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Completeness of evanescent modes in layered dielectrics

Ana María Contreras Reyes and Claudia Eberlein
Department of Physics and Astronomy, University of Sussex, Falmer, Brighton BN1 9QH, England
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In the presence of a dielectric slab, the modes of the free electromagnetic field comprise traveling modes, consisting of incoming, reflected, and transmitted parts, as well as trapped modes that are subject to repeated total internal reflection and emerge as evanescent field outside the slab. Traveling modes have a continuous range of frequencies, but trapped modes occur only at certain discrete frequencies. We solve the problem of which relative weight to use when summing over all modes, as commonly required in perturbative calculations. We demonstrate the correctness of our method by showing the completeness of electromagnetic field modes in the presence of a dielectric slab. We derive a convenient method of summing over all modes by means of a single contour integral, which is very useful in standard quantum electrodynamic calculations.

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I. INTRODUCTION AND MOTIVATION

Following the surge of nanotechnology, electrodynamic and quantum electrodynamic theory in the vicinity of various types of macroscopic structures has gained new importance. Many effects that in the past were considered of mere academic interest are now measurable, could be put to good use, or might turn out a nuisance in certain nanomachines [1]. There are a range of very powerful general methods for studying quantum electrodynamics near dielectric, reflecting, or absorbing boundaries [2,3], but applying those to any particular problem usually requires extensive numerical calculations. By contrast, for a few systems of high symmetry, the electromagnetic field can be quantized by explicit mode expansion, facilitating exact analytical calculations. The by far simplest example of such a system is that of a dielectric half-space, for which the normal modes of the electromagnetic field were first calculated by Carniglia and Mandel [4]. A nondispersive dielectric half-space is a good model for studying, e.g., interactions of an atom with a partially reflecting interface [5]. However, if one needs to take into account more than just the presence of a surface, for example in cases where the finite thickness of a reflector might matter, then a nondispersive dielectric slab is the simplest choice of model. Koshravi and Loudon have studied the electromagnetic field modes in the presence of a dielectric slab [6], and used them to work out the modified rate of spontaneous emission that an atom exhibits when placed near such a slab.

In order to work out the rate of spontaneous emission of an atom near a slab of dielectric material, or the shift in the energy levels of the atom and hence the Casimir-Polder force exerted on the atom, one needs to sum over all of the electromagnetic field modes with their correct weightings. This is not normally an issue of any difficulty, as one can usually look at the modes infinitely far away from a scatterer and then infer the correct weighting by reference to the electromagnetic field modes in free space. However, as we shall see in detail below, in the case of a slab the scenario is different. One gets two kinds of modes: traveling modes that are comprised of incident, reflected, and transmitted parts, and trapped modes that consist of waves that are subject to repeated total internal reflection *ad infinitum* inside the slab and that are evanescent outside the slab. The crucial difference between these two types of modes is that while traveling modes can have any frequency (i.e., have a continuous spectrum), trapped modes occur only at certain discrete frequencies. This leads to a problem when trying to carry out a sum over all modes, as one has to decide how to add the set of continuous modes and the set of discrete modes. Thus the "sum over modes" that is part of any perturbation calculation in such a system is then actually partly an integral and partly a discrete sum, and there is no *a priori* way of seeing how to add one to the other.

Khosravi and Loudon [6] write down an equation that suggests the use of a factor of $2\pi/L$, where L is the thickness of the slab, in front of the discrete trapped modes. The factor is written down without any argument or derivation, and it is difficult to see from their paper exactly which parts of their calculation have used this factor or not. Later researchers [7] revisiting the problem of spontaneous emission near a dielectric slab have noted that Ref. [6] contains an error in the density of trapped modes, but have not further analyzed the problem nor given any details on the correct density of modes.

The purpose of the present paper is threefold: (i) to derive the correct way of summing over the electromagnetic mode functions of a mixed continuous and discrete spectrum, with explicit calculations given for the example of a dielectric slab, (ii) to prove the completeness of the mode functions for the slab and thereby the consistency of the method, and (iii) to come up with a convenient method of summing over all modes that facilitates perturbative calculations of electromagnetic effects in the presence of a dielectric slab without resorting to complicated numerical techniques but in an exact analytical manner.

