Linear absorptive dielectrics

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Starting from Maxwell's equations for a linear, nonconducting, absorptive, and dispersive medium, characterized by the constitutive equations $\boldsymbol{D}(\mathbf{x},t)=\varepsilon_1(\mathbf{x})\boldsymbol{E}(\mathbf{x},t)+\int_{-\infty}^{t}ds\,\chi(\mathbf{x},t-s)\boldsymbol{E}(\mathbf{x},s)$ and $\boldsymbol{H}(\mathbf{x},t)=\boldsymbol{B}(\mathbf{x},t)$, a unitary time evolution and canonical formalism is obtained. Given the complex, coordinate, and frequency-dependent, electric permeability $\varepsilon(\mathbf{x},\omega)$, no further assumptions are made. The procedure leads to a proper definition of band gaps in the periodic case and a new continuity equation for energy flow. An S-matrix formalism for scattering from lossy objects is presented in full detail. A quantized version of the formalism is derived and applied to the generation of Čerenkov and transition radiation as well as atomic decay. The last case suggests a useful generalization of the density of states to the absorptive situation.
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I. INTRODUCTION

The present work deals with Maxwell's equations (ME) for a lossy, macroscopic, nonconducting, linear medium

$$\partial_t\boldsymbol{D}(\mathbf{x},t)=\partial_{\mathbf{x}}\times\boldsymbol{H}(\mathbf{x},t)-\boldsymbol{J}(\mathbf{x},t),$$
$$\partial_t\boldsymbol{B}(\mathbf{x},t)=-\partial_{\mathbf{x}}\times\boldsymbol{E}(\mathbf{x},t),\partial_{\mathbf{x}}\cdot\boldsymbol{B}(\mathbf{x},0)=0. \tag{1.1}$$

In the case where the fields are related by frequency-independent permeabilities, $\boldsymbol{D}(\mathbf{x})=\varepsilon(\mathbf{x})\boldsymbol{E}(\mathbf{x})$, $\boldsymbol{H}(\mathbf{x})=\mu(\mathbf{x})^{-1}\boldsymbol{B}(\mathbf{x})$, energy is conserved for vanishing external current $\boldsymbol{J}$. This allows the introduction of a suitable norm and corresponding Hilbert space in which the time evolution is unitary (below we refer to such systems as conservative ones). A unitary time evolution is of paramount importance since it is generated by a self-adjoint operator K. Band gaps in periodic systems and Anderson localization in random situations can then be formulated in terms of the spectral properties of K in complete analogy with the Schrödinger case. In addition a unitary time evolution can easily be quantized. This is important since processes such as decay of excited embedded atoms, require a second quantized version of the fields. The situation changes if the medium is absorptive and dispersive (shortened to absorptive or lossy below). In the simplest case, that of a linear lossy dielectric, we have $\mu=1$ and

$$\boldsymbol{D}(\mathbf{x},t)=\varepsilon_1(\mathbf{x})\boldsymbol{E}(\mathbf{x},t)+\int_{-\infty}^{t}ds\,\chi(\mathbf{x},t-s)\boldsymbol{E}(\mathbf{x},s)$$
$$=\varepsilon_1(\mathbf{x})\boldsymbol{E}(\mathbf{x},t)+\int_{t_0}^{t}ds\,\chi(\mathbf{x},t-s)\boldsymbol{E}(\mathbf{x},s), \tag{1.2}$$

where the last line holds for $\boldsymbol{E}(\mathbf{x},t)$ vanishing for $t<t_0$. This expression differs from the usual $\boldsymbol{D}(\mathbf{x},t)=E(\mathbf{x},t)+\boldsymbol{P}(\mathbf{x},t)$, where $\boldsymbol{P}$ is the polarization. However, it is the natural decomposition if we think of a system of absorptive particles in a uniform, nonabsorptive, background. Then $\varepsilon_1(\mathbf{x})$ is the background permeability outside the particles but may be different inside, thus leading to an $\mathbf{x}$ dependence. In general $\varepsilon_1(\mathbf{x})=1$ if $\mathbf{x}$ is in an absorptive region, thus ensuring the proper high-frequency behavior. In a nonabsorptive region, where $\chi(\mathbf{x},t)$ vanishes, $\varepsilon_1(\mathbf{x})$is the static permeability and may be larger than one. It is the convolution part in Eq. (1.2), leading to a complex, frequency-dependent $\varepsilon(\mathbf{x},\omega)$ in the Laplace or Fourier transformed ME, that prevents the straightforward construction of a Lagrange formalism and quantization. It is also not obvious how to define band gaps. The usual definition as a vanishing density of states in an interval becomes problematic since $\varepsilon(\mathbf{x},\omega)$ is complex, leading to complex eigenvalues and the eigenstate-counting definition is useless.

At present the situation is under active investigation. Transparent systems, i.e., systems where $\varepsilon(\mathbf{x},\omega)$ is real, so absorption is neglected, were already treated a long time ago by Jauch and Watson [1]. In recent times nonlinear transparent systems were considered by Drummond [2]. Other recent work, including absorption, and involving a nonlocal relativistic action, is due to Burgess [3]. It is also possible to approach the problem from a microscopic point of view, where the quantized electromagnetic field is coupled to a second quantized field, representing the material subsystem. This road was taken by Huttner, Barnett, and others [4–6] for spatially homogeneous situations. A different microscopic treatment by Matloob, Loudon, and co-workers [7] considers the quantized field in the presence of a quantum noise current due to the material subsystem. Here some simple spatially nonhomogeneous situations are studied, as well as systems with gain. However, there are situations that are not adequately covered in the literature, in particular for systems that are both spatially inhomogeneous and absorptive and where the precise frequency dependence of the electric permeability is important. We illustrate this by giving two examples.

The first is that of the construction of three-dimensional photonic crystals [8] built up from lossy dielectric particles on the lattice sites and here small metallic spheres offer an interesting possibility (colloids can be used to manufacture

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such objects [9]). The former behave as strongly absorptive dielectric spheres [10] and are an interesting candidate for the construction of a photonic crystal with a band gap. This raises the question of how to define band gaps in the presence of absorption. The next step is then to create some randomness in the crystal, leading to Lifshits tails in the gap that may show Anderson localization. The second example is that of transition radiation [11], the emission of electromagnetic radiation caused by the passage of energetic electrons through layered dielectrics. At present this mechanism is studied as a tool to produce x-ray radiation for technological purposes [12]. Suitable materials show strong absorption (partly used to suppress unwanted frequencies) and the actual radiation yield depends sensitively on the absorption characteristics.

As stated, quantization of absorptive dielectrics is required if one wants to study the decay properties of excited atoms or molecules embedded in a dielectric. In addition a quantized theory significantly simplifies transition radiation calculations since it can be described as a scattering process (electron, zero photons in $\rightarrow$ electron, one photon out) and a first-order calculation suffices. However, for quantization a classical Lagrange formalism has to be developed first. This is readily done for space-dependent electric and magnetic permeabilities $\varepsilon(\mathbf{x})$ and $\mu(\mathbf{x})$ in various degrees of generality [13–15] but, if the medium is absorptive *and* space dependent, only limited progress has been made [7] (for an extensive list of further references, see Ref. [16]).

In this work we present an approach that handles general space-dependent situations. The only input required is the coordinate- and frequency-dependent complex electric permeability $\varepsilon(\mathbf{x},\omega)$, which can be obtained experimentally. We shall achieve our goal by introducing auxiliary fields with the result that we obtain a new set of nonconvolutive coupled field equations, equivalent to the original ME, such that, for $\boldsymbol{J}=\mathbf{0}$, the energy of the coupled system is conserved, both globally and locally, and leading to a unitary time evolution. The idea behind this is that convolutive time evolutions often turn up if part of the system is ''integrated out,'' the standard example being the Feshbach-Zwanzig projector method. Here $\partial_t\psi(t)=-iH\psi(t)$ in some linear space $\mathcal{H}$ is rewritten as [P and $Q=1-P$ are complementary projectors, $Q\psi(0)=0$]

$$\partial_t P\psi(t)=-iPHP\psi(t)-iPHQ\psi(t),$$

$$\partial_t Q\psi(t)=-iQHP\psi(t)-iQHQ\psi(t). \tag{1.3}$$

Solving the second and substituting into the first results in the convolutive equation

$$\partial_t P\psi(t)=-iPHP\psi(t) - \int_0^t ds PHQ\exp\left[-iQHQ(t-s)\right]QHP\psi(s). \tag{1.4}$$

This expression is the starting point for the construction of generalized master equations in statistical mechanics [17], where ψ is a density operator and H the Liouville operator, i.e., the commutator with the Hamiltonian. In quantum theory ψ is the state vector and H the Hamiltonian. There the Laplace transformed version of Eq. (1.4) corresponds to the part $\mathcal{G}_P(z)=P[z-H]^{-1}P$ of the Feshbach formula [18]

$$[z-H]^{-1}=[z-QHQ]^{-1}Q +\{P+[z-QHQ]^{-1}QHP\} \times\mathcal{G}_P(z)\{P+PHQ[z-QHQ]^{-1}\},$$

$$\mathcal{G}_P(z)=[z-PHP-PHQ[z-QHQ]^{-1}QHP]^{-1} =[z-H_{eff}(z)]^{-1}, \tag{1.5}$$

featuring the effective Hamiltonian or mass operator $H_{eff}(z)$. We shall make frequent use of this formula as a technical tool.

The transition from Eqs. (1.3) to Eq. (1.4) suggests working backwards from the convolutive ME, thus ending up with a unitary time evolution with a time-independent generator and associated Lagrange formalism in a larger space. In Sec. II it is shown how this is done. As a bonus we find that we can define an energy density $e(\mathbf{x},t)=e_{em}(\mathbf{x},t)+e_{aux}(\mathbf{x},t)$ in terms of contributions from the electromagnetic ($P\psi$ in the above relations) and auxiliary fields ($Q\psi$), which satisfies a continuity equation, featuring the Poynting vector in the divergence term

$$\partial_t e(\mathbf{x},t)+\partial_{\mathbf{x}}\cdot\boldsymbol{E}(\mathbf{x},t)\times\boldsymbol{H}(\mathbf{x},t)=0. \tag{1.6}$$

This equation is a possible starting point for the development of a diffusion theory in random absorptive media. In Sec. III we use the unitary formalism for a proper definition of band gaps for lossy systems and give a result about the persistence of gaps under a lossy perturbation. Next a Lagrange-Hamilton formalism is set up in Sec. IV and quantized in Sec. V. Then we turn to some applications. In Sec. VI we apply the unitary formalism to the classical scattering of electromagnetic waves from a lossy object, whereas in Sec. VII its quantized counterpart is used for a quantum treatment of Čerenkov and transition radiation generated in a lossy dielectric. In Sec. VIII, where atomic decay is discussed, we are led to a definition of the local density of states for an absorptive system. In Sec. IX we discuss, among other matters, related work and some open problems.

Finally some remarks on notation: Below c, the speed of light in vacuum, is set equal to one, as is $\hbar$ in the quantized theory. $\boldsymbol{\epsilon}=\{\epsilon_{ijk}\}$ is the Levi-Civita pseudotensor, antisymmetric under an interchange of each pair of indices and $\epsilon_{123}=1$, whereas $\mathbf{p}=-i\partial_{\mathbf{x}}$, the momentum operator of quantum mechanics, is the generator of translations. $\Psi_{\mathcal{A}}(y)$ is the characteristic function for the set $\mathcal{A}$, i.e., $\Psi_{\mathcal{A}}(y)=1$ for $y\in\mathcal{A}$ and vanishes otherwise. Unit vectors are written as $\mathbf{e_a}=\mathbf{a}/a$, $a=|\mathbf{a}|$. Operators pertaining to the classical formalism and classical field modes entering in quantum expressions are denoted in sans serif, i.e., K, H, etc., whereas operators related to the quantum case are denoted as H, V, etc. Inner products are written as $(f,g)=\langle g|f\rangle$. Fourier and Laplace transforms $\tilde{f}(\omega)$, respectively $\hat{f}(z)$, of $f(t)$ are defined through

$$\tilde{f}(\omega)=\int_{-\infty}^{+\infty} dt\,\exp[i\omega t]f(t),$$

$$\hat{f}(z)=\begin{cases}\int_0^\infty dt\,\exp[izt]f(t), & \mathrm{Im}z>0\\ \int_0^\infty dt\,\exp[-izt]f(-t), & \mathrm{Im}z<0\end{cases} \tag{1.7}$$

so

$$\hat{f}(\omega+i0)-\hat{f}(\omega-i0)=\tilde{f}(\omega). \tag{1.8}$$

For the definition and properties of wave and scattering operators we refer to textbooks on quantum scattering theory [18,19].

II. CONSTRUCTION OF A UNITARY TIME EVOLUTION

A. Assumptions

We assume that $\varepsilon_1(\mathbf{x})$ and $\chi(\mathbf{x},t)$ are smooth, real functions of their arguments and that $0<\varepsilon_a\leqslant\varepsilon_1(\mathbf{x})\leqslant\varepsilon_b<\infty$. Following the approach given in Ref. [20], discontinuities can be obtained by a limiting procedure. We come back to this issue in the discussion section. Concerning $\chi(\mathbf{x},t)$ we make the following assumptions (the ω integrals are over $\mathbb{R}$):

A_1: $\chi(\mathbf{x},t_0)=0$,

A_2: $\chi'(\mathbf{x},t)=\partial_t\chi(\mathbf{x},t)=\int d\omega\ \nu(\mathbf{x},\omega)\exp[-i\omega t]$,

$\nu(\mathbf{x},\omega)=\nu(\mathbf{x},-\omega)\geqslant 0$,

$\chi'(\mathbf{x},0)=\int d\omega\ \nu(\mathbf{x},\omega)\leqslant c<\infty$, c $\mathbf{x}$ independent.

A_3: $\hat{\chi}(\mathbf{x},0)=\int_0^\infty dt\ \chi(\mathbf{x},t)=\int d\omega\ \nu(\mathbf{x},\omega)\omega^{-2}<\infty$.

In this section only the first two assumptions are required, whereas A_3 is needed in the Lagrange setup, see Sec. IV. These properties generally hold for linear response expressions for χ and are explicit in a case of damped two-level systems [21]. We can allow $\nu(\mathbf{x},\omega)$ to consist of an integrable part, $\nu_{ac}(\mathbf{x},\omega)$, and a sum of δ functions, $\nu_{pp}(\mathbf{x},\omega)=\Sigma_n\nu_n(\mathbf{x})\delta(\omega^2-\omega_n^2)$, $\Sigma_n\nu_n(\mathbf{x})<\infty$. The latter describes a class of systems having a phase lag but no decay in $\chi(t)$. It is convenient to write

$$m(\mathbf{x},d\omega)=\nu_{ac}(\mathbf{x},\omega)d\omega+\nu_{pp}(\mathbf{x},\omega)d\omega. \tag{2.1}$$

From a mathematical point of view m is an $\mathbf{x}$-dependent measure, consisting of an absolutely continuous part (ac) and a pure point (or atomic) part (pp). We can add a singular continuous part as well, making m a general positive measure, but there are no compelling physical reasons to do so. $\chi'(\mathbf{x},t)$, being the Fourier transform of a positive measure, has certain special properties (Bochner's theorem, see Ref. [22]). In practical cases the $\mathbf{x}$ dependence is trivial, m vanishes outside absorptive particles in a uniform nonabsorptive background and is constant within the particles. Later on we shall frequently consider the situation where $\chi(\mathbf{x},t)$ and hence $m(\mathbf{x},\omega)$ is confined to a bounded region. With this we mean that the region in space where both are nonvanishing is bounded and independent of t. In terms of m we have

A_2: $\chi'(\mathbf{x},t)=\int m(\mathbf{x},d\omega)\exp[-i\omega t]$, $m\geqslant 0$,

$m(\mathbf{x},d\omega)=m(\mathbf{x},-d\omega)$, $m(\mathbf{x},\mathbb{R})\leqslant c<\infty$,

A_3: $\hat{\chi}(\mathbf{x},0)=\int_0^\infty dt\chi(\mathbf{x},t)=\int m(\mathbf{x},d\omega)\ \omega^{-2}<\infty$.

Substitution of Eq. (1.2) into Maxwell's equations, Eqs. (1.1), and using A_1 and A_2 results in

$$\begin{aligned}\partial_t\varepsilon_1(\mathbf{x})\boldsymbol{E}(\mathbf{x},t)&=\partial_{\mathbf{x}}\times\boldsymbol{B}(\mathbf{x},t)\\&\quad-\int_{t_0}^t ds\ \chi'(\mathbf{x},t-s)\boldsymbol{E}(\mathbf{x},s)-\boldsymbol{J}(\mathbf{x},t)\\&=\partial_{\mathbf{x}}\times\boldsymbol{B}(\mathbf{x},t)-\int_{t_0}^t ds\int m(\mathbf{x},d\omega)\\&\quad\times\exp[-i\omega(t-s)]\boldsymbol{E}(\mathbf{x},s)-\boldsymbol{J}(\mathbf{x},t).\end{aligned} \tag{2.2}$$

For later reference we summarize some relations used in the text:

$$\begin{aligned}\chi(\mathbf{x},t)&=i\int m(\mathbf{x},d\omega)\omega^{-1}\exp[-i\omega t]\\&=\int m(\mathbf{x},d\omega)\omega^{-1}\sin\omega t,\end{aligned}$$

$$\chi'(\mathbf{x},t)=\int m(\mathbf{x},d\omega)\exp[-i\omega t]=\int m(\mathbf{x},d\omega)\cos\omega t,$$

$$\begin{aligned}\hat{\chi}(\mathbf{x},z)&=z^{-1}\int m(\mathbf{x},d\omega)[\omega-z]^{-1}\\&=\int m(\mathbf{x},d\omega)[\omega^2-z^2]^{-1},\end{aligned}$$

$$\hat{\chi}(\mathbf{x},\omega+i0)-\hat{\chi}(\mathbf{x},\omega-i0)=\tilde{\chi}(\mathbf{x},\omega)=2\pi i\nu(\omega)/\omega. \tag{2.3}$$

B. Unitary formalism, general *m*

We set $\boldsymbol{F}_1(\mathbf{x},t)=\sqrt{\varepsilon_1(\mathbf{x})}\boldsymbol{E}(\mathbf{x},t)$, $\boldsymbol{F}_3(\mathbf{x},t)=\boldsymbol{B}(\mathbf{x},t)$ and introduce two new auxiliary real vector fields $\boldsymbol{F}_2(\mathbf{x},\omega,t)$ and $\boldsymbol{F}_4(\mathbf{x},\omega,t)$. Next we consider the set (skipping $\mathbf{x}$ for brevity as will be done at various places)

$$\begin{aligned}
\partial_t \boldsymbol{F}_1(t) &= \varepsilon_1^{-1/2}\partial_{\mathbf{x}}\times \boldsymbol{F}_3(t) + \varepsilon_1^{-1/2}\int m(d\omega)\boldsymbol{F}_4(\omega,t) \\
&\quad - \varepsilon_1^{-1/2}\boldsymbol{J}(t), \\
\partial_t \boldsymbol{F}_2(\omega,t) &= \omega \boldsymbol{F}_4(\omega,t), \\
\partial_t \boldsymbol{F}_3(t) &= -\partial_{\mathbf{x}}\times \varepsilon_1^{-1/2}\boldsymbol{F}_1(t), \\
\partial_t \boldsymbol{F}_4(\omega,t) &= -\omega \boldsymbol{F}_2(\omega,t) - \varepsilon_1^{-1/2}\boldsymbol{F}_1(t),
\end{aligned} \tag{2.4}$$

subject to the initial conditions

$$\boldsymbol{F}_2(\omega,t_0)=0, \quad \boldsymbol{F}_4(\omega,t_0)=0. \tag{2.5}$$

Then $\boldsymbol{F}_0(\omega,t)=\boldsymbol{F}_2(\omega,t)+i\boldsymbol{F}_4(\omega,t)$ satisfies

$$\partial_t \boldsymbol{F}_0(\omega,t) = -i\omega \boldsymbol{F}_0(\omega,t) - i\varepsilon_1^{-1/2}\boldsymbol{F}_1(t),$$

and, using Eq. (2.5),

$$\begin{aligned}
\boldsymbol{F}_0(\omega,t) &= -i\varepsilon_1^{-1/2}\int_{t_0}^{t} ds\, \exp[-i\omega(t-s)]\boldsymbol{F}_1(s) \\
&= -i\int_{t_0}^{t} ds\, \exp[-i\omega(t-s)]\boldsymbol{E}(s).
\end{aligned} \tag{2.6}$$

From this we see that $\boldsymbol{F}_2$ is odd and that $\boldsymbol{F}_4$ is even in ω, so $\int m(d\omega)\boldsymbol{F}_4(\omega,t) = -i\int m(d\omega)\boldsymbol{F}_0(\omega,t)$ and substitution of Eq. (2.6) into the first of Eqs. (2.4) gives Eq. (2.2) back and we have recovered Maxwell's equations. Also

$$\boldsymbol{D}(\mathbf{x},t) = \varepsilon_1(\mathbf{x})\boldsymbol{E}(\mathbf{x},t) - \int m(\mathbf{x},d\omega)\omega^{-1}\boldsymbol{F}_2(\mathbf{x},t). \tag{2.7}$$

Given that our set of fields satisfies Eqs. (2.4) and (2.5), the auxiliary fields are unique. If we have a second such set, then the time derivative of their difference vanishes, so this difference is constant in time and hence must vanish due to Eq. (2.5).

