbf{E}$ that is causal [14] and not the separate components, this is not a convenient representation of the electric field; we would like a contribution from the photons that itself is causal. One way around this difficulty is to use the Lorentz gauge in the description of the electromagnetic field. Another route, popular in quantum optics where the emitting species are more often than not neutral atoms, is to use a decomposition of the total electric field different from Eq. (4.3). Writing the microscopic charge density in terms of a polarization potential

$$\rho(\mathbf{r})=e[\delta(\mathbf{r}-\mathbf{q})-\delta(\mathbf{r})]=-\nabla\cdot\mathbf{P}(\mathbf{r}) \ , \tag{4.4}$$

where $\mathbf{P}(\mathbf{r})$ is implicitly an operator in the Hilbert space of the electron, the approach is to write the total electric field as

$$\mathbf{E}=-4\pi\mathbf{P}+\mathbf{D} \tag{4.5}$$

rather than Eq. (4.3), where $\mathbf{D}$ is purely transverse and describes the photon field. The fields in Eq. (4.5) are of course purely microscopic; nonetheless, the analogy with macroscopic electrodynamics would suggest that $\mathbf{D}$ itself should be causal and this is indeed found to be the case. A concomitant benefit is that the Hamiltonian (4.1) is reduced to one in which the interaction of the atom with the electromagnetic field is expressed in terms of the multipole moment operators of the atom.

This approach, pioneered by Power and Thirunamachandran [15] with important contributions by Healy [16], is well known. It in itself does not relate to the issue to wave functions for photons, but it will be convenient to adopt it to then move on to that issue. For that reason we briefly summarize the approach here. Since the Hamiltonian (4.1) is essentially the same Hamiltonian that one would write down from the more usual introduction of a quantized electromagnetic field, what we do in this section is standard and conventional except for the identification of that photon fields in Eqs. (4.19) and (4.20) below.

We move from the original description (4.1) to the new one by means of a unitary transformation $S=\exp(i\sigma)$, where

$$\sigma=\frac{1}{\hbar c}\int\mathbf{P}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r})d\mathbf{r} \tag{4.6}$$

and where the (microscopic) polarization potential $\mathbf{P}(\mathbf{r})$ is given by

$$\mathbf{P}(\mathbf{r})\equiv e\mathbf{q}\int_0^1\delta(\mathbf{r}-\lambda\mathbf{q})d\lambda \ . \tag{4.7}$$

Healy [2] has investigated in detail the use of more general unitary transformations and polarization potentials, but this choice will suffice for our purposes. We find

$$\begin{aligned}&\mathbf{P}^{\rm new}(\mathbf{r})\equiv S\mathbf{P}(\mathbf{r})S^{-1}=\mathbf{P}(\mathbf{r}) \ ,\\ &\mathbf{B}^{\rm new}(\mathbf{r})\equiv S\mathbf{B}(\mathbf{r})S^{-1}=\mathbf{B}(\mathbf{r}) \ ,\\ &\mathbf{q}^{\rm new}\equiv S\mathbf{q}S^{-1}=\mathbf{q} \ ,\end{aligned} \tag{4.8}$$

while

$$\begin{aligned}&E_T^{\rm new}(\mathbf{r})\equiv S\mathbf{E}_T(\mathbf{r})S^{-1}=\mathbf{E}_T(\mathbf{r})+4\pi\mathbf{P}_T(\mathbf{r}) \ ,\\ &\mathbf{p}^{\rm new}\equiv S\mathbf{p}S^{-1}\\ &\quad=\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{q})=\frac{e}{c}\int\int_0^1\lambda\delta(\mathbf{r}-\lambda\mathbf{q})\mathbf{q}\times\mathbf{B}(\mathbf{r})d\lambda\,d\mathbf{r} \ ,\end{aligned} \tag{4.9}$$

where $\mathbf{P}_T(\mathbf{r})$ indicates the transverse part of $\mathbf{P}(\mathbf{r})$. Since the longitudinal parts of $\mathbf{P}(\mathbf{r})$ and $\mathbf{E}(\mathbf{r})$ are easily shown to satisfy

$$\mathbf{E}_L(\mathbf{r})=-4\pi\mathbf{P}_L(\mathbf{r}) \ , \tag{4.10}$$

we have

$$\mathbf{E}_T^{\rm new}(\mathbf{r})=\mathbf{E}(\mathbf{r})+4\pi\mathbf{p}(\mathbf{r})\equiv\mathbf{D}(\mathbf{r}) \ . \tag{4.11}$$