The unambiguous way to a manifestly correct prescription for adding together continuous and discrete modes is to place the whole system into a large quantization volume and impose boundary conditions at the edges. This makes all modes discrete, so that they can all be combined into a discrete sum, without any ambiguity. By considering the limit of an infinite quantization volume, one can then see traveling modes emerge, and the sum over modes turns into an integral over traveling modes plus a sum over trapped modes. In this way, the correct relative weightings of the integral and the sum

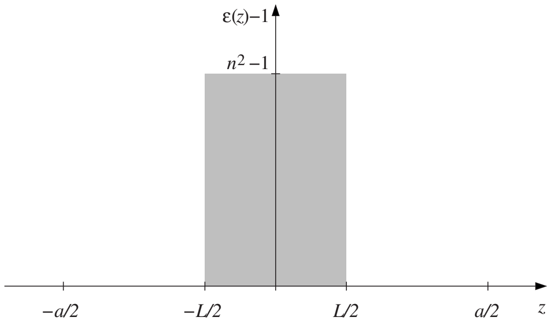

FIG. 1. The geometry considered here: the dielectric slab.

come out naturally when taking the limit of an infinite quantization volume.

We shall proceed as follows. Section II will discuss the mode functions and their general properties, and in particular the completeness relation which involves the sum over all modes. Then we shall find the traveling modes of the electromagnetic field around a dielectric slab, both in free space and in a finite quantization volume. Next we shall do the same for the trapped modes. With all modes established, we can then proceed to prove their completeness. In the process we shall show that the sum over modes can be carried out most efficiently and conveniently by deforming the integration contour in the complex k_z plane, with k_z being the component of the wave vector outside the slab that is normal to the surface of the slab. This works because the sum over trapped modes at discrete frequencies can be written as a sum of residues of an integral in the complex k_z plane, and thus, the sum over all modes, traveling and trapped, can be expressed as a contour integral in the complex k_z plane.

II. MODE FUNCTIONS AND COMPLETENESS

All explicit calculations in this paper shall be carried out for a dielectric slab of finite thickness L surrounded by vacuum. We choose a symmetric setup, as shown in Fig. 1. The dielectric will be assumed to be nondispersive and nonabsorbing, so that it is characterized just be a single number, its refractive index n, which is real and the same for all frequencies. Thus the dielectric permittivity of the configuration is

$$\varepsilon(z) = \begin{cases} n^2 & \text{for} \quad -L/2 \le z \le L/2 \\ 1 & \text{for} \quad |z| \ge L/2 \end{cases} .$$

While a highly idealized model, this system captures the essential properties of an imperfect reflector.

In order to quantize the electromagnetic field one needs to solve Maxwell's equations in the presence of the dielectric slab. A convenient way of doing this by introducing the electromagnetic potentials $\Phi(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$. In the absence of free charges one can set $\Phi(\mathbf{r},t)=0$, so that only the vector potential $\mathbf{A}(\mathbf{r},t)$ needs to be considered. In generalized Coulomb gauge,

$$\nabla \cdot [\varepsilon(z)\mathbf{A}(\mathbf{r})] = 0, \tag{1}$$

Maxwell's equations reduce to the wave equation for the vector potential,

$$\nabla \times \nabla \times \mathbf{A} + \varepsilon(\mathbf{r})\frac{\partial^2 \mathbf{A}}{\partial t^2} = \mathbf{0}. \tag{2}$$

As the dielectric function $\varepsilon(z)$ is piecewise constant, the gauge condition (1) is equivalent to the Coulomb gauge everywhere except right on the interfaces. Therefore, away from the interfaces, we can work with

$$\nabla^2 \mathbf{A} - \varepsilon(\mathbf{r})\frac{\partial^2 \mathbf{A}}{\partial t^2} = 0, \quad (z \neq \pm L/2). \tag{3}$$