Combining the four $\boldsymbol{F}_j$'s into a single (12-component) vector $\boldsymbol{F}=\oplus_{j=1}^{4}\boldsymbol{F}_j$, we can write Eqs. (2.4) as

$$\partial_t \boldsymbol{F} = \mathsf{N}\boldsymbol{F} - \boldsymbol{G}, \tag{2.8}$$

where $\boldsymbol{G}=\oplus_{j=1}^{4}\boldsymbol{G}_j$, $\boldsymbol{G}_1=\varepsilon_1^{-1/2}\boldsymbol{J}$, $\boldsymbol{G}_2=\boldsymbol{G}_3=\boldsymbol{G}_4=0$. Here $\mathsf{N}=\mathsf{N}_1+\mathsf{N}_2$ is a matrix with operator entries, explicitly given by Eqs. (2.14) and (2.16) below. As mentioned earlier it is important that N generates a unitary time evolution on a suitable Hilbert space $\mathcal{H}$. We choose $\mathcal{H}=\oplus_{j=1}^{4}\mathcal{H}_j$, $\mathcal{H}_1=\mathcal{H}_3=L^2(\mathbb{R}^3,d\mathbf{x};\mathbb{R}^3)$, the space of square integrable functions over $\mathbb{R}^3$ with value in $\mathbb{R}^3$ (i.e., they are real) and $\mathcal{H}_2=\mathcal{H}_4=L^2(\mathbb{R}^4,d\mathbf{x}\ m(\mathbf{x},d\omega;\mathbb{R}^3))$ [so for $\mathbf{f}\in\mathcal{H}_2$ its norm squared is $\int d\mathbf{x}\int m(\mathbf{x},d\omega)|\mathbf{f}(\mathbf{x},\omega)|^2$]. We denote the norm and inner product on $\mathcal{H}$ by $||\ ||$ and $(\ ,\ )$ and on $\mathcal{H}_j$ by $||\ ||_j$, $(\ ,\ )_j$. A little calculation shows that for suitable $\mathbf{f},\mathbf{g}\in\mathcal{H}$ we have $(\mathsf{N}\mathbf{f},\mathbf{g})=-(\mathbf{f},\mathsf{N}\mathbf{g})$, so for $\boldsymbol{F}$ with $\boldsymbol{F}_j\in\mathcal{H}_j$ and vanishing $\boldsymbol{G}$, $\partial_t(\boldsymbol{F},\boldsymbol{F})=(\mathsf{N}\boldsymbol{F},\boldsymbol{F})+(\boldsymbol{F},\mathsf{N}\boldsymbol{F})=0$ and

$$\mathcal{E}=\tfrac{1}{2}||\boldsymbol{F}(t)||^2 \tag{2.9}$$

is conserved in time. For vanishing χ we have $m=0$, so $\mathcal{E}$ coincides with the energy stored in the electromagnetic fields. It is therefore natural to adopt $\mathcal{E}$ as the energy of the more general system we consider here. Now energy can flow from the electromagnetic to the auxiliary fields and *vice versa*. Note that no recourse was made to cycle averaging, a procedure that becomes problematic for nonmonochromatic fields. In addition to global energy conservation there is also a local conservation law, i.e., a continuity equation. Thus let $e(\mathbf{x},t)=e_{em}(\mathbf{x},t)+e_{aux}(\mathbf{x},t)$, where

$$\begin{aligned}
e_{em}(\mathbf{x},t) &= \tfrac{1}{2}\{\varepsilon_1(\mathbf{x})\boldsymbol{E}(\mathbf{x},t)^2 + \boldsymbol{B}(\mathbf{x},t)^2\} \\
&= \tfrac{1}{2}\{\boldsymbol{F}_1(\mathbf{x},t)^2 + \boldsymbol{F}_3(\mathbf{x},t)^2\}, \\
e_{aux}(\mathbf{x},t) &= \tfrac{1}{2}\int m(\mathbf{x},d\omega)\{\boldsymbol{F}_2(\mathbf{x},\omega,t)^2 + \boldsymbol{F}_4(\mathbf{x},\omega,t)^2\}.
\end{aligned} \tag{2.10}$$

Then, for $\boldsymbol{J}=0$ and using Eqs. (2.4),

$$\partial_t e(\mathbf{x},t) + \partial_{\mathbf{x}}\cdot\boldsymbol{S}(\mathbf{x},t) = 0, \tag{2.11}$$

where $\boldsymbol{S}(\mathbf{x},t)=\boldsymbol{E}(\mathbf{x},t)\times\boldsymbol{B}(\mathbf{x},t)$. We see that the energy density has a contribution from the auxiliary fields but that the divergence term only contains the Poynting vector $\boldsymbol{S}(\mathbf{x},t)$. Note further that $e_{aux}(\mathbf{x},t)$ is nonvanishing only in those space regions where $\chi'(\mathbf{x},t)$ is nonzero.

For the discussion of spectral properties such as band gaps in periodic systems it is necessary to complexify the formalism. There we allow the components of the $\boldsymbol{F}_j$'s to be complex, so $\mathcal{H}$ becomes

$$\begin{aligned}
&\mathcal{H}=\oplus_{j=1}^{4}\mathcal{H}_j, \quad \mathcal{H}_1=\mathcal{H}_3=L^2(\mathbb{R}^3,d\mathbf{x};\mathbb{C}^3), \\
&\mathcal{H}_2=\mathcal{H}_4=L^2(\mathbb{R}^4,d\mathbf{x}\,m(\mathbf{x},d\omega);\mathbb{C}^3)
\end{aligned} \tag{2.12}$$

and we set

$$\mathsf{N}=-i\mathsf{K}, \tag{2.13}$$

where K is now symmetric. Let $\mathsf{N}=\mathsf{N}_1+\mathsf{N}_2=-i\mathsf{K}_1-i\mathsf{K}_2$ with N_1 the operator obtained from N by setting $\chi=0$. Then (recall that $\boldsymbol{\epsilon}$ is the Levi-Civita pseudotensor and $\mathbf{p}=-i\partial_{\mathbf{x}}$)

$$\begin{aligned}
\mathsf{N}_1 &= \begin{pmatrix} 0 & 0 & -\varepsilon_1^{-1/2}\boldsymbol{\epsilon}\cdot\partial_{\mathbf{x}} & 0 \\ 0 & 0 & 0 & \omega \\ \boldsymbol{\epsilon}\cdot\partial_{\mathbf{x}}\varepsilon_1^{-1/2} & 0 & 0 & 0 \\ 0 & -\omega & 0 & 0 \end{pmatrix}, \\
\mathsf{K}_1 &= \begin{pmatrix} 0 & 0 & \varepsilon_1^{-1/2}\boldsymbol{\epsilon}\cdot\mathbf{p} & 0 \\ 0 & 0 & 0 & i\omega \\ -\boldsymbol{\epsilon}\cdot\mathbf{p}\varepsilon_1^{-1/2} & 0 & 0 & 0 \\ 0 & -i\omega & 0 & 0 \end{pmatrix}.
\end{aligned} \tag{2.14}$$

Introducing the projectors P_{em} and P_{aux} upon the electromagnetic and auxiliary subspaces,

$$\mathsf{P}_{em} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathsf{P}_{aux} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{2.15}$$

we see that both commute with N_1 and K_1. Thus the latter reduce to separate operators on the individual subspaces. In Ref. [20] it is shown that the electromagnetic part of K_1 defines a self-adjoint operator. This is also the case for the auxiliary part, which has the structure $\omega\left(\begin{smallmatrix}0 & i\\ -i & 0\end{smallmatrix}\right)$ and hence $\mathbb{R}$ as spectrum. We now have $\mathsf{N}=\mathsf{N}_1+\mathsf{N}_2, \mathsf{K}=\mathsf{K}_1+\mathsf{K}_2$,

$$\mathsf{N}_2=-i\mathsf{K}_2=\begin{pmatrix} 0 & 0 & 0 & \varepsilon_1^{-1/2}\int m(\mathbf{x},d\omega)\cdots \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\varepsilon_1^{-1/2} & 0 & 0 & 0 \end{pmatrix}, \tag{2.16}$$

where the $\cdots$ in $\int m(\mathbf{x},d\omega)\cdots$ indicate an integration over $m(\mathbf{x},d\omega)$ of the object on which it acts. It is a simple matter to show that under the conditions A_1 and A_2 the operators N_2 and K_2 are bounded. Thus N is anti-self-adjoint and K is self-adjoint. An elucidation about taking adjoints might be in place. Consider an operator X with $\mathsf{X}_{41}=\phi(\omega)$. Then, in the real case, $(\mathsf{X}_{41}f_1g_4)_4=\int d\mathbf{x}\int m(d\omega)\phi(\omega)f_1(\mathbf{x})g_4(\mathbf{x},\omega)=\int d\mathbf{x}\, f_1(\mathbf{x})\int m(d\omega)\phi(\omega)g_4(\mathbf{x},\omega)=(f_1,\mathsf{X}_{14}^{*}g_4)_1$, so $\phi^{*}=\int m(d\omega)\phi(\omega)\ldots$, an example being provided by Eq. (2.16).

The present setup is quite elegant in that it combines the ac and pp situations in a single formalism and we shall use it in this form in Secs. III and IV and the first part of Sec. V. However, it has a rather awkward feature if we consider random systems [characterized by random $\varepsilon_1(\mathbf{x})$ and/or $\chi(\mathbf{x},t)$] or scattering situations. In the random case the metric may become random through the random measure $m(\mathbf{x},d\omega)$, which can be undesirable, since it varies from one realization to another. In a scattering case, where $\chi(\mathbf{x},t)$ is nonzero in a bounded region in space only, the reference system used in the definition of wave and scattering operators is obtained by setting $\chi=0$, i.e., K_1 is the generator, but now $\mathcal{H}_2$ and $\mathcal{H}_4$ collapse since the measure $m(\mathbf{x},d\omega)$ vanishes. Below we remedy this.

In conclusion we observe that, given $\varepsilon_1(\mathbf{x})$ and $\chi'(\mathbf{x},t)$ satisfying A_1 and A_2, we have constructed a formalism showing a unitary time evolution. For this purpose two auxiliary fields were introduced that are unique, given the initial conditions and the differential equations they obey. In the case $\varepsilon_1=1$ we have $\boldsymbol{D}=\boldsymbol{E}+\boldsymbol{P}$ and we can identify $\boldsymbol{P}(t)=\int m(d\omega)\ \omega^{-1}\boldsymbol{F}_2(\omega,t)$ and $\partial_t\boldsymbol{P}(t)=\int m(d\omega)\boldsymbol{F}_4(\omega,t)$. Referring back to Eq. (2.9) we note that the conserved energy *cannot* be expressed in terms of the polarization and its time derivative. From a microscopic point of view these new fields represent the material system with which the electromagnetic fields interact. See the discussion section for further comments.

C. Unitary formalism, absolutely continuous *m*

In the absolutely continuous case, where $m(\mathbf{x},d\omega)=\nu(\mathbf{x},\omega)d\omega$ the problem we noted above is easily remedied by using $d\omega$ as the measure. Replacing $\boldsymbol{F}_j$ by $\sigma(\mathbf{x},\omega)\boldsymbol{F}_j$, $j=2,4$, with $\sigma(\mathbf{x},\omega)=\nu(\mathbf{x},\omega)^{1/2}$, we have $\mathcal{H}_2=\mathcal{H}_4=L^2(\mathbb{R}^4,d\mathbf{x}\,d\omega;\mathbb{R}^3)$ and Eqs. (2.4) become

$$\begin{aligned}
\partial_t\boldsymbol{F}_1(t)&=\varepsilon_1^{-1/2}\partial_{\mathbf{x}}\times\boldsymbol{F}_3(t)+\varepsilon_1^{-1/2}\int d\omega\,\sigma(\omega)\boldsymbol{F}_4(\omega,t)\\
&\quad-\varepsilon_1^{-1/2}\boldsymbol{J}(t),\\
\partial_t\boldsymbol{F}_2(\omega,t)&=\omega\boldsymbol{F}_4(\omega,t),\\
\partial_t\boldsymbol{F}_3(t)&=-\partial_{\mathbf{x}}\times\varepsilon_1^{-1/2}\boldsymbol{F}_1(t),\\
\partial_t\boldsymbol{F}_4(\omega,t)&=-\omega\boldsymbol{F}_2(\omega,t)-\varepsilon_1^{-1/2}\sigma(\omega)\boldsymbol{F}_1(t),
\end{aligned} \tag{2.17}$$

with the corresponding changes in N and K. Thus

$$\mathsf{K}=\begin{pmatrix} 0 & 0 & \varepsilon_1^{-1/2}\boldsymbol{\epsilon}\cdot\mathbf{p} & i\varepsilon_1^{-1/2}\int d\omega\ \sigma(\mathbf{x},\omega)\cdots \\ 0 & 0 & 0 & i\omega \\ -\boldsymbol{\epsilon}\cdot\mathbf{p}\varepsilon_1^{-1/2} & 0 & 0 & 0 \\ -i\varepsilon_1^{-1/2}\sigma(\mathbf{x},\omega) & -i\omega & 0 & 0 \end{pmatrix}. \tag{2.18}$$

As before we can decompose: $\mathsf{K}=\mathsf{K}_1+\mathsf{K}_2$. Let $\mathcal{A}$ be the set of $\mathbf{x}\in\mathbb{R}^3$ for which $\chi(\mathbf{x},t)$ vanishes. Then (Ψ is a characteristic function) $\mathsf{P}_{\mathcal{A}}=\Psi_{\mathcal{A}}(\mathbf{x})\mathsf{P}_{aux}$ is a projector and

$$[\mathsf{P}_{\mathcal{A}},\mathsf{K}]=0. \tag{2.19}$$

This implies that if $\mathsf{P}_{\mathcal{A}}\boldsymbol{F}(\mathbf{x},0)=0$, then $\mathsf{P}_{\mathcal{A}}\boldsymbol{F}(\mathbf{x},t)=0$ for all other t.

The modified formalism, presented in this subsection, will be used in later sections, in particular where scattering situations are considered.

D. Unitary formalism, pure point *m*

If m is pure point, i.e., $m(\mathbf{x},\omega)=\Sigma_n\nu_n(\mathbf{x})\delta(\omega^2-\omega_n^2)$, we set $\boldsymbol{F}_{jn}=\sigma_n(\mathbf{x})\boldsymbol{F}_j(\mathbf{x},\omega_n)$, $\sigma_n(\mathbf{x})=\nu_n(\mathbf{x})^{1/2}$, $j=2,4$. Now $\mathcal{H}_2=\mathcal{H}_4=L^2(\mathbb{R}^3,d\mathbf{x})\otimes l^2$, i.e., $||\boldsymbol{F}_j||^2=\Sigma_n\int d\mathbf{x}\ |\boldsymbol{F}_{jn}(\mathbf{x})|^2$, $j=2,4$, and

$$\partial_t \boldsymbol{F}_1(t)=\varepsilon_1^{-1/2}\partial_{\mathbf{x}}\times\boldsymbol{F}_3(t)+\varepsilon_1^{-1/2}\sum_n \sigma_n \boldsymbol{F}_{4n}(t)-\varepsilon_1^{-1/2}\boldsymbol{J}(t),$$

$$\partial_t \boldsymbol{F}_{2n}(t)=\omega_n \boldsymbol{F}_{4n}(t), \tag{2.20}$$

$$\partial_t \boldsymbol{F}_3(t)=-\partial_{\mathbf{x}}\times\varepsilon_1^{-1/2}\boldsymbol{F}_1(t),$$

$$\partial_t \boldsymbol{F}_{4n}(t)=-\omega_n \boldsymbol{F}_{2n}(t)-\varepsilon_1^{-1/2}\sigma_n \boldsymbol{F}_1(t).$$

This is basically a discretized version of Eqs. (2.17). Obviously both can be combined if m is of the form Eq. (2.1).

III. BAND-GAP SYSTEMS

As is the case for electrons in periodic potentials, the spectrum of conservative periodic dielectrics has a band structure [8], which may show gaps. In this case the spectrum is determined by the eigenvalues λ^2 of the electric Helmholtz operator

$$\mathsf{H}_1=\varepsilon_1(\mathbf{x})^{-1/2}\mathsf{H}_0\varepsilon_1(\mathbf{x})^{-1/2}, \tag{3.1}$$

or

$$[\varepsilon_1(\mathbf{x})\lambda^2-\mathsf{H}_0]\boldsymbol{E}_\lambda=0. \tag{3.2}$$

Here, in dyadic notation, $\mathsf{H}_0=-\partial_{\mathbf{x}}^2\mathsf{U}+\partial_{\mathbf{x}}\partial_{\mathbf{x}}$, U being the 3×3 unit matrix. Suppose there are no solutions for $|\lambda|\in\Delta=(\lambda_a,\lambda_b)$, in which case Maxwell's equations have no eigenmodes $\boldsymbol{E}_\lambda(\mathbf{x})\exp[\pm i\lambda t]$. Then Δ and $-\Delta=(-\lambda_b,-\lambda_a)$ are a pair of band gaps. Alternatively we can define band gaps as intervals where the density of states vanishes. The situation is more complicated for absorptive systems: Using A_1 and A_2 we obtain from Eq. (2.2) and the second Eq. (1.1),

$$[z^2\varepsilon(z)-\mathsf{H}_0]\hat{\boldsymbol{E}}(z)=iz\boldsymbol{E}(0)-\partial_{\mathbf{x}}\times\boldsymbol{B}(0) \tag{3.3}$$

for the Laplace transform $\hat{\boldsymbol{E}}(z)$. Here we have taken $t_0=0$. Thus, assuming the inverse operator to exist,

$$\hat{\boldsymbol{E}}(z)=\mathsf{R}_e(z^2)\{iz\boldsymbol{E}(0)-\partial_{\mathbf{x}}\times\boldsymbol{B}(0)\}, \tag{3.4}$$

where

$$\mathsf{R}_e(z^2)=[z^2\varepsilon(z)-\mathsf{H}_0]^{-1} \tag{3.5}$$

is the resolvent associated with the electric Helmholtz equation and

$$\varepsilon(z)=\varepsilon_1+\hat{\chi}(z), \tag{3.6}$$

see also Appendix C. Suppose that $\mathsf{R}_e(z^2)$ is analytic across the real axis for $|\mathrm{Re}z|\in\Delta$. Since, according to Eq. (1.8), $\tilde{\boldsymbol{E}}(\lambda)=\hat{\boldsymbol{E}}(\lambda+i0)-\hat{\boldsymbol{E}}(\lambda-i0)$, it follows that $\tilde{\boldsymbol{E}}(\lambda)=0$ for $|\lambda|\in\Delta$ (i.e., $\boldsymbol{E}$ has no Fourier components in this interval) and we conclude that Δ is (part of) a band gap. However, $\varepsilon(\lambda\pm i0)$ are complex and it is not clear that the above analyticity assumption can be realized. In order to shed more light on this problem we return to the unitary time evolution discussed in Sec. II B. Again setting $t_0=0$, we have

$$\boldsymbol{F}(t)=\exp[-i\mathsf{K}t]\boldsymbol{F}(0), \tag{3.7}$$

where K is self-adjoint and hence has a real spectrum. Projecting upon the electromagnetic fields and using $\mathsf{P}_{aux}\boldsymbol{F}(0)=\mathbf{0}$ we have

$$\mathsf{P}_{em}\boldsymbol{F}(t)=\mathsf{P}_{em}\exp[-i\mathsf{K}t]\mathsf{P}_{em}\boldsymbol{F}(0), \tag{3.8}$$

which has the Fourier transform

$$\mathsf{P}_{em}\tilde{\boldsymbol{F}}(\lambda)=\mathsf{P}_{em}\delta(\lambda-\mathsf{K})\mathsf{P}_{em}\boldsymbol{F}(0). \tag{3.9}$$

If this quantity vanishes for $\lambda\in\Delta$, with Δ as above, then Δ is (part of) a band gap. Indeed there are no $\mathsf{P}_{em}\tilde{\boldsymbol{F}}(\lambda)$ for $\lambda\in\Delta$.

Generically K has the whole real axis as a spectrum (this being the case for the decoupled auxiliary part), so the presence of the P_{em}'s is crucial. Since the spectrum of K is real, the above definition is equivalent to $\mathsf{P}_{em}[z-\mathsf{K}]^{-1}\mathsf{P}_{em}$ being analytic across the real axis for $\mathrm{Re}z\in\Delta$. As shown in Appendix A we can recast this object according to

$$\mathsf{P}_{em}[z-\mathsf{K}]^{-1}\mathsf{P}_{em}=\begin{pmatrix}\mathsf{X}_{11}&0&\mathsf{X}_{13}&0\\0&0&0&0\\\mathsf{X}_{31}&0&\mathsf{X}_{33}&0\\0&0&0&0\end{pmatrix}, \tag{3.10}$$

where

$$\mathsf{X}_{11}=z\varepsilon_1^{1/2}\mathsf{R}_e(z^2)\varepsilon_1^{1/2},\quad \mathsf{X}_{13}=\varepsilon_1^{1/2}\mathsf{R}_e(z^2)\cdot(\boldsymbol{\epsilon}\cdot\mathbf{p}),$$

$$\mathsf{X}_{31}=-(\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot\mathsf{R}_e(z^2)\varepsilon_1^{1/2}, \tag{3.11}$$

$$\mathsf{X}_{33}=z^{-1}\{1-(\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot\mathsf{R}_e(z^2)\cdot(\boldsymbol{\epsilon}\cdot\mathbf{p})\}=z\mathsf{R}_m(z^2).$$

Here $\mathsf{R}_m(z^2)=[z^2+(\boldsymbol{\epsilon}\cdot\mathbf{p})\varepsilon(z)^{-1}\cdot(\boldsymbol{\epsilon}\cdot\mathbf{p})]^{-1}$. Since the left-hand side of Eq. (3.10) exists for $\mathrm{Im}z\neq0$, so does $\mathsf{R}_e(z^2)$ and hence $\hat{\boldsymbol{E}}(z)$ in Eq. (3.4). Now if $(\Delta,-\Delta)$ is a band-gap pair for K, then $\mathsf{R}_e(z^2)$ and $\mathsf{R}_m(z^2)$ must be analytic for z^2 crossing $\Delta^2=(\lambda_a^2,\lambda_b^2)$ and *vice versa*.

In order to see that gaps can indeed exist, consider the artificial example where $m(d\omega)=\varepsilon_1(\mathbf{x})m_0\delta(\omega^2-\omega_0^2)$ and $\varepsilon_1(\mathbf{x})=\varepsilon_1(\mathbf{x}+\mathbf{a})$ is periodic, leading to a gap $\Delta^2=(\lambda_a^2,\lambda_b^2)$ in the spectrum of $\mathsf{H}_1=\varepsilon_1^{-1/2}\mathsf{H}_0\varepsilon_1^{-1/2}$. Then $\varepsilon(\mathbf{x},z)=\varepsilon_1(\mathbf{x})z^2\{1+(m_0/\omega_0)[\omega_0^2-z^2]^{-1}\}=\varepsilon_1(\mathbf{x})\zeta^2$ and $[\varepsilon_1(\mathbf{x})\zeta^2-\mathsf{H}_0]^{-1}$ is analytic across $\mathbb{R}$ for $\mathrm{Re}\zeta^2\in\Delta^2$. But then, provided $\mu_a^2\geqslant0$ in $\mu_j^2=\omega_0^2-[m_0/\omega_0+\omega_0^2][1+\lambda_j^2]^{-1}$, $\mathsf{R}_e(z^2)$ is analytic through (μ_a^2,μ_b^2). Another case, where band gaps may exist is the situation where K_1 has a band-gap pair $(\Delta,-\Delta)$ as above and that χ is sufficiently small:

Proposition: Suppose that K_1 has the band-gap pair $(\Delta,-\Delta)$, $\Delta=(\lambda_a,\lambda_b)$ and let $0<\delta<\frac{1}{2}(\lambda_b^2-\lambda_a^2)$. If $\sup_{\mathbf{x}\in\mathbb{R}^3}\varepsilon_1(\mathbf{x})^{-1}\int_0^\infty dt|\chi(\mathbf{x},t)|\leqslant\lambda_b^{-2}\delta<1$, then $(\Delta_\delta,-\Delta_\delta)$, $\Delta_\delta=(\sqrt{\lambda_a^2+\delta},\sqrt{\lambda_b^2-\delta})$, is a band-gap pair for K.

The easy proof is given in Appendix B. Note that we did not require $\varepsilon_1(\mathbf{x})$ and $\chi(\mathbf{x},t)$ to be periodic in $\mathbf{x}$. For additional information about the eigenvectors of K^2, see Appendix C. A generalization of the concept of density of states $N(E)$ is discussed in Sec. VIII. It vanishes for E in a gap.