We can now write the Hamiltonian (4.1) in terms of the "new" variables. Dropping the superscripts "new" [but continuing to denote $\mathbf{E}_T^{\rm new}(\mathbf{r})$ by $\mathbf{D}(\mathbf{r})$] we find after some algebra the result

$$\begin{aligned}H=&\frac{1}{8\pi}\int[D^2(\mathbf{r})+B^2(\mathbf{r})]d\mathbf{r}-\tfrac{1}{2}\sum_{\mathbf{k},s}\hbar\omega_k\\ &+H^{\rm atom}-\int\mathbf{P}(\mathbf{r})\cdot\mathbf{D}(\mathbf{r})d\mathbf{r}\\ &-\int\mathbf{M}^p(\mathbf{r})\cdot\mathbf{B}(\mathbf{r})d\mathbf{r}-\tfrac{1}{2}\int\mathbf{M}^d(\mathbf{r})\cdot\mathbf{B}(\mathbf{r})d\mathbf{r} \ .\end{aligned} \tag{4.12}$$

Here

$$H^{\rm atom}=\frac{p^2}{2m}+V_c(\mathbf{q})+2\pi\int P_T^2(\mathbf{r})d\mathbf{r} \tag{4.13}$$

is the usual Hamiltonian one would write down for the bare atom, except for the inclusion of the last term involving part of the (divergent) self-energy of the atom with the electromagnetic field. Note, however, that the particle canonical momenta, the atomic Hamiltonian, and the like are now different operators from the corresponding operators that would result from the field-free version of Eq. (4.1).

Nonetheless, since the Hamiltonian (4.13) involves only variables of the electron, we can take the eigenstates to be the (partly renormalized) eigenstates of the atom. The last three terms in Eq. (4.12) describe the interaction between the atom and the radiation field. The quantities $\mathbf{M}^p(\mathbf{r})$ and $\mathbf{M}^d(\mathbf{r})$ are, respectively, the (microscopic) paramagnetization and the diamagnetization of the atom; we do not write down the expressions for them here because we will not need them. In the long-wavelength limit, where the wavelength of the radiation in resonance with the Bohr frequencies of the atom is much larger than the size of the atom, the terms in Eq. (4.12) involving the magnetizations can be neglected; in the same limit, the term involving the polarization simplifies so that we may write

$$H \approx \frac{1}{8\pi}\int [D^2(\mathbf{r})+B^2(\mathbf{r})]d\mathbf{r} - \tfrac{1}{2}\sum_{\mathbf{k},s}\hbar\omega_k + H^{\text{atom}} - \boldsymbol{\mu}\cdot\mathbf{D}(0) , \tag{4.14}$$

where

$$\boldsymbol{\mu} \equiv \int \mathbf{P}(\mathbf{r})d\mathbf{r} = e\mathbf{q} \tag{4.15}$$

is just the dipole moment operator of the atom. Equation (4.14) is the form of the Hamiltonian we shall use. From the unitary transformation involved above it is clear that the Schrödinger operators for $\mathbf{D}(\mathbf{r})$ and $\mathbf{B}(\mathbf{r})$ are given by

$$\begin{aligned}\mathbf{D}(\mathbf{r}) &= i\sum_{\mathbf{k},j}\left[\frac{2\pi\hbar\omega_k}{V}\right]^{(1/2)} \times \hat{e}_j(\hat{k})[a_j(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} - a_j^\dagger(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{r}}] , \\ \mathbf{B}(\mathbf{r}) &= i\sum_{\mathbf{k},j}\left[\frac{2\pi\hbar\omega_k}{V}\right]^{(1/2)} [\hat{k}\times\hat{e}_j(\hat{k})] \times [a_j(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} - a_j^\dagger(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{r}}] ,\end{aligned} \tag{4.16}$$