Quantization is then achieved by expanding the vector field $\mathbf{A}(\mathbf{r},t)$ in terms of normal modes,

$$\mathbf{A}(\mathbf{r},t) = \sum_{\mathbf{k},\lambda} \frac{1}{\sqrt{2\omega}}[a_{\mathbf{k}\lambda}e^{-i\omega t}\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}) + a^{\dagger}_{\mathbf{k}\lambda}e^{i\omega t}\mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r})], \tag{4}$$

where the mode functions $\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r},t)$ satisfy

$$[\varepsilon(z)\omega^2 - \nabla \times \nabla \times]\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}) = \mathbf{0}. \tag{5}$$

For our piecewise constant dielectric function $\varepsilon(z)$ this simplifies to the Helmholtz equation everywhere except right on the interfaces,

$$[\varepsilon(z)\omega^2 + \nabla^2]\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}) = \mathbf{0}, \quad (z \neq \pm L/2). \tag{6}$$

Equation (5) can be rewritten as an eigenvalue problem [8],

$$\left[\frac{1}{\sqrt{\varepsilon}}\nabla \times \nabla \times \frac{1}{\sqrt{\varepsilon}}\right]\sqrt{\varepsilon}\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}) = \omega^2\sqrt{\varepsilon}\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}). \tag{7}$$

As the operator in the square brackets is Hermitean, it follows that its eigenfunctions $\sqrt{\varepsilon}\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r})$ must form an orthogonal and complete system [8]. For traveling modes all components of $\mathbf{k}$ are continuous variables, so that the orthogonality relation is

$$\int d^3\mathbf{r}\,\varepsilon(z)\mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r}) \cdot \mathbf{f}_{\mathbf{k}'\lambda'}(\mathbf{r}) = \delta^{(3)}(\mathbf{k}-\mathbf{k}')\delta_{\lambda\lambda'}. \tag{8}$$

For trapped modes the normal component k_z is a discrete variable, and then the orthogonality relation must be written

$$\int d^3\mathbf{r}\,\varepsilon(z)\mathbf{f}^*_{\mathbf{k}\lambda}(\mathbf{r}) \cdot \mathbf{f}_{\mathbf{k}'\lambda'}(\mathbf{r}) = \delta^{(2)}(\mathbf{k}_\parallel-\mathbf{k}'_\parallel)\delta_{k_z k'_z}\delta_{\lambda\lambda'}. \tag{9}$$

The completeness relation then states that the sum over all modes of $\sqrt{\varepsilon(z)}f^i_{\mathbf{k}\lambda}(\mathbf{r})\sqrt{\varepsilon(z')}f^{*j}_{\mathbf{k}\lambda}(\mathbf{r}')$ gives an identity tensor in the subspace of functions that satisfy the gauge condition (1), which for generally spatially dependent $\varepsilon(\mathbf{r})$ would be a complicated nonlocal distribution [8]. For our piecewise constant dielectric function we again use the fact that the gauge condition is equivalent to the Coulomb gauge everywhere except right on the interfaces, so that the completeness relation can be expressed in terms of the transverse delta function,

$$\int d^2\mathbf{k}_\parallel \sum_{k_z,\lambda} \sqrt{\varepsilon(z)}f^i_{\mathbf{k}\lambda}(\mathbf{r})\sqrt{\varepsilon(z')}f^{*j}_{\mathbf{k}\lambda}(\mathbf{r}') = (\delta_{ij} - \Delta^{-1}\partial_i\partial_j)\delta^{(3)}(\mathbf{r}-\mathbf{r}'), \quad (z,z' \neq \pm L/2). \tag{10}$$

Here the sum of modes consists of an integral over the vector

$\mathbf{k}_\parallel=(k_x,k_y)$ that lies parallel to the interface, and an integral and a sum over the normal component k_z for traveling and trapped modes, respectively.