IV. LAGRANGE AND HAMILTON FORMALISM

For the quantization of the classical field equations a Lagrange formalism is required. Thus a Lagrange-Hamilton version of the set of field equations obtained in Sec. II is presented below. Here we shall need assumption A_3. Quite recently Tip [15] constructed a general Lagrange-Hamilton formalism, based upon equations of the type Eq. (2.8). We use the setup of Sec. II B for the unitary time evolution and use the subscripts e and m to refer to the first two and the last two components of vectors such as $\boldsymbol{F}$, respectively. Here e is short for electric and m for magnetic, $\boldsymbol{F}_1$ and $\boldsymbol{F}_2$ dealing with electric and $\boldsymbol{F}_3$ and $\boldsymbol{F}_4$ with magnetic fields, respectively. Since N has the structure

$$\mathsf{N}=\begin{pmatrix} 0 & \mathsf{N}_{em} \\ \mathsf{N}_{me} & 0 \end{pmatrix}, \quad \mathsf{N}_{me}=-\mathsf{N}_{em}^{*} \tag{4.1}$$

we have (see also Appendix C)

$$\mathsf{N}^2=-\mathsf{N}^{*}\mathsf{N}=\begin{pmatrix} \mathsf{N}_{em}\mathsf{N}_{me} & 0 \\ 0 & \mathsf{N}_{me}\mathsf{N}_{em} \end{pmatrix}=-\begin{pmatrix} \mathsf{H}_e & 0 \\ 0 & \mathsf{H}_m \end{pmatrix}, \tag{4.2}$$

and $\mathsf{P}=1-\mathsf{Q}$, the projector upon the null space $\mathcal{N}(\mathsf{N})$, is of the form

$$\mathsf{P}=\begin{pmatrix} \mathsf{P}_e & 0 \\ 0 & \mathsf{P}_m \end{pmatrix}=\begin{pmatrix} 1-\mathsf{Q}_e & 0 \\ 0 & 1-\mathsf{Q}_m \end{pmatrix}. \tag{4.3}$$

Further details are given in Appendix C. We now introduce the generalized coordinate field $\boldsymbol{\xi}$ through

$$\mathsf{N}\boldsymbol{\xi}=-\mathsf{Q}\boldsymbol{F}. \tag{4.4}$$

This does not fix $\boldsymbol{\xi}$ uniquely, so we add the ''gauge condition''

$$\mathsf{P}\boldsymbol{\xi}=0, \tag{4.5}$$

giving

$$\boldsymbol{\xi}=-\mathsf{N}^{-1}\mathsf{Q}\boldsymbol{F}. \tag{4.6}$$

As discussed in Ref. [15] other gauges are possible as well. There the present gauge is referred to as the C gauge since it is the natural generalization of the Coulomb gauge of electrodynamics. We introduce two further, scalar, fields ζ_e and ζ_m through

$$\mathsf{P}\boldsymbol{F}=-\mathsf{M}\boldsymbol{\zeta}=-\begin{pmatrix} \varepsilon_1^{1/2}\partial_{\mathbf{x}} & 0 \\ -\omega^{-1}\varepsilon_1^{1/2}\partial_{\mathbf{x}} & 0 \\ 0 & \partial_{\mathbf{x}} \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \zeta_e \\ \zeta_m \end{pmatrix}. \tag{4.7}$$

It is shown in Appendix C that this is the general form of $\mathsf{P}\boldsymbol{F}$. It follows from Eqs. (4.6) and (4.7) that

$$\boldsymbol{F}_m=-\mathsf{N}_{me}\boldsymbol{\xi}_e-\mathsf{M}_m\zeta_m. \tag{4.8}$$

Next we observe that ($\boldsymbol{G}_m=0$)

$$\begin{aligned}\partial_t\boldsymbol{\xi}_e&=-(\mathsf{N}^{-1}\mathsf{Q}\partial_t\boldsymbol{F})_e=-(\mathsf{N}^{-1}\mathsf{Q}[\mathsf{N}\boldsymbol{F}-\boldsymbol{G}])_e\\&=-\mathsf{Q}_e\boldsymbol{F}_e+(\mathsf{N}^{-2})_{ee}\mathsf{N}_{em}\mathsf{Q}_m\boldsymbol{G}_m=-\mathsf{Q}_e\boldsymbol{F}_e,\end{aligned}$$

so

$$\boldsymbol{F}_e=-\partial_t\boldsymbol{\xi}_e-\mathsf{M}_e\zeta_e. \tag{4.9}$$

Since $\mathsf{M}^{*}\mathsf{P}=\mathsf{M}^{*}$ we have

$$\mathsf{M}^{*}\boldsymbol{F}=-\mathsf{M}^{*}\mathsf{M}\boldsymbol{\zeta}=\begin{pmatrix} \partial_{\mathbf{x}}\cdot\varepsilon_{stat}(\mathbf{x})\partial_{\mathbf{x}}\zeta_e \\ \partial_{\mathbf{x}}^2\zeta_m \end{pmatrix}, \tag{4.10}$$

where

$$\varepsilon_{stat}(\mathbf{x})=\varepsilon_1(\mathbf{x})+\hat{\chi}(\mathbf{x},0) \tag{4.11}$$

is the static permeability [for space regions with vanishing $\hat{\chi}(\mathbf{x},0)$ this is true by our definition in Sec. I, whereas in an absorbing region $\varepsilon_1(\mathbf{x})+\hat{\chi}(\mathbf{x},0)=1+\hat{\chi}(\mathbf{x},0)$ is the static permeability by definition]. Obviously $\hat{\chi}(0)$ must be finite for Eq. (4.10) to make sense, so it is at this point that assumption A_3 must be made. Since $(\mathsf{M}^{*}\boldsymbol{F})_m=\partial_{\mathbf{x}}\cdot\boldsymbol{B}=0$, ζ_m must vanish. Also

$$\begin{aligned}(\mathsf{M}^{*}\boldsymbol{F})_e&=-\partial_{\mathbf{x}}\cdot\left\{\varepsilon_1^{1/2}\boldsymbol{F}_1-\int m(d\omega)\omega^{-1}\boldsymbol{F}_2(\omega)\right\}\\&=-\partial_{\mathbf{x}}\cdot\left\{\varepsilon_1\boldsymbol{E}-\mathrm{Im}\int m(d\omega)\omega^{-1}\right.\\&\qquad\left.\times\int_0^t ds\ \exp[-i\omega(t-s)]\boldsymbol{E}(s)\right\}\\&=-\partial_{\mathbf{x}}\cdot\boldsymbol{D}=-\rho,\end{aligned}$$

ρ being the charge density. Thus

$$-\partial_{\mathbf{x}}\cdot\varepsilon_{stat}(\mathbf{x})\partial_{\mathbf{x}}\zeta_e=\rho. \tag{4.12}$$

Equation (4.12) determines ζ_e, whereas we have for $\boldsymbol{\xi}_e$

$$\partial_t^2\boldsymbol{\xi}_e=\mathsf{N}_{em}\mathsf{N}_{me}\boldsymbol{\xi}_e-\mathsf{Q}_e\boldsymbol{G}_e. \tag{4.13}$$

These equations of motion follow from Hamilton's principle with the Lagrangian (see also Ref. [15])

$$\begin{aligned}L&=\tfrac{1}{2}(\partial_t\boldsymbol{\xi}_e+\mathsf{M}_e\zeta_e,\partial_t\boldsymbol{\xi}_e+\mathsf{M}_e\zeta_e)_e-\tfrac{1}{2}(\mathsf{N}_{me}\boldsymbol{\xi}_e,\mathsf{N}_{me}\boldsymbol{\xi}_e)_m\\&\quad-(\mathsf{Q}_e\boldsymbol{G}_e,\boldsymbol{\xi}_e)_e-(\rho,\zeta_e)_0\\&=\tfrac{1}{2}(\partial_t\boldsymbol{\xi}_e,\partial_t\boldsymbol{\xi}_e)_e+\tfrac{1}{2}(\mathsf{M}_e\zeta_e,\mathsf{M}_e\zeta_e)\\&\quad-\tfrac{1}{2}(\mathsf{N}_{me}\boldsymbol{\xi}_e,\mathsf{N}_{me}\boldsymbol{\xi}_e)_m-(\mathsf{Q}_e\boldsymbol{G}_e,\boldsymbol{\xi}_e)_e-(\rho,\zeta_e)_0.\end{aligned} \tag{4.14}$$

Here M_e and $(\ ,\ )_e$ are the component of M and the inner product for the electric subspace $\mathcal{H}_1\oplus\mathcal{H}_2$, respectively, whereas $(\ ,\ )_m$ is the inner product for the magnetic subspace $\mathcal{H}_3\oplus\mathcal{H}_4$ (both inner products are the same) and $(\ ,\ )_0$ is the inner product for $\mathcal{H}_0=L^2(\mathbb{R}^3,d\mathbf{x})$. The momentum field associated with $\boldsymbol{\xi}_e$ is given by the variational derivative

$$\boldsymbol{\pi}_e=\frac{\delta L}{\delta\partial_t\boldsymbol{\xi}_e}=\partial_t\boldsymbol{\xi}_e, \tag{4.15}$$

and the Hamiltonian is

$$H=\tfrac{1}{2}(\boldsymbol{\pi}_e,\boldsymbol{\pi}_e)_e+\tfrac{1}{2}(\mathsf{N}_{me}\boldsymbol{\xi}_e,\mathsf{N}_{me}\boldsymbol{\xi}_e)_m+\tfrac{1}{2}(\rho,\zeta_e)_0 +(\mathsf{Q}_e\boldsymbol{G}_e,\boldsymbol{\xi}_e)_e, \tag{4.16}$$

where ζ_e is the solution of Eq. (4.12). Here the situation is completely analogous to that of the Coulomb gauge in vacuum electrodynamics. In the present gauge ζ_e is a given function, determined by the external charge distribution ρ and the initial value of $\mathsf{P}_e\boldsymbol{F}_e$, whereas the gauge condition Eq. (4.5) gives

$$\partial_{\mathbf{x}}\cdot\left\{\varepsilon_1^{1/2}\boldsymbol{\xi}_1-\int m(d\omega)\omega^{-1}\boldsymbol{\xi}_2\right\}=0. \tag{4.17}$$

Comparing $\boldsymbol{F}_1=\varepsilon_1^{1/2}\boldsymbol{E}_1=-\partial_t\boldsymbol{\xi}_1-\varepsilon_1^{1/2}\partial_{\mathbf{x}}\zeta_e$ with the usual expression in terms of the vector and scalar potentials $\boldsymbol{E}=-\partial_t\boldsymbol{A}-\partial_{\mathbf{x}}\Phi$, we identify $\boldsymbol{\xi}_1=\varepsilon_1^{1/2}\boldsymbol{A}$ and $\zeta_e=\Phi$.

V. QUANTIZATION

The quantization of the Hamiltonian formalism, obtained in the preceding section, follows the pattern of Ref. [15], where an extensive discussion is given. Here we restrict ourselves by only presenting the results. Let $\{\mathbf{u}_{\lambda\alpha}\}$be the complete set of orthonormal eigenvectors, associated with the nonzero eigenvalues λ of H_e. They span $\mathcal{H}_e$ [inner product $(\ ,\ )_e$], the complex version of $\mathsf{Q}_e\{\mathcal{H}_1\oplus\mathcal{H}_2\}$. Thus

$$\mathsf{H}_e\mathbf{u}_{\lambda\alpha}=\lambda^2\mathbf{u}_{\lambda\alpha},\quad \lambda>0. \tag{5.1}$$

A discussion of this eigenvalue problem is presented in Appendix C. Let $\mathcal{F}=\mathcal{F}(\mathcal{H}_e)$ be the symmetric Fock space over $\mathcal{H}_e$ and $a^*(f)$ and $a(g)$, $f,\ g\in\mathcal{H}_e$ are creation and annihilation operators acting in $\mathcal{F}$. They satisfy the commutation relation

$$[a(g),a^*(f)]=\mathrm{Re}(f,g)_e. \tag{5.2}$$

Now

$$\boldsymbol{\xi}_e=\sum_\alpha\int d\lambda(2\lambda)^{-1/2}\{a^*(\mathbf{u}_{\lambda\alpha})\overline{\mathbf{u}}_{\lambda\alpha}+a(\mathbf{u}_{\lambda\alpha})\mathbf{u}_{\lambda\alpha}\}, \tag{5.3}$$

and denoting the first (electric) component of $\mathbf{u}_{\lambda\alpha}$ and the second (auxiliary) by $\mathbf{u}_{1\lambda\alpha}$ and $\mathbf{u}_{2\lambda\alpha}$, respectively,

$$\boldsymbol{A}(\mathbf{x})=\sum_\alpha\int d\lambda[2\lambda\varepsilon_1(\mathbf{x})]^{-1/2}\{a^*(\mathbf{u}_{\lambda\alpha})\overline{\mathbf{u}}_{1\lambda\alpha}(\mathbf{x}) +a(\mathbf{u}_{\lambda\alpha})\mathbf{u}_{1\lambda\alpha}(\mathbf{x})\}. \tag{5.4}$$

The Hamiltonian becomes

$$H=H_f+H_{ext},$$

$$H_f=\sum_\alpha\int d\lambda\ \lambda a^*(\mathbf{u}_{\lambda\alpha})a(\mathbf{u}_{\lambda\alpha}),$$

$$H_{ext}=-\sum_\alpha\int d\lambda\ (2\lambda)^{-1/2}\{(\boldsymbol{G}_e,\mathbf{u}_{\lambda\alpha})_e a^*(\mathbf{u}_{\lambda\alpha}) +(\mathbf{u}_{\lambda\alpha},\boldsymbol{G}_e)_e a(\mathbf{u}_{\lambda\alpha})\}+\tfrac{1}{2}(\rho,\zeta_e)_0 =-\int d\mathbf{x}\ \boldsymbol{J}(\mathbf{x})\cdot\boldsymbol{A}(\mathbf{x})+\tfrac{1}{2}\int d\mathbf{x}\,\rho(\mathbf{x})\Phi(\mathbf{x}). \tag{5.5}$$

Here we used the fact that only $\varepsilon_1^{-1/2}\boldsymbol{J}$, the first component of $\boldsymbol{G}_e$, is nonvanishing. In case the interaction with a set of charged scalar Schrödinger particles (mass m_j, charge e_j,coordinates $\mathbf{x}_j$, momenta $\mathbf{p}_j$) is considered, the charge and current densities originate from these particles and the Hamiltonian is now (see Ref. [15] for details)

$$H=H_m+H_f+H_{int}, \tag{5.6}$$

where

$$H_m=\sum_j\frac{1}{2m_j}\mathbf{p}_j^2+\sum_{j>h}e_je_h\Phi(\mathbf{x}_j,\mathbf{x}_h), \tag{5.7}$$

and

$$H_{int}=H_{int}(\boldsymbol{A})=-\sum_j\frac{e_j}{2m_j}\{\mathbf{p}_j\cdot\boldsymbol{A}(\mathbf{x}_j)+\boldsymbol{A}(\mathbf{x}_j)\cdot\mathbf{p}_j\} +\sum_j\frac{e_j^2}{2m_j}\boldsymbol{A}(\mathbf{x}_j)^2. \tag{5.8}$$

The potentials $\Phi(\mathbf{x},\mathbf{y})$ are the solutions of

$$-\partial_{\mathbf{x}}\cdot\varepsilon_{stat}(\mathbf{x})\partial_{\mathbf{x}}\Phi(\mathbf{x},\mathbf{y})=\delta(\mathbf{x}-\mathbf{y}). \tag{5.9}$$

In the classical formalism the auxiliary fields vanish at the initial time t_0. Here the corresponding condition consists of taking the vacuum state at the initial time. At this point we note that the states on the different Fock layers can be represented in terms of linear combinations of direct sums $f\oplus g$, $f\in\mathcal{F}(\mathcal{H}_1)$, $g\in\mathcal{F}(\mathcal{H}_2)$. Thus our initial state is of the form $f\oplus g_0$, g_0 being the vacuum state of $\mathcal{F}(\mathcal{H}_2)$ and $f\in\mathcal{F}(\mathcal{H}_1)$. The eigenstate of H_f at the eigenvalue zero is the vacuum state of $\mathcal{F}(\mathcal{H}_e)$, the direct sum of the individual vacuum states on the $\mathcal{F}(\mathcal{H}_j)$'s. Denoting the vacuum layer as the zeroth Fock layer, the first Fock layer is simply $\mathcal{H}_e$ and the restriction of H_f to this layer is $\mathsf{H}_e^{1/2}$ (for more details on the Fock space structure, see Ref. [15]). Thus the eigenstates of H_f restricted to this layer are no longer products of states from $\mathcal{H}_1$ and $\mathcal{H}_2$ and similar for higher layers.

So far, the choice for the classical unitary evolution, as discussed in Sec. II, was immaterial. As explained there, the situation changes in scattering situations, where outside a bounded region $\chi(\mathbf{x},t)$ vanishes and $\varepsilon_1=1$. Supposing that m is absolutely continuous, i.e., $m(d\omega)=\nu(\omega)d\omega$ we now use the formalism of Sec. II C. Then the reference operator

$$H^{(0)}=H_m+H_f^{(0)}+H_{int}(\boldsymbol{A}^{(0)}),$$

$$H_f^{(0)}=\sum_\alpha \int d\lambda\ \lambda a^*(\mathbf{u}_{\lambda\alpha}^{(0)})a(\mathbf{u}_{\lambda\alpha}^{(0)}), \tag{5.10}$$

$$\boldsymbol{A}^{(0)}(\mathbf{x})=\sum_\alpha \int d\lambda[2\lambda]^{-1/2}\{a^*(\mathbf{u}_{\lambda\alpha}^{(0)})\overline{\mathbf{u}}_{1\lambda\alpha}^{(0)}(\mathbf{x}) + a(\mathbf{u}_{\lambda\alpha}^{(0)})\mathbf{u}_{1\lambda\alpha}^{(0)}(\mathbf{x})\}$$

would appear in the relevant wave operators. However, there is an important subtlety. Since the null spaces of H_e and $\mathsf{H}_e^{(0)}$ differ, so do their complements $\mathcal{H}_e$ and $\mathcal{H}_e^{(0)}$, and hence the associated Fock spaces $\mathcal{F}(\mathcal{H}_e)$ and $\mathcal{F}(\mathcal{H}_e^{(0)})$. This fact leads to problems in the definition of wave operators and amends must be made. The procedure goes as follows: Suppose that H_e and $\mathsf{H}_e^{(0)}$ are related by the wave operator Ω (see Appendix C), i.e., $\mathsf{H}_e=\Omega\mathsf{H}_e^{(0)}\Omega^*$. Then $\mathcal{H}_e=\Omega\mathcal{H}_e^{(0)}$ and the eigenvectors of H_e are $\mathbf{u}_{\lambda\alpha}=\Omega\mathbf{u}_{\lambda\alpha}^{(0)}$. Also $\mathcal{F}(\mathcal{H}_e)=\Omega_F\mathcal{F}(\mathcal{H}_e^{(0)})$, where $\Omega_F=1\oplus\Omega\oplus\{\Omega\otimes\Omega\}\oplus\cdots$. Let now

$$H^{(1)}=\Omega_F H^{(0)}\Omega_F^*. \tag{5.11}$$

Since $\Omega_F H_f^{(0)}\Omega_F^*=H_f$ and

$$\boldsymbol{A}^{(1)}(\mathbf{x})=\Omega_F\boldsymbol{A}^{(0)}(\mathbf{x})\Omega_F^* =\sum_\alpha \int d\lambda[2\lambda]^{-1/2}\{a^*(\mathbf{u}_{\lambda\alpha})\overline{\mathbf{u}}_{1\lambda\alpha}^{(0)}(\mathbf{x}) + a(\mathbf{u}_{\lambda\alpha})\mathbf{u}_{1\lambda\alpha}^{(0)}(\mathbf{x})\},$$

where $\boldsymbol{A}^{(1)}(\mathbf{x})$ acts in $\mathcal{F}(\mathcal{H}_e)$, we have

$$H^{(1)}=T(\mathbf{p})+H_f+H_{int}(\boldsymbol{A}^{(1)}). \tag{5.12}$$

Now the pair H and $H^{(1)}$ act in the same space and this result will be used in Sec. VII. The $\mathbf{u}_{\lambda\alpha}^{(0)}$'s are an orthonormal set of eigenvectors of

$$\mathsf{H}_e^{(0)}=\begin{pmatrix}\mathsf{H}_0 & 0\\ 0 & \omega^2\end{pmatrix}. \tag{5.13}$$

Since the electromagnetic and auxiliary fields are decoupled, the eigenstates are of the form $\mathbf{u}_{\mathbf{k}jn}^{(0)}=c_1\mathbf{u}_{1\mathbf{k}j}^{(0)}\oplus c_2\mathbf{u}_{2n}^{(0)}$, with at least one of the c's nonzero. Here $\mathbf{u}_{1\mathbf{k}j}^{(0)}(\mathbf{x})=(2\pi)^{-3/2}\mathbf{e}_j\exp[i\mathbf{k}\cdot\mathbf{x}]$, with $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_\mathbf{k}$ mutually orthogonal and $k=\lambda$. Furthermore $\mathbf{u}_{2n}^{(0)}=\omega\delta(\lambda^2-\omega^2)\mathbf{f}_n$ with $\{\mathbf{f}_n, n=1,2,\ldots\}$ an orthogonal basis for $L^2(\mathbb{R}^3,d\mathbf{x};\mathbb{C}^3)$ (functions even in ω are also allowed but do not contribute in the present formalism). Now all eigenstates of $H_f^{(0)}$ are direct sums of states from $\mathcal{F}(\mathcal{H}_1)$ and $\mathcal{F}(\mathcal{H}_2)$ and $\Sigma_\alpha\int d\lambda$ decomposes into $\Sigma_j\int d\mathbf{k}$ and Σ_n. In Sec. VII we encounter a situation where $\mathbf{u}_{2n}^{(0)}$ vanishes. Then $\mathbf{u}=\Omega\mathbf{u}^{(0)}$ can be labeled by $\mathbf{k}$ and j, i.e., $\mathbf{u}=\mathbf{u}_{\mathbf{k}j}$ and $\Sigma_\alpha\int d\lambda\to\Sigma_j\int d\mathbf{k}$.

VI. CLASSICAL SCATTERING FROM LOSSY OBJECTS

Our first application concerns the classical scattering of an electromagnetic wave from a finite lossy object. The description of such a process involves two things. The first is the existence of the appropriate wave operators $\Omega_\pm$ and scattering operator $\mathsf{S}=\Omega_+^*\Omega_-$. We leave aside the asymptotic completeness of the wave operators, which is needed for the unitarity of S. Given S, the associated transition (T) operator and scattering amplitude follow. The second step consists of relating the scattering of a wave packet to the above scattering amplitude. This involves the scattering into cones, a subject that has been studied for Schrödinger systems but, as far as the author is aware, not for the electromagnetic case. Below we fill this gap.