[cf. Eqs. (3.18)], where again the "new" superscripts on, e.g., the $a_j(\mathbf{k})$ have been omitted; in the Heisenberg picture, it is straightforward to verify that the dynamics for the electromagnetic field that follow from the Hamiltonian (4.14) are

$$\begin{aligned} 0 &= \nabla\cdot\mathbf{D}(\mathbf{r},t) , \\ 0 &= \nabla\cdot\mathbf{B}(\mathbf{r},t) , \\ \frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t) &= c\nabla\times\mathbf{B}(\mathbf{r},t) , \\ \frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t) &= -c\nabla\times\mathbf{D}(\mathbf{r},t) + 4\pi c\nabla\times\mathcal{P}(\mathbf{r},t) ,\end{aligned} \tag{4.17}$$

where we have set

$$\mathcal{P}(\mathbf{r},t) \equiv \boldsymbol{\mu}(t)\delta(\mathbf{r}) , \tag{4.18}$$

and $\boldsymbol{\mu}(t)$ is the Heisenberg operator for $\boldsymbol{\mu}$ [Eq. (4.15)]. Finally, we note that the "new" photon fields follow from Eq. (3.17) and the unitary transformation. Again dropping the "new" superscripts, we have the new relations for the Schrödinger operators

$$\begin{aligned}\mathbf{D}(\mathbf{r}) &= \sqrt{2\pi}[\boldsymbol{\psi}_+(\mathbf{r}) + \boldsymbol{\psi}_+^\dagger(\mathbf{r}) + \boldsymbol{\psi}_-(\mathbf{r}) + \boldsymbol{\psi}_-^\dagger(\mathbf{r})] \\ &= \sqrt{2\pi}[\boldsymbol{\psi}(\mathbf{r}) + \boldsymbol{\psi}^\dagger(\mathbf{r})] , \\ \mathbf{B}(\mathbf{r}) &= -i\sqrt{2\pi}[\boldsymbol{\psi}_+(\mathbf{r}) - \boldsymbol{\psi}_+^\dagger(\mathbf{r}) - \boldsymbol{\psi}_-(\mathbf{r}) + \boldsymbol{\psi}_-^\dagger(\mathbf{r})] ,\end{aligned} \tag{4.19}$$

with of course

$$\boldsymbol{\psi}_\pm(\mathbf{r}) = \sum_{\mathbf{k}} i a_\pm(\mathbf{k})\sqrt{\hbar\omega_k}\,\mathbf{u}_\pm(\mathbf{k};\mathbf{r}) \tag{4.20}$$

[cf. Eqs. (3.13)]. Equations (4.17)–(4.20), along with the corresponding equations for $\boldsymbol{\mu}(t)$, determine the dynamics of spontaneous emission and the concomitant behavior of the photon field. It is to this we turn in the next section.

V. SPONTANEOUS EMISSION

We now turn to the calculation of the photon wave function generated as an atom spontaneously emits. We consider two eigenstates of the Hamiltonian H^{atom} of Eq. (4.13), for simplicity taking one to be the ground state $|g\rangle$ and the other one the excited state $|e\rangle$. Our interest is not in the dressing of these states by the electromagnetic field, so we assume that to a good approximation $|g\rangle|\Gamma\rangle \equiv |G\rangle$ is the ground state of the interacting atom and the electromagnetic field. We imagine the atom initially placed in the excited state with no photons present $|e\rangle|\Gamma\rangle \equiv |I(0)\rangle \equiv |I\rangle$. Again ignoring any dressing, this state will evolve by emitting a photon, leading at a later time to a ket

$$|I(t)\rangle = b(t)|e\rangle|\Gamma\rangle + \sum_{\mathbf{k},s} f_{\mathbf{k}s}(t)|g\rangle|1_{\mathbf{k}s}\rangle . \tag{5.1}$$

We work within the approximation that $|G(t)\rangle \equiv |G\rangle$ and $|I(t)\rangle$ describe evolving states of the system, satisfying

$$|I(t)\rangle = U(t)|I\rangle, \quad |G(t)\rangle = U(t)|G\rangle , \tag{5.2}$$

where $U(t)$ satisfies Eq. (3.25), but now with the full Hamiltonian (4.14); for simplicity we have taken the energy of the atomic ground state $|g\rangle$ to be zero. States of the form (5.1) are calculated, for example, within the simple Wigner-Weisskopf approximation [17] for photon emission. There the amplitude $b(t)$ is found to evolve according to

$$b(t) = e^{-i\omega_{eg}t - (1/2)\eta t} \tag{5.3}$$

for $t > 0$, where $\hbar\omega_{eg}$ is the energy difference between the atomic excited and ground states, η is the excited state decay rate, and the interaction of the atom with the photon field is assumed to be "turned on" at $t = 0$. In what follows we will require only Eq. (5.3), or some other approximate form for $b(t)$.