Transversality can be achieved by introducing polarization vectors, such that the mode functions can be written as

$$\mathbf{f}_{\mathbf{k}\lambda}(\mathbf{r}) = \hat{\mathbf{e}}_\lambda f_{\mathbf{k}\lambda}(\mathbf{r}). \tag{11}$$

The choice of polarizations we shall work with are the transverse electric (TE) mode, for which the electric field is perpendicular to the plane of incidence,

$$\hat{\mathbf{e}}_{\text{TE}} = (-\Delta_\parallel)^{-1/2}(-i\partial_y, i\partial_x, 0), \tag{12}$$

and the transverse magnetic (TM) mode, for which the magnetic field is perpendicular to the plane of incidence,

$$\hat{\mathbf{e}}_{\text{TM}} = (\Delta\Delta_\parallel)^{-1/2}(-\partial_x\partial_z, -\partial_y\partial_z, \Delta_\parallel). \tag{13}$$

The solutions of the Helmholtz Eq. (6) can be found by considering each mode to be made up from incoming, reflected, and transmitted parts and taking into account both left- and right-incident modes. The incoming, reflected, and transmitted parts of the mode are joined at the interface, where they must satisfy the continuity conditions that follow from Maxwell's equation,

$$\mathbf{E}_\parallel \text{ continuous}, \quad \mathbf{D}_\perp \text{ continuous}, \quad \mathbf{B} \text{ continuous}. \tag{14}$$

In order to distinguish waves propagating in the positive and the negative z directions, we use the following notation for the wave vector of traveling waves in free space:

$$\mathbf{k}^\pm = (k_x, k_y, \pm k_z) = (\mathbf{k}_\parallel, \pm k_z), \tag{15}$$

and likewise for the wave vector inside the dielectric,

$$\mathbf{k}_d^\pm = (\mathbf{k}_\parallel, \pm k_{dz}). \tag{16}$$

As the frequency ω and the parallel wave vector $\mathbf{k}_\parallel$ are the same on both sides of the interface, it follows that

$$k_{dz} = \sqrt{(n^2-1)k_\parallel^2 + n^2k_z^2}, \tag{17}$$

and in reverse

$$k_z = \frac{1}{n}\sqrt{k_{dz}^2 - (n^2-1)k_\parallel^2}. \tag{18}$$

Relation (18) shows that we get two types of modes: if the argument of the square root is positive then k_z is real and the modes are traveling; if the argument of the square root is negative then k_z is pure imaginary and the modes are trapped inside the slab and evanescent outside. We shall deal with each type of mode in turn.

III. TRAVELING MODES

According to Eq. (11) the mode functions for left-incident traveling waves can be written

$$f_{\mathbf{k},\lambda}^L(\mathbf{r}) = N \times \begin{cases} e^{i\mathbf{k}^+\cdot\mathbf{r}} + R_\lambda e^{i\mathbf{k}^-\cdot\mathbf{r}}, & z \le -L/2, \\ I_\lambda e^{i\mathbf{k}_d^+\cdot\mathbf{r}} + J_\lambda e^{i\mathbf{k}_d^-\cdot\mathbf{r}}, & |z| \le L/2, \\ T_\lambda e^{i\mathbf{k}^+\cdot\mathbf{r}}, & z \ge L/2. \end{cases}$$

The application of the continuity conditions [Eq. (14)] leads to the following expressions for the reflection and transmission coefficients:

$$R_\lambda = r_\lambda \frac{1-e^{2ik_{zd}L}}{1-r_\lambda^2 e^{2ik_{zd}L}} e^{-ik_zL}, \tag{19}$$

$$T_\lambda = \frac{1-r_\lambda^2}{1-r_\lambda^2 e^{2ik_{zd}L}} e^{i(k_{zd}-k_z)L}, \tag{20}$$

where r_λ are the respective Fresnel coefficients for reflection of the TE and TM polarizations at a single interface [9],

$$r_{\text{TE}} = \frac{k_z - k_{zd}}{k_z + k_{zd}} \quad \text{and} \quad r_{\text{TM}} = \frac{n^2k_z - k_{zd}}{n^2k_z + k_{zd}}. \tag{21}$$

Because of the symmetry of the system, the mode functions for right-incident modes are obtained from those for the left-incident ones simply by inverting the z axis, i.e., by letting $z \to -z$ while leaving everything else unchanged.