Thus initially an electromagnetic wave packet is moving freely towards the scatterer. We take the origin of our coordinate system somewhere inside the scatterer and shall calculate the amount of energy that finally arrives in the cone $\mathcal{C}\subset\mathbb{R}^3$ with the axis along the unit vector $\mathbf{e}$ and aperture $\vartheta_0\in(0,\pi)$, where it is recorded by a detector far away from the object. We truncate the cone to $\mathcal{C}_b$, where $x>b>0$ and b is such that the scatterer and $\mathcal{C}_b$ do not overlap. Then the energy ending up in $\mathcal{C}_b$ is purely electromagnetic. We assume m to be absolutely continuous, $\varepsilon_1=1$ and use the results of Sec. II C. The relevant wave operators are

$$\begin{aligned}\Omega_\pm&=\lim_{t\to\pm\infty}\exp[i\mathsf{K}t]\exp[-i\mathsf{K}_1t]\mathsf{P}^\perp\\ &=\left\{1+i\int_0^{\pm\infty}dt\ \exp[i\mathsf{K}t]\mathsf{K}_2\exp[-i\mathsf{K}_1t]\right\}\mathsf{P}^\perp\\ &=\left\{1+i\lim_{\delta\downarrow0}\int_0^{\pm\infty}dt\ \exp[-\delta|t|]\exp[i\mathsf{K}t]\mathsf{K}_2\right.\\ &\quad\left.\times\exp[-i\mathsf{K}_1t]\right\}\mathsf{P}^\perp,\end{aligned} \tag{6.1}$$

with $\mathsf{P}^\perp=\mathsf{P}_{em}^\perp+\mathsf{P}_{aux}$, where $\mathsf{P}_{em}^\perp$ is the projector upon the transverse parts of the electromagnetic fields. Let $\mathcal{A}\subset\mathbb{R}^3$ be the space region occupied by the scatterer and $\mathcal{A}'$ its complement in $\mathbb{R}^3$. Since $\Psi_{\mathcal{A}'}(\mathbf{x})\mathsf{P}_{aux}$ (Ψ is a characteristic function) commutes with K_1 and K_2, $\Psi_{\mathcal{A}'}(\mathbf{x})\mathsf{P}_{aux}=0$ and we have $\Omega_\pm\Psi_{\mathcal{A}'}(\mathbf{x})\mathsf{P}_{aux}=\Psi_{\mathcal{A}'}(\mathbf{x})\mathsf{P}_{aux}$. The existence proof of the remaining parts of $\Omega_\pm$ follows the usual pattern of showing that the norm $||\mathsf{K}_2\exp[-i\mathsf{K}_1t]\mathbf{f}||$ is integrable in t for a dense set of $\mathbf{f}$'s. For $||\mathsf{K}_2\exp[-i\mathsf{K}_1t]\mathsf{P}_{em}^\perp\mathbf{f}||$, see Ref. [20] and concerning $\mathsf{K}_2\exp[-i\mathsf{K}_1t]\Psi_{\mathcal{A}}(\mathbf{x})\mathsf{P}_{aux}\mathbf{f}$ we note that only its first component is nonzero and equals $\int d\omega\,\sigma(\mathbf{x},\omega)\omega\{\cos\omega t\mathbf{f}_4(\omega)+\sin\omega t\mathbf{f}_2(\omega)\}$, where $\mathbf{f}_j$ is the jth component of $\mathbf{f}$. Choosing the $\mathbf{f}_j$'s properly, its norm is an integrable function of t. Note that here the $\mathbf{x}$ dependence of $\sigma(\mathbf{x},\omega)$ and $\Psi_{\mathcal{A}}(\mathbf{x})$ is immaterial, so $\Omega_\pm\mathsf{P}_{aux}$ exists for spatially homogeneous and periodic systems as well. The scattering operator is

$$\begin{aligned}\mathsf{S}&=\Omega_+^*\Omega_-=\Omega_+^*\Omega_++\Omega_+^*\{\Omega_+-\Omega_-\}\\&=\mathsf{P}^\perp+i\Omega_+^*\int_{-\infty}^{+\infty}dt\ \exp[i\mathsf{K}t]\mathsf{K}_2\exp[-i\mathsf{K}_1t]\mathsf{P}^\perp\\&=\mathsf{P}^\perp+i\int_{-\infty}^{+\infty}dt\ \exp[i\mathsf{K}_1t]\Omega_+^*\mathsf{K}_2\exp[-i\mathsf{K}_1t]\mathsf{P}^\perp\\&=\mathsf{P}^\perp+i\int_{-\infty}^{+\infty}dt\ \exp[i\mathsf{K}_1t]\mathcal{T}\exp[-i\mathsf{K}_1t]\mathsf{P}^\perp\\&=\mathsf{P}^\perp+2\pi i\overline{\mathcal{T}}\mathsf{P}^\perp,\end{aligned}\tag{6.2}$$

with $\mathcal{T}=\Omega_+^*\mathsf{K}_2$ and where we used the intertwining property $\Omega_+^*\mathsf{K}=\mathsf{K}_1\Omega_+^*$. We have $\boldsymbol{F}(t)=\exp[-i\mathsf{K}t]\boldsymbol{F}(0)$, and, since initially the wave packet is moving freely, there exists an $\boldsymbol{F}_{in}$ such that

$$\begin{aligned}&\lim_{t\to-\infty}\{\boldsymbol{F}(t)-\exp[-i\mathsf{K}_1t]\boldsymbol{F}_{in}\}\\&\qquad=\lim_{t\to-\infty}\{\exp[-i\mathsf{K}t]\boldsymbol{F}(0)-\exp[-i\mathsf{K}_1t]\boldsymbol{F}_{in}\}=0,\end{aligned}$$

so $\boldsymbol{F}(0)=\Omega_-\boldsymbol{F}_{in}$. Also $\boldsymbol{F}(t)\sim\mathsf{P}_{em}\boldsymbol{F}(t)$, since $\boldsymbol{F}(t)$ becomes purely electromagnetic as $t\to-\infty$. Hence, since P_{em} and K_1 commute, $\boldsymbol{F}_{in}=\mathsf{P}_{em}\boldsymbol{F}_{in}$ and its (electromagnetic) components are transverse.

Let $\Theta(\cdot)$ be the Heaviside step function and $\Psi_{\mathcal{C}_b}(\mathbf{x})=\Theta(\mathbf{e}\cdot\mathbf{e}_\mathbf{x}-a)\Theta(x-b)$, $a=\cos\vartheta_0$, the characteristic function for the set $\mathcal{C}_b$. It defines the projector $\mathsf{P}_{\mathcal{C}_b}=\Psi_{\mathcal{C}_b}(\mathbf{x})$ in $\mathcal{H}$. Then the energy $\mathcal{E}_{\mathcal{C}_b}(t)$, contained in $\mathcal{C}_b$ at time t, is

$$\begin{aligned}\mathcal{E}_{\mathcal{C}_b}(t)&=\tfrac{1}{2}\langle\boldsymbol{F}(t)|\mathsf{P}_\mathcal{C}|\boldsymbol{F}(t)\rangle\\&=\tfrac{1}{2}\langle\boldsymbol{F}_{in}|\Omega_-^*\exp[i\mathsf{K}t]\{\Psi_{\mathcal{C}_b}(\mathbf{x})\mathsf{P}_{aux}+\Psi_{\mathcal{C}_b}(\mathbf{x})\mathsf{P}_{em}\}\\&\quad\times\exp[-i\mathsf{K}t]\Omega_-|\boldsymbol{F}_{in}\rangle.\end{aligned}\tag{6.3}$$

According to Eq. (2.19), $\Psi_{\mathcal{C}_b}(\mathbf{x})\mathsf{P}_{aux}$ commutes with K and K_0 and hence with $\Omega_\pm$. Since $\mathsf{P}_{aux}\boldsymbol{F}_{in}=\mathbf{0}$ we are left with

$$\begin{aligned}\mathcal{E}_{\mathcal{C}_b}(t)&=\tfrac{1}{2}\langle\boldsymbol{F}_{in}|\Omega_-^*\exp[i\mathsf{K}t]\Psi_{\mathcal{C}_b}(\mathbf{x})\mathsf{P}_{em}\exp[-i\mathsf{K}t]\Omega_-|\boldsymbol{F}_{in}\rangle\\&=\tfrac{1}{2}\langle\boldsymbol{F}_{in}|\Omega_-^*\exp[i\mathsf{K}t]\exp[-i\mathsf{K}_1t]\\&\quad\times\exp[+i\mathsf{K}_1t]\Psi_{\mathcal{C}_b}(\mathbf{x})\exp[-i\mathsf{K}_1t]\\&\quad\times\mathsf{P}_{em}\exp[+i\mathsf{K}_1t]\exp[-i\mathsf{K}t]\Omega_-|\boldsymbol{F}_{in}\rangle.\end{aligned}$$

As shown in Appendix D,

$$\begin{aligned}&\lim_{t\to\infty}\exp[+i\mathsf{K}_1t]\Psi_{\mathcal{C}_b}(\mathbf{x})\exp[-i\mathsf{K}_1t]\mathsf{P}_{em}\\&\qquad=\Theta(\mathbf{e}\cdot\mathbf{e}_\mathbf{p}-a)\mathsf{P}_++\Theta(-\mathbf{e}\cdot\mathbf{e}_\mathbf{p}-a)\mathsf{P}_-\\&\qquad=\Theta_+\mathsf{P}_++\Theta_-\mathsf{P}_-,\end{aligned}\tag{6.4}$$

where $\mathsf{P}_\pm\subset\mathsf{P}_{em}$, project upon the eigenspaces of $\mathbf{K}_0=\mathsf{K}_1\mathsf{P}_{em}$ with positive and negative eigenvalues, respectively. They are given explicitly in Appendix D. Note that the single cone in coordinate space gives rise to two cones in momentum space. This is different from the Schrödinger case and is connected with the spectrum of K_1 being the whole real axis, rather than its positive half as in the Schrödinger situation.

The complete sets of orthonormal eigenvectors $\mathbf{f}_{\mathbf{k}j}^\pm\in\mathsf{P}_\pm\mathcal{H}$, $\mathbf{K}_0\mathbf{f}_{\mathbf{k}j}^\pm=\pm k\mathbf{f}_{\mathbf{k}j}^\pm$, $j=1,2$, are ($\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_\mathbf{k}$ are mutually orthogonal unit vectors)

$$\mathbf{f}_{\mathbf{k}j}^\pm(\mathbf{x})=\langle\mathbf{x}|\mathbf{f}_{\mathbf{k}j}^\pm\rangle=(2\pi)^{-3/2}2^{-1/2}\begin{pmatrix}\mathbf{e}_j\\\mathbf{e}_\mathbf{k}\times\mathbf{e}_j\end{pmatrix}\exp[\pm i\mathbf{k}\cdot\mathbf{x}],\tag{6.5}$$

with normalization

$$\langle\mathbf{f}_{\mathbf{k}j}^\pm|\mathbf{f}_{\mathbf{k}'j'}^\pm\rangle=\delta(\mathbf{k}-\mathbf{k}')\,\delta_{jj'}.\tag{6.6}$$

Let the conjugation operator C be defined by

$$(\mathsf{C}\boldsymbol{F})_j(\mathbf{x})=\overline{\boldsymbol{F}_j(\mathbf{x})}.\tag{6.7}$$

Then $\mathbf{f}_{\mathbf{k}j}^-(\mathbf{x})=(\mathsf{C}\mathbf{f}_{-\mathbf{k}j}^+)(\mathbf{x})$, and, since $\mathsf{K}=i\mathsf{N}$ and $\mathsf{K}_n=i\mathsf{N}_n$, $n=1,2$, with N and N_n real operators,

$$\mathsf{CKC}=-\mathsf{K},\mathsf{CK}_n\mathsf{C}=-\mathsf{K}_n,\quad n=1,2.\tag{6.8}$$

For the T operator

$$\begin{aligned}\mathsf{T}(z)&=\mathsf{K}_2+\mathsf{K}_2[z-\mathsf{K}]^{-1}\mathsf{K}_2\\&=[z-\mathsf{K}_2][z-\mathsf{K}]^{-1}[z-\mathsf{K}_2]-[z-\mathsf{K}_2],\end{aligned}\tag{6.9}$$

we then have

$$\mathsf{CT}(z)\mathsf{C}=-\mathsf{T}(-\overline{z}).\tag{6.10}$$

Returning to $\mathcal{E}_{\mathcal{C}_b}(t)$ we obtain, using the fact that S commutes with K_1 and hence with $\mathsf{P}_\pm$,

$$\begin{aligned}\mathcal{E}_\mathcal{C}&=\lim_{t\to\infty}\mathcal{E}_{\mathcal{C}_b}(t)=\tfrac{1}{2}\langle\boldsymbol{F}_{in}|\mathsf{S}^*\{\Theta_+\mathsf{P}_++\Theta_-\mathsf{P}_-\}\mathsf{S}|\boldsymbol{F}_{in}\rangle\\&=\tfrac{1}{2}\langle\boldsymbol{F}_{in}|\mathsf{P}_+\mathsf{S}^*\Theta_+\mathsf{P}_+\mathsf{S}\mathsf{P}_+|\boldsymbol{F}_{in}\rangle+\tfrac{1}{2}\langle\boldsymbol{F}_{in}|\mathsf{P}_-\mathsf{S}^*\Theta_-\mathsf{P}_-\mathsf{S}\mathsf{P}_-|\boldsymbol{F}_{in}\rangle=\mathcal{E}_\mathcal{C}^+-\mathcal{E}_\mathcal{C}^-.\end{aligned}\tag{6.11}$$

Inserting the complete sets $\{\mathbf{f}_{\mathbf{k}'j'}^\pm\}$ we have, assuming $\boldsymbol{F}_{in}\perp\Theta_\pm\mathsf{P}_\pm\mathcal{H}$,

$$\mathcal{E}_{\mathcal{C}}^{\pm}=\tfrac{1}{2}\langle \boldsymbol{F}_{in}|\mathsf{P}_{\pm}\mathsf{S}^{*}\Theta_{\pm}\mathsf{P}_{\pm}\mathsf{S}\mathsf{P}_{\pm}|\boldsymbol{F}_{in}\rangle=\tfrac{1}{2}\langle \boldsymbol{F}_{in}|\mathsf{P}_{\pm}\overline{\mathcal{T}}^{*}\Theta_{\pm}\mathsf{P}_{\pm}\overline{\mathcal{T}}\mathsf{P}_{\pm}|\boldsymbol{F}_{in}\rangle$$

$$=2\pi^{2}\sum_{j'}\int d\mathbf{k}'\ \Theta_{\pm}(\mathbf{e}_{\mathbf{k}'})\langle \boldsymbol{F}_{in}|\,\delta(\pm k'-\mathsf{K}_1)\mathcal{T}^{*}|\mathbf{f}^{\pm}_{\mathbf{k}'j'}\rangle\langle\mathbf{f}^{\pm}_{\mathbf{k}'j'}|\mathcal{T}\delta(\pm k'-\mathsf{K}_1)|\boldsymbol{F}_{in}\rangle.$$

Since

$$\langle\mathbf{f}^{\pm}_{\mathbf{k}'j'}|\mathcal{T}=\langle\mathbf{f}^{\pm}_{\mathbf{k}'j'}|\Omega^{*}_{+}\mathsf{K}_2=\langle\mathbf{f}^{\pm}_{\mathbf{k}'j'}|\mathsf{P}^{\perp}\left\{1-i\lim_{\delta\downarrow 0}\int_0^{+\infty}dt\ \exp[-\delta t]\exp[i\mathsf{K}_1 t]\mathsf{K}_2\exp[-i\mathsf{K}t]\right\}\mathsf{K}_2$$

$$=\langle\mathbf{f}^{\pm}_{\mathbf{k}'j'}|\left\{1-i\lim_{\delta\downarrow 0}\int_0^{+\infty}dt\ \exp[-\delta t]\exp[\pm ik' t]\mathsf{K}_2\exp[-i\mathsf{K}t]\right\}\mathsf{K}_2=\langle\mathbf{f}^{\pm}_{\mathbf{k}j}|\mathsf{T}(\pm k'+i0),$$

we arrive at

$$\mathcal{E}_{\mathcal{C}}^{\pm}=2\pi^{2}\sum_{j'}\int d\mathbf{k}'\ \Theta_{\pm}(\mathbf{e}_{\mathbf{k}'})\langle \boldsymbol{F}_{in}|\,\delta(\pm k'-\mathsf{K}_1)\mathsf{T}(\pm k'-i0)|\mathbf{f}^{\pm}_{\mathbf{k}'j'}\rangle\langle\mathbf{f}^{\pm}_{\mathbf{k}'j'}|\mathsf{T}(\pm k'+i0)\,\delta(\pm k'-\mathsf{K}_1)|\boldsymbol{F}_{in}\rangle.$$

Taking $\boldsymbol{F}_{in}(\mathbf{x})$ real, so $|\boldsymbol{F}_{in}\rangle=\mathsf{C}|\boldsymbol{F}_{in}\rangle$,

$$\mathcal{E}_{\mathcal{C}}^{-}=2\pi^{2}\sum_{j'}\int d\mathbf{k}'\ \Theta_{-}(\mathbf{e}_{\mathbf{k}'})\langle \boldsymbol{F}_{in}|\mathsf{C}\delta(-k'-\mathsf{K}_1)\mathsf{T}(-k'-i0)|\mathbf{f}^{-}_{\mathbf{k}'j'}\rangle\langle\mathbf{f}^{-}_{\mathbf{k}'j'}|\mathsf{T}(k'+i0)\,\delta(-k'-\mathsf{K}_1)\mathsf{C}|\boldsymbol{F}_{in}\rangle$$

$$=2\pi^{2}\sum_{j'}\int d\mathbf{k}'\ \Theta_{-}(\mathbf{e}_{\mathbf{k}'})\langle \boldsymbol{F}_{in}|\,\delta(k'-\mathsf{K}_1)\mathsf{T}(k'-i0)|\mathbf{f}^{+}_{-\mathbf{k}'j'}\rangle\langle\mathbf{f}^{+}_{-\mathbf{k}'j'}|\mathsf{T}(k'+i0)\,\delta(k'-\mathsf{K}_1)|\boldsymbol{F}_{in}\rangle$$

$$=2\pi^{2}\sum_{j'}\int d\mathbf{k}'\ \Theta_{+}(\mathbf{e}_{\mathbf{k}'})\langle \boldsymbol{F}_{in}|\,\delta(k'-\mathsf{K}_1)\mathsf{T}(k'-i0)|\mathbf{f}^{+}_{\mathbf{k}'j'}\rangle\langle\mathbf{f}^{+}_{\mathbf{k}'j'}|\mathsf{T}(k'+i0)\,\delta(k'-\mathsf{K}_1)|\boldsymbol{F}_{in}\rangle=\mathcal{E}_{\mathcal{C}}^{+},$$

and

$$\mathcal{E}_{\mathcal{C}}=(2\pi)^{2}\sum_{j'}\int d\mathbf{k}'\Theta_{+}(\mathbf{e}_{\mathbf{k}'})\langle \boldsymbol{F}_{in}|\,\delta(k'-\mathsf{K}_1)\mathsf{T}(k'-i0)|\mathbf{f}^{+}_{\mathbf{k}'j'}\rangle\langle\mathbf{f}^{+}_{\mathbf{k}'j'}|\mathsf{T}(k'+i0)\,\delta(k'-\mathsf{K}_1)|\boldsymbol{F}_{in}\rangle. \tag{6.12}$$

Next we make a special choice for $\boldsymbol{F}_{in}$. Let $\Delta=[-\delta,\delta]$, $\delta>0$ and $\Psi_{\Delta}(\ )$ its characteristic function. We set

$$\boldsymbol{F}_{in}(\mathbf{x})=\tfrac{1}{2}\Psi_{\Delta}(\mathbf{e}_{\mathbf{k}}\cdot\mathbf{x})\{\mathbf{f}^{+}_{\mathbf{k}j}(\mathbf{x})+\mathbf{f}^{-}_{\mathbf{k}j}(\mathbf{x})\}=(2\pi)^{-3/2}2^{-1/2}\Psi_{\Delta}(\mathbf{e}_{\mathbf{k}}\cdot\mathbf{x})\begin{pmatrix}\mathbf{e}_j\\ \mathbf{e}_{\mathbf{k}}\times\mathbf{e}_j\end{pmatrix}\cos\mathbf{k}\cdot\mathbf{x}. \tag{6.13}$$

Note that $\boldsymbol{F}_{in}(\mathbf{x})$ is real and $\boldsymbol{F}_{in}\perp\mathsf{P}_{\mathcal{C}_b}\mathcal{H}$ for b sufficiently large. Also $\boldsymbol{F}_{in}\perp\Theta_{\pm}\mathsf{P}_{\pm}\mathcal{H}$ by taking $\mathbf{k}$ outside the cone $\mathcal{C}$. Using

$$\langle\mathbf{f}^{+}_{\mathbf{k}'j'}|\boldsymbol{F}_{in}\rangle=\langle\boldsymbol{F}_{in}|\mathbf{f}^{-}_{\mathbf{k}'j'}\rangle=(2\pi)^{-1}\delta(\mathbf{e}_j\cdot\mathbf{k}')\,\delta(\mathbf{e}_{\mathbf{k}}\times\mathbf{e}_j\cdot\mathbf{k}')\,\delta(\mathbf{e}_{\mathbf{k}}\cdot\mathbf{k}')\,\zeta(k,k',\delta)\,\delta_{jj'}, \tag{6.14}$$

where

$$\zeta(k,k',\delta)=\pi^{-1}\left\{\frac{\sin(k-k')\,\delta}{k-k'}+\frac{\sin(k+k')\,\delta}{k+k'}\right\}, \tag{6.15}$$

we obtain, by inserting complete sets,

$$\exp[-i\mathbf{K}_0 t]\boldsymbol{F}_{in}(\mathbf{x})=\tfrac{1}{4}\pi^{-5/2}\int_0^{\infty}dk'\ \xi(k,k',\delta)\times\begin{pmatrix}\mathbf{e}_j\\ \mathbf{e}_{\mathbf{k}}\times\mathbf{e}_j\end{pmatrix}\cos(k'\mathbf{e}_{\mathbf{k}}\cdot\mathbf{x}-k't), \tag{6.16}$$

a wave that moves towards the scatterer if $\mathbf{k}$ points into its direction. We obtain the scattering cross section by dividing $\mathcal{E}_C=\mathcal{E}_C(\delta)$ by the total incident flux $\Phi(\delta)$ that has passed through a plane orthogonal to $\mathbf{k}$ in the limit $\delta\to\infty$ (where the incident wave becomes a plane wave). Here

$$\Phi(\delta)=\int_{-\infty}^{+\infty}dt\ \boldsymbol{E}(\mathbf{x},t)\times\boldsymbol{B}(\mathbf{x},t)\ \cdot\mathbf{e}_{\mathbf{k}}, \tag{6.17}$$

with $\boldsymbol{E}(\mathbf{x},t)$ and $\boldsymbol{B}(\mathbf{x},t)$ given by Eq. (6.16). A little calculation shows that

$$\Phi(\delta)\overset{\delta\to\infty}{\sim}\tfrac{1}{2}(2\pi)^{-3}\delta. \tag{6.18}$$

Again using Eq. (6.14),

$$\delta(k'-\mathsf{K}_1)|\boldsymbol{F}_{in}\rangle=(2\pi)^{-1}\zeta(k,k',\delta)|\mathbf{f}^+_{k'\mathbf{e}_\mathbf{k}j}\rangle.$$

Since for smooth functions $g(k)$,

$$\int dk'\ \zeta(k,k',\delta)^2 g(k') \overset{\delta\to\infty}{\sim} \delta g(k),$$

we have

$$\begin{aligned}\mathcal{E}_\mathcal{C}(\delta)&=\sum_{j'}\int d\mathbf{k}'\ \zeta(k,k',\delta)^2\Theta_+(\mathbf{e}_{\mathbf{k}'})\\&\quad\times|\langle\mathbf{f}^+_{\mathbf{k}'j'}|\mathsf{T}(k'+i0)|\mathbf{f}^+_{k'\mathbf{e}_\mathbf{k}j}\rangle|^2\\&\overset{\delta\to\infty}{\sim}\delta\pi k^2\sum_{j'}\int d\mathbf{e}_{\mathbf{k}'}\ \Theta_+(\mathbf{e}_{\mathbf{k}'})\\&\quad\times|\langle\mathbf{f}^+_{\mathbf{k}'j'}|\mathsf{T}(k+i0)|\mathbf{f}^+_{\mathbf{k}j}\rangle|^2\\&=\delta\pi\sum_{j'}\int d\mathbf{e}'\ \Theta_+(\mathbf{e}')|f(\mathbf{k}j\to\mathbf{k}'j')|^2,\end{aligned}$$

where in the last two lines $\mathbf{k}'=k\mathbf{e}_{\mathbf{k}'}=k\mathbf{e}'$ and

$$f(\mathbf{k}j\to\mathbf{k}'j')=k\langle\mathbf{f}^+_{\mathbf{k}'j'}|\mathsf{T}(k+i0)|\mathbf{f}^+_{\mathbf{k}j}\rangle \tag{6.19}$$

is the scattering amplitude for the transition $\mathbf{k}j\to\mathbf{k}'j'$. Now

$$\begin{aligned}\mathcal{E}_\mathcal{C}(\delta)/\Phi(\delta)&\overset{\delta\to\infty}{\to}(2\pi)^4\sum_{j'}\int d\mathbf{e}'\Theta_+(\mathbf{e}')|f(\mathbf{k}j\to\mathbf{k}'j')|^2\\&=\sigma(\mathbf{k},j\to\mathcal{C}),\end{aligned} \tag{6.20}$$

the cross section for scattering into the cone $\mathcal{C}$. From this we see that the differential cross section for scattering into the direction $\mathbf{e}$ is

$$\sigma(\mathbf{k}j\to k\mathbf{e}j')=(2\pi)^4|f(\mathbf{k}j\to k\mathbf{e}j')|^2, \tag{6.21}$$

summed over the final polarization directions j'.