Now as the state $|I(t)\rangle$ evolves we obviously have

$$\begin{aligned}\langle I(t)|\boldsymbol{\mu}|I(t)\rangle &= \langle I|\boldsymbol{\mu}(t)|I\rangle = \mathbf{0} , \\ \langle I(t)|\mathbf{D}(\mathbf{r})|I(t)\rangle &= \langle I|\mathbf{D}(\mathbf{r},t)|I\rangle = \mathbf{0} ,\end{aligned} \tag{5.4}$$

etc., where for simplicity we have assumed that the atom has no "permanent" dipole moment in its ground or excited state. Analogous to the treatment at the end of Sec. III, we now introduce quantities

$$\mathbf{D}_{GI}(\mathbf{r},t) \equiv \langle G(t)|\mathbf{D}(\mathbf{r})|I(t)\rangle = \langle G|\mathbf{D}(\mathbf{r},t)|I\rangle . \tag{5.5}$$

These quantities do not vanish as $|I(t)\rangle$ evolves. In fact, we find, for example,

$$\boldsymbol{\mu}_{\text{GI}}(t) \equiv \langle G(t)|\boldsymbol{\mu}|I(t)\rangle = b(t)\boldsymbol{\mu}_{ge} , \tag{5.6}$$

where the matrix element $\boldsymbol{\mu}_{ge} \equiv \langle g|\boldsymbol{\mu}|e\rangle$. Bracketing Eqs. (4.17) between $\langle G|$ and $|I\rangle$ we find the equations

$$
\begin{aligned}
0&=\nabla\cdot\mathbf{D}_{GI}(\mathbf{r},t)\ ,\\
0&=\nabla\cdot\mathbf{B}_{GI}(\mathbf{r},t)\ ,\\
\frac{\partial}{\partial t}\mathbf{D}_{GI}(\mathbf{r},t)&=c\nabla\times\mathbf{B}_{GI}(\mathbf{r},t)\ ,\\
\frac{\partial}{\partial t}\mathbf{B}_{GI}(\mathbf{r},t)&=-c\nabla\times\mathbf{D}_{GI}(\mathbf{r},t)+4\pi c\nabla\times\mathcal{P}_{GI}(\mathbf{r},t)\ ,
\end{aligned}
\tag{5.7}
$$

where

$$
\mathcal{P}_{GI}(\mathbf{r},t)\equiv\mu_{ge}b(t)\delta(\mathbf{r})\ . \tag{5.8}
$$

Since the $f_{\mathbf{k}s}(t)$ in Eq. (5.1) vanish at $t=0$, the "*GI*" fields are found from the solution of Eqs. (4.7) subject to the initial conditions

$$
\mathbf{D}_{GI}(\mathbf{r},0)=0,\quad \mathbf{B}_{GI}(\mathbf{r},0)=0\ . \tag{5.9}
$$

Equations (5.7), subject to the initial conditions (5.9), are just the classical equations for the displacement $\mathbf{D}_{GI}(\mathbf{r},t)$ and magnetic field $\mathbf{B}_{GI}(\mathbf{r},t)$ driven by a (admittedly complex) polarization $\mathcal{P}_{GI}(\mathbf{r},t)$. The resulting quantities $\mathbf{D}_{GI}(\mathbf{r},t)$ and $\mathbf{B}_{GI}(\mathbf{r},t)$ will obviously be causal fields, i.e., for any t they will not extend a distance beyond the origin greater than $r=ct$.

Turning now to the photon field, as in Sec. III we extract the photon wave function $\Psi(\mathbf{r},t)$ as

$$
\Psi(\mathbf{r},t)=\langle G(t)|\boldsymbol{\psi}(\mathbf{r})|I(t)\rangle=\langle G|\boldsymbol{\psi}(\mathbf{r},t)|I\rangle \tag{5.10}
$$

and note that the expectation value of the energy density in the evolving state $|I(t)\rangle$ is indeed given by

$$
\begin{aligned}
\Psi^*(\mathbf{r},t)\cdot\Psi(\mathbf{r},t)&=\langle I(t)|\boldsymbol{\psi}^\dagger(\mathbf{r})\cdot\boldsymbol{\psi}(\mathbf{r})|I(t)\rangle\\
&=\langle I|\boldsymbol{\psi}^\dagger(\mathbf{r},t)\cdot\boldsymbol{\psi}(\mathbf{r},t)|I\rangle\ .
\end{aligned}
\tag{5.11}
$$

Finally, from Eqs. (4.19) and (5.10) we see that

$$
\Psi(\mathbf{r},t)=\left[\frac{1}{2\pi}\right]^{1/2}\mathbf{D}_{GI}(\mathbf{r},t)\ . \tag{5.12}
$$