A short and straightforward calculation shows that these mode functions satisfy the orthogonality relation (8) if the normalization factor is chosen as

$$N = \frac{1}{(2\pi)^{3/2}}, \tag{22}$$

as one would expect by comparison with the limit of a vanishing dielectric, $n \to 1$, where $R_\lambda \to 0$ and $T_\lambda \to 1$.

As explained earlier, we wish to discretize these modes [10] by putting our system into a quantization volume $[-a/2, a/2]$ and imposing Dirichlet boundary conditions onto the mode functions at $z=\pm a/2$. As left- and right-incident modes are incompatible with such boundary conditions, we form symmetric and antisymmetric combinations of them, which amounts to a rotation in the Hilbert space of these mode functions.

$$f_{\mathbf{k}\lambda}^{S,A}(\mathbf{r}) = \frac{N^{S,A}}{\sqrt{2}} \times \begin{cases} e^{i\mathbf{k}^+\cdot\mathbf{r}} + (R_\lambda \pm T_\lambda)e^{i\mathbf{k}^-\cdot\mathbf{r}}, & z \le -L/2, \\ (I_\lambda \pm J_\lambda)(e^{i\mathbf{k}_d^+\cdot\mathbf{r}} \pm e^{i\mathbf{k}_d^-\cdot\mathbf{r}}), & |z| \le L/2, \\ e^{i\mathbf{k}^-\cdot\mathbf{r}} + (R_\lambda \pm T_\lambda)e^{i\mathbf{k}^+\cdot\mathbf{r}}, & z \ge L/2. \end{cases}$$

Here the $\pm$ signs apply to the symmetric (S) and antisymmetric (A) modes, respectively. Applying Dirichlet boundary conditions, $f_{\mathbf{k}\lambda}^{S,A}(z=\pm a/2)=0$, leads to the dispersion relations,

$$-e^{-ik_za} = R_\lambda \pm T_\lambda \quad \text{for } S(A) \text{ modes}, \tag{23}$$

which, for any given $\mathbf{k}_\parallel$, are satisfied only by certain discrete values of k_z. Normalization according to Eq. (9) then yields in the limit of a large quantization volume,

$$\lim_{a\to\infty} N^{S,A} = \frac{1}{2\pi\sqrt{a}}. \tag{24}$$

In order to see what happens to the sum over all modes in the limit of an infinitely large quantization volume, let us look at a particular mode function. For example, the symmetric mode to the right of the slab is described by

$$f^S_{\mathbf{k}\lambda}(z \geq L/2) = \frac{N^S}{\sqrt{2}} e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel}[(R_\lambda + T_\lambda + 1)\cos k_z z + i(R_\lambda + T_\lambda - 1)\sin k_z z]. \quad (25)$$

Since $|R_\lambda|^2+|T_\lambda|^2=1$ and also $R_\lambda T^*_\lambda + R^*_\lambda T_\lambda = 0$, which is easy to see from Eqs. (19)–(21), it follows that $|R_\lambda + T_\lambda| = 1$, so that one can write

$$R_\lambda + T_\lambda = e^{2i\delta_S} \quad \text{with} \quad \delta_S \ \text{real}. \quad (26)$$

Thus we can write the mode function as

$$f^S_{\mathbf{k}\lambda}(z \geq L/2) = \sqrt{2}N^S e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel + i\delta_S}\cos(k_z z + \delta_S). \quad (27)$$

This shows explicitly that the presence of the slab in the quantization volume leads to a phase shift δ_S of the mode compared to the empty quantization volume. Dirichlet boundary conditions at $z=a/2$ then lead to

$$\frac{k_z a}{2} + \delta_S = \left(n + \frac{1}{2}\right)\pi \quad \text{with} \quad n \ \text{integer}. \quad (28)$$

This, together with Eq. (26), is a re-expression of the dispersion relation (23) for the modes. In the limit of a very large quantization volume these discrete modes move closer and closer together, so that the sum over all modes can then be turned into an integral, which, according to Eq. (28), can be expressed as an integral over k_z.

$$\sum_n \underset{a\to\infty}{\longrightarrow} \int dn = \int dk_z \left(\frac{a}{2\pi} + \frac{1}{\pi}\frac{\partial\delta}{\partial k_z}\right). \quad (29)$$

Since the derivative of the phase shift stays finite as $a\to\infty$, one can ignore the second term under the k_z integral in this limit.