We can simplify the above expressions further by noting that only the restriction of T to $\mathsf{P}_+\mathcal{H}\subset\mathsf{P}_{em}\mathcal{H}$ contributes. As shown in Appendix D,

$$\mathsf{P}_{em}z\mathsf{T}(z)\mathsf{P}_{em}=\mathsf{t}(z)\mathsf{P}_{el},$$

$$\begin{aligned}\mathsf{t}(z)&=-z^2\hat\chi(z)+z^4\hat\chi(z)[z^2\varepsilon(z)-\mathsf{H}_0]^{-1}\hat\chi(z)\\&=-z^2\hat\chi(z)+z^4\hat\chi(z)\mathsf{R}_e(z^2)\hat\chi(z),\end{aligned} \tag{6.22}$$

where $\mathsf{P}_{el}=\{(\mathsf{P}_{el})_{kl}\}=\{\delta_{k1}\delta_{l1}\}$ projects upon the first (electric field) component of $\boldsymbol{F}$. Thus, with $\mathbf{f}^\pm_{\mathbf{k}j1}$ the electric (first) component of $\mathbf{f}^\pm_{\mathbf{k}j}$,

$$f(\mathbf{k}j\to\mathbf{k}'j')=\langle\mathbf{f}^+_{\mathbf{k}'j'1}|\mathsf{t}(k+i0)|\mathbf{f}^+_{\mathbf{k}j1}\rangle. \tag{6.23}$$

Note that $\mathsf{t}(z)$ has the usual T-matrix structure, the potential being $-z^2\hat\chi(z)$. $\mathsf{t}(z)$, as given by Eq. (6.22) is often taken as the starting point for the description of electromagnetic scattering. Here we have presented a precise justification. For spherically symmetric systems a further reduction of $\mathsf{t}(z)$ can be made. A systematic approach has recently been discussed by the author [23]. If the system is an absorptive Mie sphere the formulas given there for conservative systems are readily adapted to the present situation.

VII. TRANSITION RADIATION

Our second application makes use of the quantized formalism developed in Sec. V. It deals with the generation of photons caused by the passage of fast electrons through dielectric layers. We distinguish Čerenkov radiation and the less well known transition radiation. Čerenkov radiation is generated throughout the medium provided the speed of the charged particle exceeds that of the radiation in the medium, whereas this condition is not required for transition radiation. The latter is created at places where a steep gradient in $\varepsilon(\mathbf{x})$ occurs, typically at the interfaces in stacks consisting of parallel layers with different electric permeability. At present there is some interest in the use of transition radiation as an x-ray source [12] and for technological reasons strongly absorptive and dispersive materials are considered. We apply the present formalism for a quantum description of the phenomenon. Thus we consider a model of an energetic charged particle (typically in the MeV region) without spin (spin does not play a significant role and can safely be neglected), which moves through a finite piece of absorptive dielectric. In actual experiments only single photon production is observed, so we can restrict ourselves to a calculation to first order in the fine structure constant, i.e., in e. Since we are dealing with fast electrons, we use the expression for the energy of a relativistic scalar particle

$$\begin{aligned}H_m+H_{int}&=[(\mathbf{p}-e\boldsymbol{A}(\mathbf{x}))^2+m^2]^{1/2}\\&=[\mathbf{p}^2+m^2]^{1/2}-(e/2)[\mathbf{p}^2+m^2]^{-1/4}\\&\quad\times\{\mathbf{p}\cdot\boldsymbol{A}(\mathbf{x})+\boldsymbol{A}(\mathbf{x})\cdot\mathbf{p}\}[\mathbf{p}^2+m^2]^{-1/4}+O(e^2)\\&=T(\mathbf{p})-(e/2)T(\mathbf{p})^{-1/2}\{\mathbf{p}\cdot\boldsymbol{A}(\mathbf{x})+\boldsymbol{A}(\mathbf{x})\cdot\mathbf{p}\}\\&\quad\times T(\mathbf{p})^{-1/2}+O(e^2)\\&=T(\mathbf{p})+W(\boldsymbol{A})+O(e^2)\approx T(\mathbf{p})+W(\boldsymbol{A}),\end{aligned} \tag{7.1}$$

where $\boldsymbol{A}(\mathbf{x})$ is given by Eq. (5.4) and $\mathbf{x}$ and $\mathbf{p}$ are the electron coordinate and momentum, respectively. We shall consider two cases, finite dielectrics and stacks of parallel layers with incident electron momentum normal to the boundary surface. Both can be treated as scattering situations, but, due to the translation invariance in two orthogonal directions, the second case slightly differs from the first. The full Hamiltonian, acting in $\mathcal{H}=\mathcal{H}_m\otimes\mathcal{H}_f$, where $\mathcal{H}_m$ and $\mathcal{H}_f$ are the Hilbert spaces for the material system and fields, respectively, is now

$$H=T(\mathbf{p})+H_f+W(\boldsymbol{A}). \tag{7.2}$$

Initially an electron coupled to the free electromagnetic field moves towards the target material and finally we again have an asymptotic motion determined by the coupled electron-free field Hamiltonian

$$H^{(0)}=T(\mathbf{p})+H_f^{(0)}+W(\boldsymbol{A}^{(0)}), \tag{7.3}$$

with $H_f^{(0)}$ and $\boldsymbol{A}^{(0)}$ given in Sec. V. However, as discussed in Sec. V, they do not act in the same Hilbert space since the Fock spaces are different. For the state vector $\psi(t)$ we do not have $\psi(t)-\exp[-iH^{(0)}t]\psi_{in}\to 0$ as $t\to-\infty$, but rather $\psi(t)-\Omega_F\exp[-iH^{(0)}t]\psi_{in}=\psi(t)-\exp[-iH^{(1)}t]\Omega_F\psi_{in}\to 0$, so $\psi(0)=\Omega_-\Omega_F\psi_{in}$. Here (see Sec. V for notation)

$$H^{(1)}=\Omega_F H^{(0)}\Omega_F^*=T(\mathbf{p})+H_f+W(\boldsymbol{A}^{(1)}), \tag{7.4}$$

and the scattering and wave operators for the process at hand are

$$S=\Omega_+^*\Omega_-,\quad \Omega_\pm=\lim_{t\to\pm\infty}\exp[iHt]\exp[-iH^{(1)}t]. \tag{7.5}$$

Note that the interaction $H-H^{(1)}=W(\boldsymbol{A}-\boldsymbol{A}^{(1)})$ is of order e. Let P be a projector, such that $\lim_{t\to\infty}\exp[iH^{(0)}t]P\exp[-iH^{(0)}t]=P_\infty$ exists. Then $P^{(1)}=\Omega_F P_\infty\Omega_F^*$ commutes with $H^{(1)}$ and the probability to find the system in $P^{(1)}\mathcal{H}$ at time t is

$$\begin{aligned}\mathcal{W}_P(t)&=\langle\psi_{in}|\Omega_F^*\Omega_-{}^*\exp[iHt]P^{(1)}\exp[-iHt]\Omega_-\Omega_F|\psi_{in}\rangle\\&=\langle\psi_{in}|\Omega_F^*\Omega_-{}^*\exp[iHt]\\&\quad\times\exp[-iH^{(1)}t]P^{(1)}\exp[iH^{(1)}t]\\&\quad\times[-iHt]\Omega_-\Omega_F|\psi_{in}\rangle\\&\overset{t\to\infty}{\to}\langle\psi_{in}|\Omega_F^*S^*P^{(1)}S\Omega_F|\psi_{in}\rangle=\mathcal{W}_P.\end{aligned} \tag{7.6}$$

Assuming that $\Omega_F|\psi_{in}\rangle\perp P^{(1)}\mathcal{H}$ this becomes

$$\begin{aligned}\mathcal{W}_P&=\langle\psi_{in}|\Omega_F^*\{1-2\pi i(\overline{\mathcal{T}})^*\}P^{(1)}\{1+2\pi i\overline{\mathcal{T}}\}\Omega_F|\psi_{in}\rangle\\&=(2\pi)^2\langle\psi_{in}|\Omega_F^*(\overline{\mathcal{T}})^*P^{(1)}\overline{\mathcal{T}}\Omega_F|\psi_{in}\rangle,\end{aligned}$$

where

$$\begin{aligned}\overline{\mathcal{T}}&=(2\pi)^{-1}\int_{-\infty}^{+\infty}dt\,\exp[iH^{(1)}t](\Omega_+)^*\{W(\boldsymbol{A})-W(\boldsymbol{A}^{(1)})\}\\&\quad\times\exp[-iH^{(1)}t]\\&=(2\pi)^{-1}\int_{-\infty}^{+\infty}dt\,\exp[iH^{(2)}t]\{W(\boldsymbol{A})-W(\boldsymbol{A}^{(1)})\}\\&\quad\times\exp[-iH^{(2)}t]+O(e^2)\\&=\overline{\mathcal{T}_1}+O(e^2),\end{aligned} \tag{7.7}$$

with

$$H^{(2)}=T(\mathbf{p})+H_f. \tag{7.8}$$

Hence, to leading (i.e., second) order in e,

$$\mathcal{W}_P=(2\pi)^2\langle\psi_{in}|\Omega_F^*(\overline{\mathcal{T}_1})^*P^{(1)}\overline{\mathcal{T}_1}\Omega_F|\psi_{in}\rangle.$$

However, since $\overline{\mathcal{T}_1}$ is of first order in e we can take $P^{(1)}$ to zeroth order in e, i.e., a projector commuting with $H^{(2)}$, whereas for ψ_{in} we can take $\psi_{in}=\psi_m\otimes\psi_{vac}$ with ψ_m the initial electron state and ψ_{vac} the vacuum state for the fields. This is typical for the approximation we have made. For $\psi_{in}=\psi_m\otimes\psi_{vac}$ the expression $\psi(t)-\Omega_F\exp[-iH^{(0)}t]\psi_{in}$ no longer tends to zero to higher order in e. Since Ω_F reduces to the unit operator on the zeroth Fock layer we have $\Omega_F|\psi_{in}\rangle=|\psi_{in}\rangle$, so that

$$\mathcal{W}_P=(2\pi)^2\langle\psi_{in}|(\overline{\mathcal{T}_1})^*P^{(1)}\overline{\mathcal{T}_1}|\psi_{in}\rangle. \tag{7.9}$$

We are interested in photon production, so we consider a detector that measures the photons emerging in a cone $\mathcal{C}_b$ (for the definition of objects such as $\mathcal{C}_b$, Θ_+, and Ψ_Δ, see Sec. VI) in coordinate space and does not measure the auxiliary fields. In general the translation to a projector, which now acts in the Fock space connected with the fields is far from trivial. The second problem is to relate the cone $\mathcal{C}_b$ in coordinate space to the cone $\mathcal{C}$ in momentum space. However, since $\overline{\mathcal{T}_1}$ only contains creation operators to linear order and ψ_{in} contains the vacuum state, $P^{(1)}$ is restricted to the first Fock layer. Thus, taking

$$P=\Psi_{\mathcal{C}_b}(\mathbf{x}')\begin{pmatrix}1&0\\0&0\end{pmatrix}=\Psi_{\mathcal{C}_b}(\mathbf{x}')P_1 \tag{7.10}$$

for the restriction of P to the first Fock layer, we obtain (note that here and below $\mathbf{x}'$ and $\mathbf{p}'$ are operators in $\mathcal{H}_e^{(0)}$ and not electron coordinate and momentum)

$$P_\infty=\lim_{t\to\infty}\exp[i\mathsf{H}_e^{(0)}t]P\exp[-i\mathsf{H}_e^{(0)}t]=\Theta_+(\mathbf{e}\cdot\mathbf{e}_{\mathbf{p}'})P_1, \tag{7.11}$$

and $P^{(1)}=\Omega_F P_\infty\Omega_F^*$ reduces to

$$P^{(1)}=\Omega\Theta_+(\mathbf{e}\cdot\mathbf{e}_{\mathbf{p}'})P_1\Omega^* \tag{7.12}$$

on the first Fock layer. Let the complete orthonormal sets of eigenvectors of $T(\mathbf{p})$ be $\{|\mathbf{k}\rangle\}$, so $\langle\mathbf{x}|\mathbf{k}\rangle=(2\pi)^{-3/2}\exp[i\mathbf{k}\cdot\mathbf{x}]$ and that of $\mathsf{H}_0=\mathbf{p}^2\boldsymbol{\Delta}_\mathbf{p}$ be $\{\mathbf{u}_{1\mathbf{k}j}^{(0)}(\mathbf{x})=(2\pi)^{-3/2}\mathbf{e}_j\exp[i\mathbf{k}\cdot\mathbf{x}]\}$, where $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_\mathbf{k}$ are mutually orthogonal (see also Sec. V). Since P_1 in $P_\infty=\Theta_+(\mathbf{e}\cdot\mathbf{e}_{\mathbf{p}'})P_1$ projects away the auxiliary components of the eigenvectors $\mathbf{u}^{(0)}$ of $\mathsf{H}_e^{(0)}$, we have, with

$$\mathbf{u}_{\mathbf{k}j}^{(0)}=\begin{pmatrix}\mathbf{u}_{1\mathbf{k}j}^{(0)}\\0\end{pmatrix},$$

that

$$\begin{aligned}P^{(1)}&=\sum_{j_2}\int d\mathbf{k}_1\int d\mathbf{k}_2\Omega|\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}^{(0)}\rangle\Theta_+(\mathbf{e}\cdot\mathbf{e}_{\mathbf{k}_2})\langle\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}^{(0)}|\Omega^*\\&=\sum_{j_2}\int d\mathbf{k}_1\int d\mathbf{k}_2|\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}\rangle\Theta_+(\mathbf{e}\cdot\mathbf{e}_{\mathbf{k}_2})\langle\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}|.\end{aligned}$$

Noting that $H^{(2)}|\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}\rangle=\{T(\mathbf{k}_1)+k_2\}|\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}\rangle$, we now obtain

$$\mathcal{W}_P=(2\pi)^2\sum_{j_2}\int d\mathbf{k}_1\int d\mathbf{k}_2\langle\psi_{in}|\delta(H^{(2)}-T(\mathbf{k}_1)-k_2)\mathcal{T}_1^*|\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}\rangle\Theta_+(\mathbf{e}\cdot\mathbf{e}_{\mathbf{k}_2})\langle\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}|\mathcal{T}_1\delta(H^{(2)}-T(\mathbf{k}_1)-k_2)|\psi_{in}\rangle$$

$$=(2\pi)^2\sum_{j_2}\int d\mathbf{k}_1\int d\mathbf{k}_2\langle\psi_{in}|\delta(T(\mathbf{p})-T(\mathbf{k}_1)-k_2)\mathcal{T}_1^*|\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}\rangle\Theta_+(\mathbf{e}\cdot\mathbf{e}_{\mathbf{k}_2})\langle\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}|\mathcal{T}_1\delta(T(\mathbf{p})-T(\mathbf{k}_1)-k_2)|\psi_{in}\rangle$$

$$=(2\pi)^2\sum_{j_2}\int d\mathbf{k}_2\Theta_+(\mathbf{e}\cdot\mathbf{e}_{\mathbf{k}_2})\int d\mathbf{k}_1|X(\mathbf{k}_1,\mathbf{k}_2,j_2,\psi_{in})|^2=\sum_{j_2}\int d\mathbf{k}_2\Theta_+(\mathbf{e}\cdot\mathbf{e}_{\mathbf{k}_2})w(\mathbf{k}_2,j_2),\tag{7.13}$$

where $w(\mathbf{k}_2,j_2)$ is the probability density for the transition into the state $\mathbf{k}_2,j_2$ and

$$X=\langle\mathbf{k}_1\mathbf{u}_{\mathbf{k}_2j_2}|\mathcal{T}_1\delta(T(\mathbf{p})-T(\mathbf{k}_1)-k_2)|\psi_{in}\rangle\{\varepsilon_1^{-1/2}\overline{\mathbf{u}}_{1\mathbf{k}'j'}(\mathbf{x})-\overline{\mathbf{u}}^{(0)}_{1\mathbf{k}'j'}(\mathbf{x})\}|\psi_{vac}\rangle\cdot(\mathbf{k}_1+\mathbf{p})\,\delta(T(\mathbf{p})-T(\mathbf{k}_1)-k_2)|\psi_m\rangle$$

$$=-(e/2)(2k_2)^{-1/2}T(\mathbf{k}_1)^{-1/2}[T(\mathbf{k}_1)+k_2]^{-1/2}\langle\mathbf{k}_1|\{\varepsilon_1^{-1/2}\overline{\mathbf{u}}_{1\mathbf{k}_2j_2}-\overline{\mathbf{u}}^{(0)}_{1\mathbf{k}_2j_2}\}\cdot(\mathbf{k}_1+\mathbf{p})\,\delta(T(\mathbf{p})-T(\mathbf{k}_1)-k_2)|\psi_m\rangle.\tag{7.14}$$

For $|\psi_m\rangle$ we take

$$|\psi_m\rangle=\Psi_{\mathcal{A}}(\mathbf{x}^\perp)\Psi_\Delta(\mathbf{e}_\mathbf{k}\cdot\mathbf{x})|\mathbf{k}\rangle,\tag{7.15}$$

where $\mathbf{x}^\perp$ is the component of $\mathbf{x}$ orthogonal to $\mathbf{k}$ (we shall take the X_3 axis along $\mathbf{k}$ in the following, so $\mathbf{k}=k\mathbf{e}_3$, $k>0$), $\mathcal{A}=[-\gamma,\gamma]\times[-\gamma,\gamma]$ and $\Delta=[-\delta,\delta]$. Then $|\psi_m\rangle$ tends to the plane wave state $|\mathbf{k}\rangle$ as $\gamma,\delta\to\infty$. Now $\langle\mathbf{a}|\psi_m\rangle=f_\gamma(\mathbf{a}^\perp)g_\delta(k-a_3)$, where $f_\gamma(\mathbf{a}^\perp)=[\sin(a_1\gamma)/\pi a_1]\sin(a_2\gamma)/\pi a_2$ for finite γ and $f_\gamma(\mathbf{a}^\perp)=\delta(\mathbf{a}^\perp)$ for $\gamma=\infty$, whereas $g_\delta(b)=\sin(b\delta)/\pi b$.

At this point we have to distinguish between the two cases. For layered stacks we can take the normalized state $|\hat{\psi}_m\rangle=\pi^{3/2}\gamma^{-1}\delta^{-1/2}|\psi_m\rangle$ and take the limit $\gamma,\delta\to\infty$ in $w=w_{\gamma\delta}$. Although ψ_m becomes spread out in coordinate space, the electron will always hit the stack if it propagates in the right direction. This is not the case with a finite target. Here $w_{\gamma\delta}$ would tend to zero, since the probability that the electron hits the target tends to zero as the normalized state spreads out. Thus we set $\gamma=\infty$. Then ψ_m is no longer square integrable as $\gamma\to\infty$ and does not represent a single electron but rather a pulsed beam of electrons with width 2δ. Then the current due to the free motion generated by $T(\mathbf{p})$,

$$\mathbf{j}(\mathbf{x},t)=\langle\mathbf{x}|Y(t)\mathbf{p}+\mathbf{p}Y(t)|\mathbf{x}\rangle,$$

$$\langle\mathbf{k}_1|Y(t)|\mathbf{k}_2\rangle=[k_1^2-k_2^2]^{-1}[T(\mathbf{k}_1)-T(\mathbf{k}_2)]\exp[-i\{T(\mathbf{k}_1)-T(\mathbf{k}_2)\}t]\langle\mathbf{k}_1|\psi_m\rangle\times\langle\psi_m|\mathbf{k}_2\rangle\tag{7.16}$$

is still finite and so is

$$\mathbf{\Phi}_\delta(\mathbf{x})=\int_{-\infty}^{\infty}dt\;\mathbf{j}(\mathbf{x},t)\overset{\delta\to\infty}{\sim}\delta(2\pi)^{-2}\pi^{-1}\mathbf{e}_3=\Phi_\delta\mathbf{e}_3.\tag{7.17}$$

It represents the total flux that has passed through a unit surface orthogonal to $\mathbf{k}$ in the course of time. The cross section is then obtained as the ratio w_δ/Φ_δ as $\delta\to\infty$. Thus, for finite dielectrics, taking $\gamma=\infty$,

$$X\overset{\delta\to\infty}{\sim}-e(2k_2)^{-1/2}T(\mathbf{k}_1)^{-1/2}[T(\mathbf{k}_1)+k_2]^{1/2}\langle\mathbf{k}_1|\{\varepsilon_1^{-1/2}\overline{\mathbf{u}}_{1\mathbf{k}_2j_2}-\overline{\mathbf{u}}^{(0)}_{1\mathbf{k}_2j_2}\}|\mathbf{k}\rangle\cdot(\mathbf{k}_1+\mathbf{k})\int dk_{33}\delta(k_{33}^2-k_0^2)g_\delta(k-k_{33}),\tag{7.18}$$

where $k_0>0$ is determined by

$$[k_0^2+m^2]^{-1/2}=[k_1^2+m^2]+k_2.\tag{7.19}$$

Then

$$w=w_\delta\overset{\delta\to\infty}{\sim}\delta\frac{\pi e^2k_1}{2k_2k}\int d\mathbf{e}_1|\langle\mathbf{k}_1|\varepsilon_1^{-1/2}\overline{\mathbf{u}}_{1\mathbf{k}_2j_2}|\mathbf{k}\rangle\cdot(\mathbf{k}_1+\mathbf{k})|^2,\tag{7.20}$$

where $\mathbf{e}_1=\mathbf{e}_{\mathbf{k}_1}$ and k_1 is determined by $[k^2+m^2]^{1/2}=[k_1^2+m^2]^{1/2}+k_2$ and the cross section $\sigma(\mathbf{k}\to\mathbf{k}_2,j_2)$ becomes

$$\sigma(\mathbf{k}\to\mathbf{k}_2,j_2)=\lim_{\delta\to\infty}\frac{w_\delta}{\Phi_\delta}=\frac{2\pi^4e^2k_1}{k_2k}\times\int d\mathbf{e}_1|\langle\mathbf{k}_1|\varepsilon_1^{-1/2}\overline{\mathbf{u}}_{1\mathbf{k}_2j_2}|\mathbf{k}\rangle\cdot(\mathbf{k}_1+\mathbf{k})|^2.\tag{7.21}$$

Note that the contribution from $\overline{\mathbf{u}}^{(0)}_{1\mathbf{k}_2j_2}$ has disappeared.