Thus we find that the photon wave function $\Psi(\mathbf{r},t)$ is indeed a causal field, propagating out from the emitting atom at the speed of light. It is obtained by essentially solving for the displacement field in a classical radiation problem, but with a complex polarization source (5.8). At any time t we identify the integral over all space of $\Psi^*(\mathbf{r},t)\cdot\Psi(\mathbf{r},t)$ as the energy "in the photon field"; as t approaches infinity this integral approaches the expectation value of the energy emitted by the atom. For finite times there is a divergent contribution to this energy, but that is associated in a well-known way with part of the renormalization of the transition [18]. All these results are of course implicit in the solution (5.1) to the spontaneous emission problem; developing the connection with the *GI* fields here merely allowed us to see the nature of the solution in a simple way and in practice would give a simple way to calculate it if, for example, the form of $b(t)$ were assumed or postulated.

We can conclude this section by confirming that indeed $\Phi(\mathbf{r},t)$ is not a reasonable candidate for the photon wave function, as discussed in Sec. II. Comparing Eq. (2.10) with Eq. (2.14) and following through our analysis up to this point we are led to the relation

$$
\Phi(\mathbf{r},t)=\int w(\mathbf{r}-\mathbf{r}')\Psi(\mathbf{r}',t)d\mathbf{r}'\ , \tag{5.13}
$$

where

$$
w(\mathbf{r})=\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\hbar ck}} \tag{5.14}
$$

is essentially the nonlocal kernel employed by, e.g., Cook [10]. For $\mathbf{r}\neq0$ the expression (5.14) can be directly integrated; we find

$$
w(\mathbf{r})=\frac{1}{2(2\pi)^{(3/2)}\sqrt{\hbar cr^{(5/2)}}}\ , \tag{5.15}
$$

a result with in fact a sufficiently weak divergence as $r\to0$ that it can be integrated over. But in any case, since w is nonvanishing for $\mathbf{r}\neq0$ and $\Psi(\mathbf{r},t)$ is causal function in the sense described above, $\Phi(\mathbf{r},t)$ will not be: At arbitrarily early times it will extend out to values of $\mathbf{r}\neq0$.

VI. SUMMARY

We have argued that it is physically reasonable to introduce a position-representation wave function $\Psi(\mathbf{r},t)$ for a photon such that

$$
\Psi^*(\mathbf{r},t)\cdot\Psi(\mathbf{r},t)d\mathbf{r} \tag{6.1}
$$

is the expected value of the photon energy in a region $d\mathbf{r}$ about $\mathbf{r}$. On the basis of this we have constructed a wave-function theory for a single photon, second quantized it to yield a quantum theory for the free radiation field, and shown that in a spontaneous emission process the wave function $\Psi(\mathbf{r},t)$ generated is a causal field, propagating out from the emitting atom at the speed of light. Perhaps not surprisingly, the wave function $\Psi(\mathbf{r},t)$ calculated for this process is essentially the displacement field that would be found in a kind of semiclassical calculation of spontaneous emission. That it is the displacement field rather than the electric field itself follows at a technical level from the Power-Healy transformation [2] that is used to help solve the problem. But physically this could also have been expected: The total "field" associated with the photon must be both causal and transverse. Clearly the classical electric field emitted by a dipole does not satisfy these properties, but the associated displacement field does.

The route we have taken to construct the wave function $\Psi(\mathbf{r},t)$ is apparently not unique. The adoption of Eq. (2.15) can be seen as a kind of "minimum modification" of the function Eq. (2.6) that might more naively have been expected to be the appropriate wave function; other equations could have been written down. And connections with the electromagnetic fields other than Eq. (3.17) could have been chosen [19]. Yet in the end our route does lead to causal photon wave-function generation during spontaneous emission.

It could be argued that this result is contrived. One can certainly expect the electromagnetic field energy generated in spontaneous emission to propagate in a causal way and the construction of $\Psi(\mathbf{r},t)$ such that Eq. (6.1)

gives that energy almost guarantees that $\Psi(\mathbf{r},t)$ will also propagate in causal way. Indeed, in a sense the result is contrived. In fact, our object is precisely to contrive a way of associating wave functions with photons such that those wave functions behave in a physically meaningful way and thus can be of some use in understanding the quantum processes involved. We believe we have succeeded with respect to the spontaneous emission of a single photon. The crucial question is whether something like this approach can be contrived to yield few-photon wave functions that are physically meaningful in describing the quantum processes that generate or modify them.

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