Now it is straightforward to calculate the contribution to the completeness relation (10) from the sum over all traveling modes in the limit of a large quantization volume. Here we are interested in the region outside the slab, $z, z' > L/2$, where one obtains the desired transverse delta function plus an extra term,

$$\int d^2\mathbf{k}_\parallel \sum_{k_z,\lambda} \sqrt{\varepsilon(z)} f^i_{\mathbf{k}\lambda}(\mathbf{r}) \sqrt{\varepsilon(z')} f^{*j}_{\mathbf{k}\lambda}(\mathbf{r}')\Big|_{\text{trav.}} = (\delta_{ij} - \Delta^{-1}\partial_i\partial_j)\delta^{(3)}(\mathbf{r}-\mathbf{r}') + \frac{1}{(2\pi)^3}\sum_\lambda \hat{e}^i_\lambda(\partial_r)\hat{e}^{*j}_\lambda(\partial_{r'})\int d^2\mathbf{k}_\parallel \times \int_{-\infty}^{\infty} dk_z R_\lambda(k_z,\mathbf{k}_\parallel) e^{ik_z(z+z') + i\mathbf{k}_\parallel\cdot(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)}. \quad (30)$$

Equation (29) shows that this expression is the same for the discrete sum over modes with the normalization factor [Eq. (24)] in a large quantization volume and for the k_z integral over the continuous set of modes with the normalization factor [Eq. (22)] in free space.

IV. TRAPPED MODES

If a wave inside the dielectric strikes the interface with the vacuum outside at a very large angle of incidence, then it suffers total internal reflection. Because of the symmetry of the slab, once this happens on one interface, it will then also happen on the opposite side, and so forth. Thus, the repeated total internal reflections lead to a standing wave (in z direction) inside the dielectric, which is flanked by evanescent waves on the outside. These are trapped-mode solutions to the Helmholtz Eq. (6).

More specifically, this situation arises when $k_{dz} < (n^2 - 1)k^2_\parallel$, which causes the argument of the square root in Eq. (18) to become negative and hence the normal component of the wave vector outside the slab to become pure imaginary, $k_z = \pm i\kappa$. These trapped modes can be either symmetric or antisymmetric with respect to the middle of the slab,

$$f^{S,A}_{\mathbf{k}\lambda}(\mathbf{r}) = M_\lambda \times \begin{cases} \pm L^{S,A}_\lambda e^{i\mathbf{k}_\parallel\cdot\mathbf{r}+\kappa z}, & z < -L/2, \\ e^{i\mathbf{k}^+_d\cdot\mathbf{r}} \pm e^{i\mathbf{k}^-_d\cdot\mathbf{r}}, & |z| \leq L/2, \\ L^{S,A}_\lambda e^{i\mathbf{k}_\parallel\cdot\mathbf{r}-\kappa z}, & z > L/2. \end{cases}$$

Imposing the continuity conditions [Eq. (14)] at the vacuum-dielectric interface leads to the coefficients $L^{S,A}_\lambda$ and also to additional constraints on the allowed values of κ and k_{dz} in the form of dispersion relations,

$$\kappa = \begin{cases} k_{dz}\tan(k_{dz}L/2) & \text{for } (S), \quad \lambda = \text{TE}, \\ -k_{dz}\cot(k_{dz}L/2) & \text{for } (A), \quad \lambda = \text{TE}, \\ -k_{dz}\cot(k_{dz}L/2)/n^2 & \text{for } (S), \quad \lambda = \text{TM}, \\ k_{dz}\tan(k_{dz}L/2)/n^2 & \text{for } (A), \quad \lambda = \text{TM}. \end{cases} \quad (31)$$

For each mode the respective dispersion relation has to be satisfied together with Eq. (18), which gives

$$\kappa = \frac{1}{n}\sqrt{(n^2-1)k^2_\parallel - k^2_{dz}}. \quad (32)$$

Thus there are only a limited number of discrete solutions for κ and k_{dz} for each mode [11].