Next we consider stacks with finite width consisting of parallel layers of dielectric materials with boundary surfaces orthogonal to $\mathbf{k}//\mathbf{X}_3$. Now $\varepsilon_1(\mathbf{x})$ and $\chi(\mathbf{x},t)$ only depend on x_3 and the mode functions are of the form $\mathbf{u}_{1\mathbf{k}_2j_2}(\mathbf{x})=\exp[i\mathbf{k}^\perp\cdot\mathbf{x}^\perp]\mathbf{v}_{\mathbf{k}_2j_2}(x_3)$ and $\mathbf{u}^{(0)}_{1\mathbf{k}_2j_2}=\exp[i\mathbf{k}^\perp\cdot\mathbf{x}^\perp]\mathbf{v}^{(0)}_{\mathbf{k}_2j_2}(x_3)$. We set $\phi_{\mathbf{k}_2j_2}(x_3)=\varepsilon_1(x_3)^{-1/2}\overline{\mathbf{u}}_{1\mathbf{k}_2j_2}(\mathbf{x})-\overline{\mathbf{u}}^{(0)}_{1\mathbf{k}_2j_2}(\mathbf{x})$. In this case we have

$$X \overset{\gamma,\delta\to\infty}{\sim} -e(2k_2)^{-1/2}T(\mathbf{k}_1)^{-1/2}[T(\mathbf{k}_1)+k_2]^{1/2}f_\gamma(\mathbf{k}_3^\perp) \times\langle k_{13}|\phi_{\mathbf{k}_2 j_2}|k\rangle\cdot(\mathbf{k}_1+\mathbf{k}_3^\perp+k\mathbf{e}_3)(2k_0)^{-1} \times\{g_\delta(k-k_0)+g_\delta(k+k_0)\}|_{\mathbf{k}_3^\perp=\mathbf{k}_1^\perp+\mathbf{k}_2^\perp}, \tag{7.22}$$

where $\langle x_3|k\rangle=(2\pi)^{-1/2}\exp[ikx_3]$. Then

$$w_{\gamma\delta} \overset{\gamma,\delta\to\infty}{\sim} \gamma^2\delta\frac{e^2}{2\pi k_{13}k} \times|\langle k_{13}|\varepsilon_1(x_3)^{-1/2}\mathbf{v}_{\mathbf{k}_2 j_2}(x_3)|k\rangle\cdot(\mathbf{k}_1+\mathbf{k})|^2. \tag{7.23}$$

Here $\mathbf{k}_1^\perp=-\mathbf{k}_2^\perp$ and k_{13} is determined by $[k^2+m^2]^{1/2}=[k_{13}^2+m^2]^{1/2}+k_2$. Defining $\sigma(\mathbf{k}\to\mathbf{k}_2,j_2)$ as the ratio $w_{\gamma\delta}/\langle\psi_m|\psi_m\rangle$ (i.e., in $w_{\gamma\delta}$ the state ψ_m is replaced by its normalized version $\hat{\psi}_m$) in the limit $\gamma,\delta\to\infty$:

$$\sigma(\mathbf{k}\to\mathbf{k}_2,j_2)=\lim_{\gamma,\delta\to\infty} w_{\gamma\delta}/\langle\psi_m|\psi_m\rangle =\frac{e^2\pi^2}{2k_{13}k}\langle k_{13}|\varepsilon_1(x_3)^{-1/2}\mathbf{v}_{\mathbf{k}_2 j_2}(x_3)|k\rangle\cdot(\mathbf{k}_1+\mathbf{k})|^2. \tag{7.24}$$

The detailed calculations leading to Eqs. (7.21) and (7.24) are not given here but are available from the author [24]. Our final results describe both Čerenkov and transition radiation. We have calculated the Čerenkov and transition radiation yield for the case of stacks of parallel layers [25]. The results agree with those obtained from the classical ME with the charged particle entering through a given external current, provided the photon energy is much smaller than the initial electron energy. In the classical case the electron velocity is usually assumed to be constant, a condition that is not required in the present setup: The latter can also handle large photon energies. For a discussion of Čerenkov radiation generated in transparent media and including spin effects, see Ref. [26].

VIII. ATOMIC RADIATIVE DECAY AND THE DENSITY OF STATES

In Ref. [15] the author studied the decay of an excited atom embedded in a conservative dielectric under a number of simplifying assumptions. Here we do the same for the lossy case. Thus we consider a hydrogen atom with an infinitely heavy nucleus at the position $\mathbf{X}$. For the fields we make the long wavelength approximation, i.e., in Eq. (5.9) $\varepsilon_1(\mathbf{x})$ and $\hat{\chi}(\mathbf{x},0)$ are taken in $\mathbf{x}=\mathbf{X}$ as is the vector potential $\boldsymbol{A}(\mathbf{x})$. In addition we neglect all atomic states except the $1s$ and $2p$ states. The coupling with the electromagnetic field causes the $2p$ states to turn into resonances, i.e., their eigenvalues acquire an imaginary part $\Gamma(\mathbf{X})$, which determines their decay back to the ground state. In general the three $2p$ substates can split up due to symmetry breaking effects of the $\mathbf{x}$-dependent dielectric. To leading order the perturbed eigenvalues are the solutions z of

$$z\mathsf{U}=\lambda_2\mathsf{U}+\kappa(\mathbf{X})\sum_\alpha\int d\lambda\, s(\lambda)\lambda^{-1}[z-\lambda_1-\lambda]^{-1} \times\overline{\mathbf{u}}_{1\lambda\alpha}(\mathbf{X})\mathbf{u}_{1\lambda\alpha}(\mathbf{X}), \tag{8.1}$$

where U is the unit 3×3 matrix and $s(\lambda)$ is a cutoff function, which can be set equal to one in the expression for $\mathrm{Im}z$. Furthermore $\kappa(\mathbf{X})=(e/3m)^2[2\varepsilon_1(\mathbf{X})]^{-1}|\langle\varphi_1|\mathbf{p}\cdot\boldsymbol{\varphi}_2\rangle|^2$, where φ_1 is the unperturbed atomic ground state (eigenvalue λ_1) and φ_2 are the three unperturbed $2p$ states (eigenvalue λ_2), which are taken to be real and combined into a single vector, see Ref. [15]. The derivation follows the lines of [15]; the only difference from the conservative case is the appearance of $\mathbf{u}_{1\lambda\alpha}(\mathbf{X})$ rather than an eigenvector of H_1. Making an isotropy approximation, i.e., $\overline{\mathbf{u}}_{1\lambda\alpha}(\mathbf{X})\mathbf{u}_{1\lambda\alpha}(\mathbf{X}) \to\frac{1}{3}|\mathbf{u}_{1\lambda\alpha}(\mathbf{X})|^2\mathsf{U}$, the calculation made in Ref. [15] can be repeated with the result that to leading order in e [cf. Ref. [15], Eq. (8.13)],

$$\Gamma(\mathbf{X})=-\frac{\pi}{3}\kappa(\mathbf{X})\omega_0^{-1}\sum_\alpha\int d\lambda\,\delta(\omega_0-\lambda)|\mathbf{u}_{1\lambda\alpha}(\mathbf{X})|^2, \tag{8.2}$$

where $\omega_0=\lambda_2-\lambda_1$. We can rewrite $\Gamma(\mathbf{X})$ as (for P_{el} see Sec. VI)

$$\Gamma(\mathbf{X})=-\frac{\pi}{3}\kappa(\mathbf{X})\omega_0^{-1}\langle\mathbf{X}|\mathsf{P}_{el}\delta(\omega_0-\mathsf{H}_e)\mathsf{P}_{el}|\mathbf{X}\rangle =-\frac{\pi}{3}\kappa(\mathbf{X})\omega_0^{-1}N_f(\omega_0,\mathbf{X}), \tag{8.3}$$

where $N_f(\omega_0,\mathbf{X})$ is the generalization of the local density of states for the field to the absorptive situation. In this spirit a generalized density of states $N_f(E)$ can be defined as

$$N_f(E)=\int d\mathbf{x}\,\langle\mathbf{x}|\mathsf{P}_{el}\delta(E-\mathsf{H}_e)\mathsf{P}_{el}|\mathbf{x}\rangle=\mathrm{tr}\mathsf{P}_{el}\delta(E-\mathsf{H}_e)\mathsf{P}_{el}. \tag{8.4}$$

This definition is consistent with our results in Sec. III, where we found that if E falls in a band gap $\mathsf{P}_{el}\delta(E-\mathsf{H}_e)\mathsf{P}_{el}=0$ and hence $N_f(E)=0$. Using the relations $2\pi\delta(\lambda-\mathsf{H}_e)=[\lambda-i0-\mathsf{H}_e]^{-1}-[\lambda-i0-\mathsf{H}_e]^{-1}$ and $\mathsf{P}_{el}[z-\mathsf{H}_e]^{-1}\mathsf{P}_{el}=\mathsf{R}_e(z^2)\mathsf{P}_{el}$ we obtain

$$\Gamma(\mathbf{X})=-\frac{\kappa(\mathbf{X})}{6\pi\omega_0}\mathrm{Im}\langle\mathbf{X}|\mathsf{R}_e(\lambda^2-i0)|\mathbf{X}\rangle =-\frac{\kappa(\mathbf{X})}{6\pi\omega_0}\mathrm{Im}\mathsf{G}_e(\mathbf{X},\mathbf{X},\lambda^2-i0) \tag{8.5}$$

and

$$N_f(E)=(2\pi)^{-1}\mathrm{Im}\,\mathrm{tr}\,\mathsf{R}_e(\lambda^2-i0) =(2\pi)^{-1}\mathrm{Im}\int d\mathbf{x}\,\mathsf{G}_e(\mathbf{x},\mathbf{x},\lambda^2-i0), \tag{8.6}$$

where

$$\mathsf{G}_e(\mathbf{x},\mathbf{y},z)=\langle\mathbf{x}|\mathsf{R}_e(z^2)|\mathbf{y}\rangle. \tag{8.7}$$

Once more we end up with expressions featuring the electric Helmholtz resolvent $\mathsf{R}_e(z^2)$ but again we had to start from the full formalism. In case the isotropy assumption is not justified a more elaborate approach, as in Ref. [15], can be used. The results of that reference for atoms in conservative band-gap dielectrics are also easily generalized. Since there are no essential changes in the results obtained there, we shall not repeat the calculations.

IX. DISCUSSION

A. Summary of results

Starting from the phenomenological Maxwell's equations for a linear absorptive medium characterized by the constitutive equation

$$\boldsymbol{D}(\mathbf{x},t)=\varepsilon_1(\mathbf{x})\boldsymbol{E}(\mathbf{x},t)+\int_{t_0}^{t} ds\,\chi(\mathbf{x},t-s)\boldsymbol{E}(\mathbf{x},s), \quad (9.1)$$

we constructed a unitary time evolution in a larger space by introducing two essentially unique, real, auxiliary fields. The only inputs required were $\varepsilon_1(\mathbf{x})$ and $\chi(\mathbf{x},t)$ or, equivalently, the complex electric permeability $\varepsilon(\mathbf{x},\omega)$, which can be obtained experimentally. Another feature is that cycle averaging procedures were not required. This is important since in general electromagnetic waves are not monochromatic and a cycle is not well defined. The formalism allowed us to give a proper definition of band gaps in Sec. III and to construct a classical scattering formalism based upon wave and scattering operators in Sec. VI. We also showed that a sufficiently small absorptive perturbation of a conservative system possessing a band gap can still posses a band gap. More challenging is the direct establishment of a band gap for the absorptive case. Its investigation is rather straightforward in the point interaction limit (not unreasonable in the metallic sphere example mentioned in the Introduction) as in the conservative situation [27]. It is not *a priori* obvious how to define the density of states. However, in Sec. VIII, where we discussed the decay of an excited atom in a lossy dielectric, we were led in a natural way to a generalization of the density of states for a conservative medium. There and in the definition of band gaps the problem is that in the Helmholtz eigenvalue problem

$$[z^2\varepsilon(z)-\mathsf{H}_0]\mathbf{f}=\mathbf{0}, \quad (9.2)$$

the electric permeability $\varepsilon(z)$ is complex, even for real z, so we cannot exclude complex eigenvalues. The unitary formalism, although having a self-adjoint generator with real spectrum, did not directly solve this problem since the electromagnetic fields are coupled to the auxiliary fields. In the decoupled situation the latter have a real spectrum covering the whole real axis, so one does not expect band gaps for the full system. However, a projection upon the electromagnetic subspace took care of this. At the same time the Helmholtz operator and its resolvent $\mathsf{R}_e(z)=[z^2\varepsilon(z)-\mathsf{H}_0]^{-1}$ reappeared in the formalism but now the interpretation has become clear: It can only be singular for $z\in\mathbb{R}$. Given the unitary evolution a Lagrange-Hamilton formalism and its quantization directly followed by applying the results of a recent paper by the author [15]. In Sec. VII the quantized formalism was used to describe Čerenkov and transition radiation caused by fast electrons passing through a lossy dielectric and in Sec. VIII it was used again to study the decay of an excited atom surrounded by an absorptive dielectric. The decay constant Γ featured an object $N(\mathbf{x},z)$ that could be considered as a generalization of the local density of states for a conservative system. It can be expressed in terms of the Green's function $\mathsf{G}(\mathbf{x},\mathbf{x}',z)=\langle\mathbf{x}|\mathsf{R}_e(z)|\mathbf{x}'\rangle$.

B. Generalizations

Although we did not do so, it will be clear that a linear, absorptive magnetic system can be handled along the same lines as well as the combined case. This is also true if χ is nonlocal in coordinate space: $\chi(\mathbf{x},t-s)\boldsymbol{E}(\mathbf{x},s)\rightarrow\int d\mathbf{y}\,\chi(\mathbf{x}-\mathbf{y},t-s)\boldsymbol{E}(\mathbf{y},s)$. The present model does not include temperature effects, such as heat conduction. In the continuity equation for the energy density of the complete system $e(\mathbf{x},t)$, i.e., including the auxiliary fields,

$$\partial_t e(\mathbf{x},t)+\partial_{\mathbf{x}}\cdot\boldsymbol{S}(\mathbf{x},t)=0, \quad (9.3)$$

so that, as observed earlier in Ref. [4] , energy is only carried out of a volume through the Poynting vector $\boldsymbol{S}(\mathbf{x},t)=\boldsymbol{E}(\mathbf{x},t)\times\boldsymbol{B}(\mathbf{x},t)$. This can be traced back to the absence of space derivatives $\partial_{\mathbf{x}}\boldsymbol{F}_{2,4}$ in the equations of motion for the auxiliary fields. Continuity equations and Poynting vector have been the subject of much recent activity, see Refs. [28–30] for other aspects.

The extension of the present formalism to include nonlinear situations (in terms of nonlinear susceptibilities) is far from obvious. We can still introduce auxiliary fields to remove the time convolutions, leaving a set of coupled nonlinear equations of motion, see Sec. IX F below. However, if the medium is transparent, i.e., the system is dispersive but absorption can be neglected, so $\varepsilon=\varepsilon(\mathbf{x},\omega)$ is real, Drummond [2], extending results of Hillery and Mlodinow [31], obtained for the conservative case, has constructed a Lagrange formalism. He starts off with the assumption that ε is piecewise constant as a function of ω and generalizes later on to the case of a slowly varying envelope situation.

Above we did not consider discontinuities in the $\mathbf{x}$ dependence of $\varepsilon_1(\mathbf{x})$ and $\chi(\mathbf{x},t)$. In Ref. [20], using a limiting procedure, an approach is presented that can be taken over to the present case. It allows quite general situations, such as fractal shaped objects, where normals and tangents relative to the boundary surface are no longer meaningful. A common, more pedestrian, approach consists of obtaining boundary conditions from the Laplace transformed equations of motion, the only difference with the conservative situation being their frequency dependence. In applications, as in Secs. VII and VIII, they play a role in the determination of the mode functions $\mathbf{u}_{\lambda\alpha}$.

C. Microscopic and macroscopic approaches

So far we have taken the phenomenological Maxwell's equations at face value. We started out with a space and frequency dependent $\varepsilon(\mathbf{x},\omega)$ and were led in a natural way to a formalism where energy conservation is restored by introducing new auxiliary fields. A quite different route was taken by Burgess [3], who discusses a relativistic covariant

formalism. He does not introduce additional fields but relates the equations of motion to an action, which is nonlocal in the field. In its general form it is given by his Eq. (79). As a consequence, the creation and annihilation operators in a plane wave expansion of the field not only depend on the wave vector $\mathbf{k}$, but also on $\mathbf{x}$ and t, see his Eqs. (5)–(7). After a discussion of some fundamental matters the formalism is applied to the phenomenon of squeezed states (see also Ref. [32]), initially for scalar fields, whereupon the electromagnetic case is treated.

An alternative is to start directly from a microscopic quantum formalism for the combined matter-field system. This approach was taken by Hopfield [33], who considered the interaction of the electromagnetic field with a crystal. Among other matters he discusses the route by which electromagnetic energy is transferred to the lattice phonon modes. The matter part enters the formalism as a second field and for the interaction a special choice is made. The Hopfield model is also at the basis of further work by Huttner and Barnett [5] and Gruner and Welsh [6]. Here we note that in the above microscopic theories only spatially homogeneous situations are considered. Comparing the microscopic results with the present approach in its quantized form, we see that in both cases a second field, representing the matter system, appears. The main difference is that these authors only consider spatially homogeneous systems, allowing the use of the Coulomb gauge. Another, equivalent, way to describe the quantum situation is in terms of a quantum noise current, as was done by Matloob, Loudon, and co-workers in a series of papers [7]. Here some simple spatially inhomogeneous situations are considered, such as slab configurations with normal incident field, as well as systems with gain. Vacuum field fluctuations and power spectrum are given in explicit form.

Considering the various approaches, we think that our setup, starting from the macroscopic Maxwell equations and featuring the experimentally obtainable $\varepsilon(\mathbf{x},\omega)$, is quite useful in situations where the spatial inhomogeneity is important. Our approach results in general expressions, the space dependence entering through the classical mode functions $\mathbf{u}_{\lambda\alpha}$. Obviously the latter must be evaluated numerically in complicated situations. This is, for instance, the case for the description of transition radiation. The latter is very sensitive to the precise space and frequency dependence of $\varepsilon(\mathbf{x},\omega)$. Conversely this aspect can be used to obtain $\varepsilon(\omega)$ for a material from transition radiation data. Especially in the x-ray region $\varepsilon(\omega)$ is not well known for a number of materials.

D. Atomic radiative decay

As we have seen the properties of an atom interacting with a quantized absorbing dielectric are affected in two ways. The first is a change in the atomic levels due to the presence of $\varepsilon_{stat}(\mathbf{x})$ in Eq. (5.9), which determines the potentials. This effect is related to the nonpropagating field modes (the longitudinal modes in a spatially homogeneous situation) and is the same as in the conservative case. The second is due to the modified propagating field modes in the quantized fields and in Sec. VIII we discussed the radiative decay of a model atom. The final result is similar to the conservative case. The only difference comes from the change in ε in $\mathsf{R}_e(z^2)$, which is now frequency dependent and complex. The experimental observation of these effects is doubtful in spatially homogeneous situations or for atoms buried deeply in large pieces of lossy material. In the latter case nearly all radiation will have been absorbed before it leaves the material on its way to an outside detector. Thus atoms at the boundary of a lossy material are a better proposition [34]. The spatially homogeneous situation has been considered in terms of a different formalism by Barnett *et al.* [16]. In that work the longitudinal modes are related to a decay mechanism for an atomic excited state, whereas here they lead to a modification of the Coulomb potential (and hence the atomic eigenvalues) through $\varepsilon_{stat}(\mathbf{x})$. It is at present not clear whether the two are equivalent. In [16] local field corrections are considered as well. One case is that of an atom in an empty cavity for which the atomic decay rate is considered. In the present formalism the presence of the cavity is taken into account automatically since it leads to different classical mode functions $\mathbf{u}_{\lambda\alpha}(\mathbf{x})$ and hence to a modified local density of states.

E. Initial assumptions and validity of the formalism

As noted earlier the assumptions A_1–A_3 are satisfied in relevant physical situations. Two crucial requirements are involved. The first is that $\chi'(\mathbf{x},0)=m(\mathbf{x},\mathbb{R})\leqslant c<\infty$ in A_2, which is quite acceptable. The second is A_3, which states that the static susceptibility $\hat{\chi}(\mathbf{x},0)=\int_0^\infty dt\,\chi(\mathbf{x},t)<\infty$. This relation usually holds except for critical points in the thermodynamic case, where ε depends on temperature and density. We have seen that it is not needed in the construction of a unitary formalism but it is required for a Lagrange setup. In order to get some further insight into this matter consider the situation where

$$m(d\omega)=\nu(\omega)d\omega$$

$$=\pi^{-1}\int n(d\omega')\gamma(\omega')[(\omega-\omega')^2+\gamma(\omega')^2]^{-2}d\omega, \tag{9.4}$$

with $\gamma(\omega)\geqslant 0$ and n satisfying A_1–A_3. Then m satisfies A_1 and A_2 but not A_3. In this case we can obtain a version of Eqs. (2.4), featuring n instead of m, but the motion has become dissipative, since now

$$\partial_t \boldsymbol{F}_0(\omega,t)=-\{\gamma(\omega)+i\omega)\}\boldsymbol{F}_0(\omega,t)-i\varepsilon_1^{-1/2}\boldsymbol{F}_1(t). \tag{9.5}$$

Thus in this special case either the motion is unitary and A_3 is not satisfied or we have the opposite situation.

Although an approach starting from the phenomenological ME or a microscopic equivalent can give valuable information about the behavior of certain material systems coupled to radiation fields, the method has its limitations. In the transition radiation case the electrons can scatter from the individual atoms or molecules constituting the dielectric. This leads to a loss of active electrons, diminishing the actual radiation yield, a mechanism that plays an important role in experimental setups. Atoms embedded in dielectrics will also be affected by their immediate surroundings in ways that are not accounted for in the phenomenological ME. The latter

can be looked upon as a crude approximation to a more detailed transport equation (see Ref. [15] for other comments). In fact it is quite remarkable that they give a satisfactory description of many physical situations in terms of a single parameter, the permeability ε.

F. Outlook and open problems

The existence of a continuity equation for the energy density is crucial for the occurrence of diffusion in a random situation. In the conservative case, after averaging over the randomness, indicated by $\langle\ \rangle$, we have

$$\partial_t\langle e(\mathbf{x},t)\rangle+\partial_{\mathbf{x}}\cdot\langle \boldsymbol{S}(\mathbf{x},t)\rangle=0. \tag{9.6}$$

In a diffusive situation, for large t and an appropriate initial situation, the current $\boldsymbol{S}$ is assumed to become proportional to the gradient of the energy density

$$\langle \boldsymbol{S}(\mathbf{x},t)\rangle\sim -D\partial_{\mathbf{x}}\langle e(\mathbf{x},t)\rangle,\quad D>0, \tag{9.7}$$

leading to a diffusion equation for e. In the absorptive case further investigation is necessary. It is not *a priori* clear whether $\langle e\rangle$ in Eq. (9.7) should be the full or only the electromagnetic energy density.

The opposite situation is that of Anderson localization, which results in a vanishing diffusion coefficient in the conservative case. The mathematical definition of localization is that of spectral intervals with a dense point spectrum for the generator of the motion, each point of this spectrum corresponding with a square integrable (usually exponentially decaying) eigenvector [35]. Recently it has been found that in conservative systems possessing a band gap, localization intervals in the gap can develop if the system is randomized [36,37]. In the lossy case we run into the same problem as with the definition of gaps and the density of states, i.e., we expect $\sigma(\mathsf{K})$, the spectrum of K, to cover the whole real axis. However, we can again consider the restriction $\mathsf{P}_{em}[z-\mathsf{K}]^{-1}\mathsf{P}_{em}$ to the electromagnetic subspace and we can try to define a localization interval Δ as an interval where this operator has a dense set of poles and no other singularities. If $\sigma(\mathsf{K})$ is absolutely continuous outside the point 0, $\mathsf{P}_{em}[z-\mathsf{K}]^{-1}\mathsf{P}_{em}$ will have no poles in Δ, excluding localization in the above sense. Thus $\sigma(\mathsf{K})$ must be more complicated for the existence of Anderson localization. This makes the study of random absorptive systems an interesting open mathematical problem (think of a random conservative system for which Δ is a localization interval, which is subject to an absorptive perturbation).

If it turns out that localization occurs, i.e., $\mathsf{P}_{em}[z-\mathsf{K}]^{-1}\mathsf{P}_{em}$ has a dense set of poles in some sets Δ, there exists the further problem of how to disentangle localization effects from absorptive attenuation in an experimental setup where a light beam travels through a slab and the transmitted beam is studied as a function of slab thickness. For instance, in the recent experimental work on light localization by Wiersma *et al.* [38], the avoidance of absorption is an important issue.

Finally we briefly sketch how the convolution term can be removed in a simple nonlinear situation. Suppose that

$$\boldsymbol{D}(t)=\boldsymbol{E}(t)+\int_0^t ds\int_0^t du\,\boldsymbol{\chi}(t-s,t-u):\boldsymbol{E}(s)\boldsymbol{E}(u), \tag{9.8}$$

where the nonlinear susceptibility $\boldsymbol{\chi}$ has the usual properties $\boldsymbol{\chi}(t_1,t_2)=\boldsymbol{\chi}(t_2,t_1)$ is real and $\boldsymbol{\chi}(t,0)=0$. Since only nonnegative t_1 and t_2 appear, we can define $\boldsymbol{\chi}(-t_1,t_2)=-\boldsymbol{\chi}(t_1,t_2)$, so $\boldsymbol{\chi}(-t_1,-t_2)=\boldsymbol{\chi}(t_1,t_2)$ and in terms of

$$\hat{\boldsymbol{\chi}}(\omega_1,\omega_2)=(2\pi)^{-2}\int dt_1dt_2\exp[i(\omega_1t_1+\omega_2t_2)]\boldsymbol{\chi}(t_1,t_2),$$

and [cf. Eq. (2.6)]

$$\begin{aligned}\boldsymbol{F}_0(t,\omega)&=-i\int_0^t ds\exp[-i\omega(t-s)]\boldsymbol{E}(s)\\&=\boldsymbol{F}_2(t,\omega)+i\boldsymbol{F}_4(t,\omega),\end{aligned}$$

we have, since $\hat{\boldsymbol{\chi}}(\omega_1,\omega_2)$ is odd in each ω_j, and using that $\boldsymbol{F}_2(t,\omega)$ is odd in ω and $\boldsymbol{F}_4(t,\omega)$ even,

$$\begin{aligned}\boldsymbol{D}(t)&=\boldsymbol{E}(t)-\int d\omega_1d\omega_2\,\hat{\boldsymbol{\chi}}(\omega_1,\omega_2):\boldsymbol{F}_0(t,\omega_1)\boldsymbol{F}_0(t,\omega_2)\\&=\boldsymbol{E}(t)-\int d\omega_1d\omega_2\,\hat{\boldsymbol{\chi}}(\omega_1,\omega_2):\boldsymbol{F}_2(t,\omega_1)\boldsymbol{F}_2(t,\omega_2).\end{aligned} \tag{9.9}$$

Differentiation leads to Eqs. (2.4) for $\boldsymbol{J}=0$ and $\varepsilon_1=1$, except for the first, which now becomes nonlinear:

$$\begin{aligned}\partial_t\boldsymbol{F}_1(t)&=\partial_{\mathbf{x}}\times\boldsymbol{F}_3(t)\\&\quad-2\int d\omega_1d\omega_2\,\omega_1\hat{\boldsymbol{\chi}}(\omega_1,\omega_2):\boldsymbol{F}_4(t,\omega_1)\boldsymbol{F}_2(t,\omega_2).\end{aligned} \tag{9.10}$$

Higher-order nonlinearities can be handled in the same way. The remaining, open, problem consists of finding a Lagrange formalism that reproduces these equations of motion and leads to a Hamiltonian H that can be identified as the energy of the system. Note that it is not obvious that such an H exists, there may be no constants of the motion at all.

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APPENDIX A: THE OPERATOR $\mathsf{P}_{em}[z-\mathsf{K}]^{-1}\mathsf{P}_{em}$

Below we use the notation given in Sec. III. Since P_{em} and P_{aux} are complementary projectors, $\mathsf{P}_{em}+\mathsf{P}_{aux}=1$, we can apply the Feshbach formula, Eq. (1.5), to obtain (Im$z\neq 0$, $\mathsf{A}=\{A_{jh}\}$)

$$\mathsf{X}(z)=\mathsf{P}_{em}[z-\mathsf{K}]^{-1}\mathsf{P}_{em}=[z-\mathsf{P}_{em}\mathsf{K}\mathsf{P}_{em}-\mathsf{Y}(z)]^{-1}\mathsf{P}_{em}, \tag{A1}$$

where

$$\begin{aligned}\mathsf{Y}(z)&=\mathsf{P}_{em}\mathsf{K}\mathsf{P}_{aux}[z-\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{aux}]^{-1}\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{em}\\&=\mathsf{P}_{em}\mathsf{K}\mathsf{P}_{aux}[z+\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{aux}][z^2-(\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{aux})^2]^{-1}\\&\quad\times\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{em}.\end{aligned} \tag{A2}$$

Now

$$\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{aux}=\begin{pmatrix}0&0&0&0\\0&0&0&i\omega\\0&0&0&0\\0&-i\omega&0&0\end{pmatrix},$$

so $(\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{aux})^2=\omega^2\mathsf{P}_{aux}$ and $\mathsf{Y}(z)=\mathsf{P}_{em}\mathsf{K}\mathsf{P}_{aux}[z+\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{aux}][z^2-\omega^2]^{-1}\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{em}$. Evaluating this expression we have

$$\begin{aligned}Y_{jh}(z)&=zK_{14}[z^2-\omega^2]^{-1}K_{41}\delta_{j1}\delta_{h1}\\&=z\varepsilon_1^{-1}\int m(d\omega)[z^2-\omega^2]^{-1}\delta_{j1}\delta_{h1}\\&=-z\varepsilon_1^{-1}\hat{\chi}(z)\,\delta_{j1}\delta_{h1}.\end{aligned} \tag{A3}$$

Since only the K_{13} and K_{31} elements survive in $\mathsf{P}_{em}\mathsf{K}\mathsf{P}_{em}$ we have

$$\mathsf{X}(z)=\begin{bmatrix}z\varepsilon(z)&0&K_{13}&0\\0&z&0&0\\K_{31}&0&z&0\\0&0&0&z\end{bmatrix}^{-1}\mathsf{P}_{em}. \tag{A4}$$

The operator $\mathsf{W}=\begin{pmatrix}z\varepsilon(z)&K_{31}\\K_{13}&z\end{pmatrix}$ has the inverse (recall that $\mathsf{R}_e(z^2)=[z^2\varepsilon(z)-\mathsf{H}_0]^{-1}$)

$$\begin{aligned}&\mathsf{W}^{-1}\\&=\begin{pmatrix}z\varepsilon_1^{1/2}\mathsf{R}_e(z^2)\varepsilon_1^{1/2}&\varepsilon_1^{1/2}\mathsf{R}_e(z^2)\cdot(\boldsymbol{\epsilon}\cdot\mathbf{p})\\-(\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot\mathsf{R}_e(z^2)\varepsilon_1^{1/2}&z^{-1}\{1-(\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot\mathsf{R}_e(z^2)\cdot(\boldsymbol{\epsilon}\cdot\mathbf{p})\}\end{pmatrix}\\&=\begin{pmatrix}\mathsf{X}_{11}&\mathsf{X}_{13}\\\mathsf{X}_{31}&\mathsf{X}_{33}\end{pmatrix},\end{aligned} \tag{A5}$$

as is readily verified by solving $\mathbf{g}=\mathsf{W}\mathbf{f}$ for $\mathbf{f}$ in terms of $\mathbf{g}$. Thus we have

$$\mathsf{X}(z)=\begin{pmatrix}\mathsf{X}_{11}&0&\mathsf{X}_{13}&0\\0&0&0&0\\\mathsf{X}_{31}&0&\mathsf{X}_{33}&0\\0&0&0&0\end{pmatrix}, \tag{A6}$$

with the X_{jh}'s as in Eq. (A5). Finally we note that $z^{-1}\{1-(\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot\mathsf{R}_e(z^2)\cdot(\boldsymbol{\epsilon}\cdot\mathbf{p})\}=z\mathsf{R}_m(z^2)$, so we have verified Eq. (3.10).

APPENDIX B: PROOF OF THE PROPOSITION

We have $\mathsf{K}=\mathsf{K}_1+\mathsf{K}_2$ with K_1 having the band gap pair $(\Delta,-\Delta)$, $\Delta=(\lambda_a,\lambda_b)$, $\lambda_a\geqslant 0$, or, equivalently, $\mathsf{H}_1=\varepsilon_1^{-1/2}\mathsf{H}_0\varepsilon_1^{-1/2}$ has the gap $\Delta^2=(\lambda_a^2,\lambda_b^2)$. For $\mathrm{Im}z\neq 0$ we can write

$$\begin{aligned}\mathsf{R}_e(z^2)&=\varepsilon_1^{-1/2}[z^2-\mathsf{H}_1+z^2\varepsilon_1^{-1}\hat{\chi}(z)]^{-1}\varepsilon_1^{-1/2}\\&=\varepsilon_1^{-1/2}[z^2-\mathsf{H}_1]^{-1}[1+z^2\varepsilon_1^{-1}\hat{\chi}(z)\\&\quad\times[z^2-\mathsf{H}_1]^{-1}]^{-1}\varepsilon_1^{-1/2}.\end{aligned} \tag{B1}$$

Since $[z^2-\mathsf{H}_1]^{-1}$ is analytic through the gap Δ^2, $\mathsf{R}_e(z^2)$ will be analytic through a subset of Δ^2 for which $\lambda^2\varepsilon_1^{-1}\hat{\chi}(\lambda)[\lambda^2-\mathsf{H}_1]^{-1}$ remains strictly smaller than 1 in norm. Taking $\Delta_\delta^2=(\lambda_a^2+\delta,\lambda_b^2-\delta)$, $0<\delta<(\lambda_b^2-\lambda_a^2)/2$, it is easy to verify that the norm $||\lambda^2[\lambda^2-\mathsf{H}_1]^{-1}||\leqslant\lambda_b^2\delta^{-1}$, $\lambda^2\in\Delta_\delta^2$, since λ^2 keeps a minimal distance δ from the spectrum of H_1. Next we note that if for $\lambda^2\in\Delta_\delta^2$,

$$\begin{aligned}&||\lambda^2\varepsilon_1^{-1}\hat{\chi}(\lambda)[\lambda^2-\mathsf{H}_1]^{-1}||\\&\leqslant||\varepsilon_1^{-1}\hat{\chi}(\lambda)||\;||\lambda^2[\lambda^2-\mathsf{H}_1]^{-1}||\\&\leqslant\sup_{\mathbf{x}\in\mathbb{R}^3}\varepsilon_1(\mathbf{x})^{-1}\int_0^\infty dt\;|\chi(\mathbf{x},t)|\lambda_b^2\delta^{-1}\leqslant c<1,\end{aligned}$$

or, since $\varepsilon(\mathbf{x})=1$ for those $\mathbf{x}$ for which $\chi(\mathbf{x},\omega)$ is nonzero,

$$\sup_{\mathbf{x}\in\mathbb{R}^3}\int_0^\infty dt\;|\chi(\mathbf{x},t)|<\lambda_b^{-2}\delta,$$

then $\mathsf{R}_e(z^2)$ is analytic through Δ_δ^2, implying that $(\Delta_\delta,-\Delta_\delta)$, $\Delta_\delta=(\sqrt{\lambda_a^2+\delta},\sqrt{\lambda_b^2-\delta})$ is a band-gap pair for K.

APPENDIX C: SPECTRAL PROPERTIES

1. Relation between K and the pair H_e, H_m

Since K is of the form

$$\mathsf{K}=\begin{pmatrix}0&\mathsf{K}_{em}\\\mathsf{K}_{me}&0\end{pmatrix},\quad \mathsf{K}_{me}=\mathsf{K}_{em}^* \tag{C1}$$

we have

$$\mathsf{K}^*\mathsf{K}=\begin{pmatrix}\mathsf{K}_{em}\mathsf{K}_{em}^*&0\\0&\mathsf{K}_{em}^*\mathsf{K}_{em}\end{pmatrix}=\begin{pmatrix}\mathsf{H}_e&0\\0&\mathsf{H}_m\end{pmatrix}, \tag{C2}$$

where, using $\int m(d\omega)=\chi'(0)$ and denoting $\mathsf{H}_1=\varepsilon_1^{-1/2}\mathsf{H}_0\varepsilon_1^{-1/2}$,

$$\mathsf{H}_e=\begin{pmatrix} \mathsf{H}_1+\varepsilon_1^{-1}\chi'(0) & \varepsilon_1^{-1/2}\int m(d\omega)\omega\cdots \\ \varepsilon_1^{-1/2}\omega & \omega^2 \end{pmatrix},$$

$$\mathsf{H}_m=\begin{pmatrix} (\boldsymbol{\epsilon}\cdot\mathbf{p})\cdot\varepsilon_1^{-1}(\boldsymbol{\epsilon}\cdot\mathbf{p}) & -i\varepsilon_1^{-1}(\boldsymbol{\epsilon}\cdot\mathbf{p})\int m(d\omega)\ \omega\cdots \\ -i\varepsilon_1^{-1}(\boldsymbol{\epsilon}\cdot\mathbf{p}) & \omega^2+\varepsilon_1^{-1}\int m(d\omega)\cdots \end{pmatrix}. \tag{C3}$$

It is known from general principles [39] that the spectra of $\mathsf{K}_{em}\mathsf{K}_{em}^*$ and $\mathsf{K}_{em}^*\mathsf{K}_{em}$ coincide, except for, possibly, the point 0. These expressions refer to the setup of Sec. II B, whereas for Sec. II C

$$\mathsf{H}_e=\begin{pmatrix} \mathsf{H}_1+\varepsilon_1^{-1}\chi'(0) & \varepsilon_1^{-1/2}\int d\omega\,\sigma(\omega)\omega\cdots \\ \varepsilon_1^{-1/2}\omega\sigma(\omega) & \omega^2 \end{pmatrix}$$

$$=\begin{pmatrix} \mathsf{H}_1+\chi'(0) & \int d\omega\,\sigma(\omega)\omega\cdots \\ \omega\sigma(\omega) & \omega^2 \end{pmatrix}, \tag{C4}$$

where we used the fact that $\varepsilon_1(\mathbf{x})=1$ for those $\mathbf{x}$ for which $\chi(\mathbf{x},\omega)$ is nonzero.

2. Eigenvectors related by a wave operator

Let

$$H=H_0+V \tag{C5}$$

and suppose the wave operators

$$\Omega_\pm=\lim_{t\to\pm\infty}\exp[iHt]\exp[-iH_0t]$$

$$=1+i\int_0^{\pm\infty}dt\exp[iHt]V\exp[-iH_0t]$$

$$=1+i\lim_{\delta\to 0}\int_0^{\pm\infty}dt\exp[-\delta|t|]\exp[iHt]V\exp[-iH_0t] \tag{C6}$$

exist. Then, if $H_0f_0=\lambda f_0$ and $f^\pm=\Omega_\mp f_0$, also $Hf^\pm=\lambda f^\pm$ and from Eq. (C6), in the limit $\delta\downarrow 0$,

$$f^\pm=f_0+[\lambda\pm i\delta-H]^{-1}Vf_0. \tag{C7}$$

Conversely, from $\Omega_\mp^*f^\pm=f_0$,

$$\{1-[\lambda\pm i\delta-H_0]^{-1}V\}f^\pm=f_0, \tag{C8}$$

an abstract form of the Lippmann-Schwinger equations. Let P_1 and $P_2=1-P_1$ two complementary projectors, which commute with H_0, $H_0=H_{01}P_1+H_{02}P_2$ so $H_{0j}P_jf_0=\lambda P_jf_0$. Assume further that $V_{22}=0$. Then, with $g_j=P_jg$, $\mathsf{X}_{jh}=P_j\mathsf{X}P_h$ and

$$V_{eff}(z)=V_{11}+V_{12}[z-H_{02}]^{-1}V_{21},$$

$$V_{eff}^\pm(\lambda)=\lim_{\delta\to 0}V_{eff}(\lambda\pm i\delta), \tag{C9}$$

we obtain from the Feshbach formula

$$P_1f^\pm=P_1f_0+[\lambda\pm i0-H_{01}-V_{eff}^\pm(\lambda)]^{-1}$$
$$\times\{P_1Vf_0+P_1VP_2[\lambda\pm i0-H_{02}]^{-1}P_2Vf_0\}$$
$$=P_1f_0+[\lambda\pm i0-H_{01}-V_{eff}^\pm(\lambda)]^{-1}$$
$$\times\{P_1V_{eff}^\pm(\lambda)P_1f_0+P_1VP_2f_0\},$$

$$P_2f^\pm=P_2f_0+[\lambda\pm i0-H_{02}]^{-1}P_2VP_1\{f^\pm-f_0\}$$

or

$$f_1^\pm=f_{01}+[\lambda\pm i0-H_{01}-V_{eff}^\pm(\lambda)]^{-1}\{V_{eff}^\pm(\lambda)f_{01}+V_{12}f_{02}\},$$

$$f_2^\pm=f_{02}+[\lambda+i0-H_{02}]^{-1}V_{21}(f_1^\pm-f_{01}). \tag{C10}$$

Let f^a be the solution for which $f_{02}=0$ and f^b the one for which $f_{01}=0$. Then, since both f_0's are orthogonal and the wave operators, being isometric, preserve orthogonality, also $f^a\perp f^b$. The above results hold for the case the wave operators exist. In other situations the above relations still define eigenvectors of H. However, if the wave operators exist the formal manipulations involved (i.e., $\delta\downarrow 0$) are better controlled. The crucial point is the existence of $V_{eff}^\pm(\lambda)=\lim_{\delta\to 0}V_{eff}(\lambda\pm i\delta)$.

3. Spectral properties of H_e

We now consider the eigenvalue problem for H_e for the case $m(\mathbf{x},d\omega)=\nu(\mathbf{x},\omega)d\omega$ and use the formulation of Sec. II C. Thus

$$\mathsf{H}_e\mathbf{u}=\lambda^2\mathbf{u},\quad \lambda>0. \tag{C11}$$

Since H_e is a real operator we note that along with $\mathbf{u}=\begin{pmatrix}\mathbf{u}_1\\ \mathbf{u}_2(\omega)\end{pmatrix}$, $\overline{\mathbf{u}}=\begin{pmatrix}\overline{\mathbf{u}}_1\\ \overline{\mathbf{u}}_2(\omega)\end{pmatrix}$ is an eigenvector at the same eigenvalue and this is also the case for $\begin{pmatrix}\mathbf{u}_1\\ -\mathbf{u}_2(-\omega)\end{pmatrix}$. Taking linear combinations we can restrict ourselves to real $\mathbf{u}$ of the type $\mathbf{u}=\begin{pmatrix}\mathbf{u}_1\\ \mathbf{u}_2(\omega)\end{pmatrix}$ with $\mathbf{u}_2(\omega)$ odd in ω and $\mathbf{u}=\begin{pmatrix}0\\ \mathbf{u}_2(\omega)\end{pmatrix}$ with $\mathbf{u}_2(\omega)$ even in ω. In the second case we have $\omega^2\mathbf{u}_2(\omega)=\lambda^2\mathbf{u}_2(\omega)$ so $\mathbf{u}_2(\omega)\sim\delta(\omega^2-\lambda^2)$ and it remains to consider the first. We do so by writing [see Eq. (C4)]

$$\mathsf{H}_e=\begin{pmatrix}\mathsf{H}_1 & 0\\ 0 & \omega^2\end{pmatrix}+\begin{pmatrix}\chi'(0) & \int d\omega\,\sigma(\omega)\omega\cdots\\ \omega\sigma(\omega) & 0\end{pmatrix}$$

$$=\mathsf{H}_e^{(0)}+\mathsf{V}. \tag{C12}$$

We assume that $\nu(\mathbf{x},\omega)$, and hence $\sigma(\mathbf{x},\omega)$, is confined to a bounded region in space. Let Q be the projector upon the complement of the null space of $\mathsf{H}_e^{(0)}$, i.e., $\varepsilon_1^{-1/2}$ times the first component of $\mathsf{Q}\mathbf{f}$ is transverse. Then the wave operators $\Omega_\pm=\lim_{t\to\pm\infty}\exp[i\mathsf{H}_et]\exp[-i\mathsf{H}_e^{(0)}t]\mathsf{Q}$ exist and we can apply the results of the preceding subsection to $\mathbf{u}_\lambda^\pm=\Omega_\mp\mathbf{u}_\lambda^{(0)}$,

erwhere $\mathsf{H}_e^{(0)}\mathbf{u}_\lambda^{(0)}=\lambda^2\mathbf{u}_\lambda^{(0)}$. Since $\omega^2\mathbf{u}_{2\lambda}^{(0)}(\mathbf{x},\omega)=\lambda^2\mathbf{u}_{2\lambda}^{(0)}(\mathbf{x},\omega)$, we have $\mathbf{u}_{2\lambda}^{(0)}(\mathbf{x},\omega)=\omega\delta(\omega^2-\lambda^2)\mathbf{g}(\mathbf{x})$, where $\mathbf{g}(\mathbf{x})$ is arbitrary. Using the specific structure of the operators involved we obtain from Eq. (C10)

$$\begin{aligned}\mathbf{u}_{\lambda 1}^{\pm}&=\mathbf{u}_{\lambda 1}^{(0)}+\mathsf{R}^{\pm}(\lambda^2)\Big\{-\lambda^2\hat{\chi}^{\pm}(\lambda)\mathbf{u}_{\lambda 1}^{(0)}\\&\quad+\int d\omega\ \sigma(\omega)\omega\mathbf{u}_{\lambda 2}^{(0)}(\omega)\Big\}\\&=\mathbf{u}_{\lambda 1}^{(0)}+\mathsf{R}^{\pm}(\lambda^2)\{-\lambda^2\hat{\chi}^{\pm}(\lambda)\mathbf{u}_{\lambda 1}^{(0)}+\lambda\sigma(\lambda)\mathbf{g}\},\\\mathbf{u}_{\lambda 2}^{\pm}(\omega)&=\omega\delta(\omega^2-\lambda^2)\mathbf{g}+\omega[\lambda^2\pm i0-\omega^2]^{-1}\\&\quad\times\sigma(\omega)\{\mathbf{u}_{\lambda 1}^{\pm}-\mathbf{u}_{\lambda 1}^{(0)}\},\end{aligned}\tag{C13}$$

where

$$\begin{aligned}\mathsf{R}^{\pm}(\lambda^2)&=\lim_{\delta\to 0}\mathsf{R}_e(\lambda^2\pm i\delta),\\\mathsf{R}_e(z^2)&=[z^2\varepsilon(z)-\mathsf{H}_0]^{-1}.\end{aligned}\tag{C14}$$

For real $\mathbf{u}^{(0)}$ the functions $\mathbf{u}_{1\lambda}^{\pm}$ are complex conjugate, so we can obtain real eigenvectors of H_e by taking the appropriate linear combinations. As before we have two types of orthogonal solutions. The first is obtained by setting $\mathbf{u}_{2\lambda}^{(0)}=0$ or $\mathbf{g}=0$ and the second by $\mathbf{u}_{1\lambda}^{(0)}=0$. Note that the requirement $V_{eff}(\lambda)=\lim_{\delta\to 0}V_{eff}(\lambda+i\delta)$ exists of the preceding subsection amounts here to the existence of $\lim_{\delta\downarrow 0}\hat{\chi}(\lambda\pm i\delta)=\int_0^\infty dt\exp[\pm i\lambda t]\chi(\pm t)$, which is the case if $|\chi(t)|$ is integrable.

If $\nu(\mathbf{x},\omega)$ is not confined to a bounded region in space, as in spatially homogeneous or periodic systems, the above expressions can still be used. In the spatially homogeneous case with nontrivial χ [so $\mathrm{Im}\hat{\chi}(\lambda)>0$] and setting $\varepsilon_1=1$, we have, for the transverse case, $\mathsf{R}^{\pm}(\lambda^2)=[\lambda^2\{1+\hat{\chi}^{\pm}(\lambda)\}-\mathbf{p}^2]^{-1}=[\xi_{\pm}^2-\mathbf{p}^2]^{-1}$, which has the kernel $\langle\mathbf{x}|\mathsf{R}^{\pm}(\lambda^2)|\mathbf{y}\rangle=-\exp[i\xi_{\pm}|\mathbf{x}-\mathbf{y}|]/(4\pi|\mathbf{x}-\mathbf{y}|)$, where $\mathrm{Im}\xi_{\pm}>0$. This results in $\mathbf{u}_\lambda$'s which remain bounded as functions of $\mathbf{x}$, contrary to the solutions of the Helmholtz equation,

$$[\lambda^2\{1+\chi^{\pm}(\lambda)\}-\mathbf{p}^2]f=0,\tag{C15}$$

which diverge for large $\mathbf{x}$. From $\mathsf{K}_{em}\mathsf{K}_{em}^*\mathbf{u}=\lambda^2\mathbf{u}$ it follows that $\mathsf{H}_m\mathsf{K}_{em}^*\mathbf{u}=\mathsf{K}_{em}^*\mathsf{K}_{em}\mathsf{K}_{em}^*\mathbf{u}=\mathsf{K}_{em}^*\mathsf{H}_e\mathbf{u}=\lambda^2\mathsf{K}_{em}^*\mathbf{u}$ so $\mathsf{K}_{em}^*\mathbf{u}$ is the corresponding eigenvector of H_m.

4. The eigenvalue zero and gauge condition

In the present case 0 is an eigenvalue of K. As is readily verified, the corresponding eigenvectors are of the form

$$\mathbf{f}=\begin{pmatrix}-\varepsilon_1^{1/2}\partial_{\mathbf{x}}\zeta_e\\ \omega^{-1}\varepsilon_1^{1/2}\partial_{\mathbf{x}}\zeta_e\\ -\partial_{\mathbf{x}}\zeta_m\\ 0\end{pmatrix}=-\begin{pmatrix}\varepsilon_1^{1/2}\partial_{\mathbf{x}} & 0\\ -\omega^{-1}\varepsilon_1^{1/2}\partial_{\mathbf{x}} & 0\\ 0 & \partial_{\mathbf{x}}\\ 0 & 0\end{pmatrix}\cdot\begin{pmatrix}\zeta_e\\ \zeta_m\end{pmatrix}=-\mathsf{M}\boldsymbol{\zeta},\tag{C16}$$

where the ζ_j's are scalar functions. Its first two components give the corresponding eigenvectors of H_e and the second of H_m. The projector upon $\mathcal{N}(\mathsf{H}_e)$, the null space of H_e, and on $\mathcal{N}(\mathsf{H}_m)$ are

$$\mathsf{P}_e=\begin{pmatrix}\mathsf{P}_{11} & -\mathsf{P}_{11}\int m(d\omega')(\omega')^{-1}\varepsilon_1^{-1/2}\\ -\varepsilon_1^{-1/2}\omega^{-1}\mathsf{P}_{11} & \omega^{-1}\int m(d\omega')(\omega')^{-1}\varepsilon_1^{-1/2}\mathsf{P}_{11}\varepsilon_1^{-1/2}\end{pmatrix},\quad \mathsf{P}_m=\begin{pmatrix}\mathsf{P}_0 & 0\\ 0 & 0\end{pmatrix}.\tag{C17}$$

Here $\mathsf{P}_{11}=\mathsf{P}[\mathsf{P}\{1+\varepsilon_1^{-1}\hat{\chi}(0)\}\mathsf{P}]^{-1}\mathsf{P}$ with P the projector upon $\mathcal{N}(\mathsf{H}_1)$, see Refs. [15,20],

$$\mathsf{P}=\varepsilon_1^{1/2}\mathsf{P}_0[\mathsf{P}_0\varepsilon_1\mathsf{P}_0]^{-1}\mathsf{P}_0\varepsilon_1^{1/2},\tag{C18}$$

where P_0 is the projector upon the null space $\mathcal{N}(\mathsf{H}_0)$ of H_0, i.e., the longitudinal functions. The vectors $\mathbf{u}_\lambda^{\pm}$, discussed above, being eigenvectors of H_e at eigenvalue $\lambda^2\neq 0$, satisfy $\mathsf{P}_e\mathbf{u}_\lambda^{\pm}=0$, which is equivalent to the gauge condition Eq. (4.17), as can be checked explicitly. We finally note that

$$\mathsf{M}^*=\begin{pmatrix}-\partial_{\mathbf{x}}\varepsilon_1^{1/2} & \partial_{\mathbf{x}}\int m(d\omega)\omega^{-1} & 0 & 0\\ 0 & 0 & -\partial_{\mathbf{x}} & 0\end{pmatrix},$$

$$\mathsf{M}^*\mathsf{M}=\begin{pmatrix}-\partial_{\mathbf{x}}\cdot\varepsilon_{stat}(\mathbf{x})\partial_{\mathbf{x}} & 0\\ 0 & -\partial_{\mathbf{x}}^2\end{pmatrix}.\tag{C19}$$

APPENDIX D: CLASSICAL ELECTROMAGNETIC SCATTERING

1. Scattering into cones

We are interested in the asymptotic behavior for large t of

$$\mathbf{U}(t)^*\Theta(\mathbf{e}\cdot\mathbf{e}_{\mathbf{x}}-a)\Theta(x-b)\mathbf{U}(t),\tag{D1}$$

where $\mathbf{U}(t)=\exp[-i\mathbf{K}_0t]$ with $\mathbf{K}_0$ the restriction of K_1 for $\varepsilon_1=1$ to the electromagnetic subspace, i.e.,

$$\mathbf{K}_0=\mathbf{K}_0(\mathbf{p})=\begin{pmatrix}0 & \boldsymbol{\epsilon}\cdot\mathbf{p}\\ -\boldsymbol{\epsilon}\cdot\mathbf{p} & 0\end{pmatrix}.\tag{D2}$$

We note that $\mathbf{K}_0(\mathbf{p})=p\mathbf{P}_+-p\mathbf{P}_-$, where $\mathbf{P}_\pm$ are the projectors upon the eigenspaces of $\mathbf{K}_0$ with positive and negative eigenvalues, respectively. In explicit form

$$\mathbf{P}_{\pm}=\tfrac{1}{2}\begin{pmatrix}\boldsymbol{\Delta}_{\mathbf{p}} & \pm\boldsymbol{\epsilon}\cdot\mathbf{e}_{\mathbf{p}}\\ \mp\boldsymbol{\epsilon}\cdot\mathbf{e}_{\mathbf{p}} & \boldsymbol{\Delta}_{\mathbf{p}}\end{pmatrix} \tag{D3}$$

and

$$\mathbf{U}(t)=\exp[-ipt]\mathbf{P}_{+}+\exp[ipt]\mathbf{P}_{-}\,. \tag{D4}$$

Since, for $t>0$,

$$\Theta(\mathbf{e}\cdot\mathbf{e}_{\mathbf{x}}-a)=\Theta[(t^{-1}(\mathbf{e}\cdot\mathbf{x}-ax))],$$

$$\Theta(x-b)=\Theta[(t^{-1}(x-b))], \tag{D5}$$

we have to determine how $\mathbf{U}(t)*t^{-1}\mathbf{e}\cdot\mathbf{x}\mathbf{U}(t)$ and $\mathbf{U}(t)*(x/t)\mathbf{U}(t)$ behave. By differentiation and integration we obtain, using $i[\mathbf{K}_0(\mathbf{p}),\mathbf{e}\cdot\mathbf{x}]=\mathbf{K}_0(\mathbf{e})$,

$$\begin{aligned}\mathbf{U}(t)*t^{-1}\mathbf{e}\cdot\mathbf{x}\mathbf{U}(t)&=t^{-1}\mathbf{e}\cdot\mathbf{x}+t^{-1}\int_0^t du\ \mathbf{U}(u)*i[\mathbf{K}_0(\mathbf{p}),\mathbf{e}\cdot\mathbf{x}]\mathbf{U}(u)\\&=t^{-1}\mathbf{e}\cdot\mathbf{x}+t^{-1}\int_0^t du\ \mathbf{U}(u)*\mathbf{K}_0(\mathbf{e})\mathbf{U}(u)\\&=t^{-1}\mathbf{e}\cdot\mathbf{x}+t^{-1}\int_0^t du\ \{\exp[ipu]\mathbf{P}_{+}+\exp[-ipu]\mathbf{P}_{-}\}\mathbf{K}_0(\mathbf{e})\{\exp[-ipu]\mathbf{P}_{+}+\exp[ipu]\mathbf{P}_{-}\}\\&\overset{t\to\infty}{\to}\mathbf{P}_{+}\mathbf{K}_0(\mathbf{e})\mathbf{P}_{+}+\mathbf{P}_{-}\mathbf{K}_0(\mathbf{e})\mathbf{P}_{-}\\&=\mathbf{e}_{\mathbf{p}}\cdot\mathbf{e}(\mathbf{P}_{+}-\mathbf{P}_{-}).\end{aligned} \tag{D6}$$

In a similar way, with $i[\mathbf{K}_0(\mathbf{p}),x^2]=2\mathbf{K}_0(\mathbf{x})$,

$$\mathbf{U}(t)*(x/t)^2\mathbf{U}(t)=(x/t)^2+2t^{-2}\int_0^t du\ \{\exp[ipu]\mathbf{P}_{+}+\exp[-ipu]\mathbf{P}_{-}\}\mathbf{K}_0(\mathbf{x})\ \{\exp[-ipu]\mathbf{P}_{+}+\exp[ipu]\mathbf{P}_{-}\}.$$

But $\exp[ipu]\mathbf{K}_0(\mathbf{x})\exp[-ipu]=\mathbf{K}_0(\exp[ipu]\mathbf{x}\exp[-ipu])=\mathbf{K}_0(\mathbf{x}+\mathbf{e}_{\mathbf{p}}u)$, so

$$\begin{aligned}\mathbf{U}(t)*(x/t)^2\mathbf{U}(t)&=(x/t)^2+2t^{-2}\int_0^t du\ \{\exp[ipu]\mathbf{P}_{+}+\exp[-ipu]\mathbf{P}_{-}\}\{\exp[-ipu]\mathbf{K}_0(\mathbf{x})\mathbf{P}_{+}+\exp[ipu]\mathbf{K}_0(\mathbf{x})\mathbf{P}_{-}\}\\&\quad+2t^{-2}\int_0^t du\ u\{\exp[ipu]\mathbf{P}_{+}+\exp[-ipu]\mathbf{P}_{-}\}\{\exp[-ipu]\mathbf{K}_0(\mathbf{e}_{\mathbf{p}})\mathbf{P}_{+}-\exp[ipu]\mathbf{K}_0(\mathbf{e}_{\mathbf{p}})\mathbf{P}_{-}\}\\&=(x/t)^2+2t^{-2}\int_0^t du\ \{\exp[ipu]\mathbf{P}_{+}+\exp[-ipu]\mathbf{P}_{-}\}\{\exp[-ipu]\mathbf{K}_0(\mathbf{x})\mathbf{P}_{+}+\exp[ipu]\mathbf{K}_0(\mathbf{x})\mathbf{P}_{-}\}\\&\quad+2t^{-2}\int_0^t du\ u\{\exp[ipu]\mathbf{P}_{+}+\exp[-ipu]\mathbf{P}_{-}\}\{\exp[-ipu]\mathbf{P}_{+}+\exp[ipu]\mathbf{P}_{-}\}\\&\overset{t\to\infty}{\to}\boldsymbol{\Delta}_{\mathbf{p}}\begin{pmatrix}1&0\\0&1\end{pmatrix}.\end{aligned} \tag{D7}$$

Hence

$$\lim_{t\to\infty}\mathbf{U}(t)*(x/t)\mathbf{U}(t)=\boldsymbol{\Delta}_{\mathbf{p}}\begin{pmatrix}1&0\\0&1\end{pmatrix}, \tag{D8}$$

and

$$\begin{aligned}\lim_{t\to\infty}\mathbf{U}(t)*\Theta(\mathbf{e}\cdot\mathbf{e}_{\mathbf{x}}-a)\Theta(x-b)\mathbf{U}(t)&=\lim_{t\to\infty}\mathbf{U}(t)*\Theta(\mathbf{e}\cdot\mathbf{e}_{\mathbf{x}}-a)\mathbf{U}(t)\mathbf{U}(t)*\Theta(x-b)\mathbf{U}(t)\\&=\{\Theta(\mathbf{e}\cdot\mathbf{e}_{\mathbf{p}}-a)\mathbf{P}_{+}+\Theta(-\mathbf{e}\cdot\mathbf{e}_{\mathbf{p}}-a)\mathbf{P}_{-}\}\boldsymbol{\Delta}_{\mathbf{p}}\begin{pmatrix}1&0\\0&1\end{pmatrix}\\&=\Theta(\mathbf{e}\cdot\mathbf{e}_{\mathbf{p}}-a)\mathbf{P}_{+}+\Theta(-\mathbf{e}\cdot\mathbf{e}_{\mathbf{p}}-a)\mathbf{P}_{-}\,,\end{aligned} \tag{D9}$$

which is Eq. (6.4).

2. Reduction of $\mathsf{T}(z)$

We reduce $\mathsf{P}_{em}\mathsf{T}(z)\mathsf{P}_{em}$ to an object $\mathsf{t}(z)$ that only acts on electric fields by applying the Feshbach formula twice. We have ($\mathbf{K}_0$ is defined above)

$$\begin{aligned}\mathsf{X}&=\mathsf{P}_{em}\mathsf{T}(z)\mathsf{P}_{em}=[z-\mathbf{K}_0]\mathsf{P}_{em}[z-\mathsf{K}]^{-1}\mathsf{P}_{em}[z-\mathbf{K}_0]-[z-\mathbf{K}_0]\mathsf{P}_{em}\\&=[z-\mathbf{K}_0]\mathsf{P}_{em}[z-\mathbf{K}_0-\mathsf{P}_{em}\mathsf{K}\mathsf{P}_{aux}[z-\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{aux}]^{-1}\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{em}]^{-1}\mathsf{P}_{em}[z-\mathbf{K}_0]-[z-\mathbf{K}_0]\mathsf{P}_{em}.\end{aligned}\tag{D10}$$

Since $\mathsf{P}_{em}\mathsf{K}\mathsf{P}_{aux}=\{\mathsf{K}_{14}\delta_{k1}\delta_{l4}\}$ and $\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{em}=\{\mathsf{K}_{41}\delta_{k4}\delta_{l1}\}$, whereas ($\mathsf{K}_{1aux}=\mathsf{P}_{aux}\mathsf{K}_1\mathsf{P}_{aux}$)

$$[z-\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{aux}]^{-1}=[z+\mathsf{K}_{1aux}][z^2-(\mathsf{K}_{1aux})^2]^{-1}=[z^2-\omega^2]^{-1}\begin{pmatrix}z&0&0&0\\0&z&0&i\omega\\0&0&z&0\\0&-i\omega&0&z\end{pmatrix},$$

we obtain

$$\mathsf{P}_{em}\mathsf{K}\mathsf{P}_{aux}[z-\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{aux}]^{-1}\mathsf{P}_{aux}\mathsf{K}\mathsf{P}_{em}=z\mathsf{K}_{14}[z^2-\omega^2]^{-1}\mathsf{K}_{41}\mathsf{P}_{el}=z\int d\omega\ \nu(\omega)[z^2-\omega^2]^{-1}\mathsf{P}_{el}=-z\hat{\chi}(z)\mathsf{P}_{el},\tag{D11}$$

where $\mathsf{P}_{el}=\{\delta_{k1}\delta_{l1}\}$ is the projector upon the electric field (first) component of $\boldsymbol{F}$. Thus, rearranging terms and again applying the Feshbach formula,

$$\begin{aligned}\mathsf{X}&=[z-\mathbf{K}_0]\mathsf{P}_{em}[z-\mathbf{K}_0+z\hat{\chi}(z)\mathsf{P}_{el}]^{-1}\mathsf{P}_{em}[z-\mathbf{K}_0]-[z-\mathbf{K}_0]\mathsf{P}_{em}\\&=\mathsf{P}_{em}[z-\mathbf{K}_0+z\hat{\chi}(z)\mathsf{P}_{el}-z\hat{\chi}(z)\mathsf{P}_{el}]\mathsf{P}_{em}[z-\mathbf{K}_0+z\hat{\chi}(z)\mathsf{P}_{el}]^{-1}\mathsf{P}_{em}[z-\mathbf{K}_0]-[z-\mathbf{K}_0]\mathsf{P}_{em}\\&=-\mathsf{P}_{em}z\hat{\chi}(z)\mathsf{P}_{el}[z-\mathbf{K}_0+z\hat{\chi}(z)\mathsf{P}_{el}]^{-1}\mathsf{P}_{em}[z-\mathbf{K}_0+z\hat{\chi}(z)\mathsf{P}_{el}-z\hat{\chi}(z)\mathsf{P}_{el}]\mathsf{P}_{em}\\&=-z\hat{\chi}(z)\mathsf{P}_{el}+z^2\hat{\chi}(z)\mathsf{P}_{el}[z-\mathbf{K}_0+z\hat{\chi}(z)\mathsf{P}_{el}]^{-1}\mathsf{P}_{el}\hat{\chi}(z)\\&=-z\hat{\chi}(z)\mathsf{P}_{el}+z^2\hat{\chi}(z)\mathsf{P}_{el}[z-\mathsf{P}_{el}\mathbf{K}_0\mathsf{P}_{el}+z\hat{\chi}(z)\mathsf{P}_{el}-\mathsf{P}_{el}\mathbf{K}_0\mathsf{P}_{mag}[z-\mathsf{P}_{mag}\mathbf{K}_0\mathsf{P}_{mag}]^{-1}\mathsf{P}_{mag}\mathbf{K}_0\mathsf{P}_{el}]^{-1}\mathsf{P}_{el}\hat{\chi}(z)\\&=\{-z\hat{\chi}(z)+z^2\hat{\chi}(z)[z\varepsilon(z)-\mathsf{P}_{el}\mathbf{K}_0\mathsf{P}_{mag}z^{-1}\mathsf{P}_{mag}\mathbf{K}_0\mathsf{P}_{el}]^{-1}\}\mathsf{P}_{el}\\&=\{-z\hat{\chi}(z)+z^3\hat{\chi}(z)[z^2\varepsilon(z)-\mathsf{H}_0]^{-1}\}\mathsf{P}_{el}=\mathsf{t}(z)\mathsf{P}_{el}.\end{aligned}\tag{D12}$$

Here $\mathsf{P}_{em}=\mathsf{P}_{el}+\mathsf{P}_{mag}$ and we used the relations $\mathsf{P}_{el}\mathbf{K}_0\mathsf{P}_{el}=\mathsf{P}_{mag}\mathbf{K}_0\mathsf{P}_{mag}=0$, $\mathsf{P}_{el}\mathbf{K}_0=\mathsf{P}_{el}\mathbf{K}_0\mathsf{P}_{mag}$, $\mathsf{P}_{mag}\mathbf{K}_0\mathsf{P}_{el}=\mathbf{K}_0\mathsf{P}_{el}$, and $\mathsf{P}_{el}\mathbf{K}_0\mathsf{P}_{mag}\mathbf{K}_0\mathsf{P}_{el}=\mathsf{P}_{el}\mathbf{K}_0^2\mathsf{P}_{el}=\mathsf{H}_0\mathsf{P}_{el}$.

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