Since the trapped modes are discrete anyway, it makes no difference whether one uses a quantization volume $[-a,a]$ or quantizes in free space. The introduction of a quantization volume merely shifts the frequencies of the trapped modes by some amount, but in the limit $a\to\infty$ of a large quantization volume these shifts of course all vanish.

The contribution to the completeness relation (10) from the sum over all trapped modes in the region outside the slab, $z, z' > L/2$, is

$$\int d^2\mathbf{k}_\parallel \sum_{k_z\lambda} \sqrt{\varepsilon(z)} f^i_{\mathbf{k}\lambda}(\mathbf{r}) \sqrt{\varepsilon(z')} f^{*j}_{\mathbf{k}\lambda}(\mathbf{r}')\Big|_{\text{evan.}} = \sum_\lambda \hat{e}^i_\lambda(\partial_r)\hat{e}^j_\lambda(\partial_{r'})\int d^2\mathbf{k}_\parallel \sum_{k_z} |M_\lambda|^2 |L_\lambda|^2 e^{-\kappa(z+z') + i\mathbf{k}_\parallel\cdot(\mathbf{r}_\parallel - \mathbf{r}'_\parallel)}, \quad (33)$$

where $|L_\lambda|$ carries no upper index as it turns out that $|L^S_\lambda| = |L^A_\lambda|$. The normalization factors $M_{\text{TE}}, M_{\text{TM}}$ are determined by Eq. (9). The combinations with $|L_\lambda|$, as needed above, come out as

$$|M_{\mathrm{TE}}|^2|L_{\mathrm{TE}}|^2=\frac{k_{dz}^2e^{\kappa L}}{(2\pi)^2(n^2-1)\left[n^2\frac{L}{2}(k_\parallel^2-\kappa^2)+k_\parallel^2/\kappa\right]},\tag{34}$$

$$|M_{\mathrm{TM}}|^2|L_{\mathrm{TM}}|^2=\frac{k_{dz}^2e^{\kappa L}}{(2\pi)^2(n^2-1)\left[\frac{L}{2}(k_\parallel^2+n^2\kappa^2)+k_\parallel^2/\kappa\right]}.\tag{35}$$

V. PROOF OF COMPLETENESS

In order to prove the completeness relation (10) we need to sum over all modes, both traveling and trapped. In a finite quantization volume there is no ambiguity in how to carry out this sum, as all modes are discrete. In the limit of a large quantization volume one obtains from adding Eqs. (30) and (33) in the region outside the slab $z,z'>L/2$,

$$\begin{aligned}&\int d^2\mathbf{k}_\parallel\sum_{k_z,\lambda}\sqrt{\varepsilon(z)}f^i_{\mathbf{k}\lambda}(\mathbf{r})\sqrt{\varepsilon(z')}f^{*j}_{\mathbf{k}\lambda}(\mathbf{r}')\\&=(\delta_{ij}-\Delta^{-1}\partial_i\partial_j)\delta^{(3)}(\mathbf{r}-\mathbf{r}')+\sum_\lambda\hat{e}^i_\lambda(\partial_r)\hat{e}^{*j}_\lambda(\partial_{r'})\int d^2\mathbf{k}_\parallel\\&\quad\times\left[\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}dk_zR_\lambda(k_z,\mathbf{k}_\parallel)e^{ik_z(z+z')+i\mathbf{k}_\parallel\cdot(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)}\right.\\&\quad\left.+\sum_{k_z}|M_\lambda|^2|L_\lambda|^2e^{-\kappa(z+z')+i\mathbf{k}_\parallel\cdot(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)}\right].\end{aligned}\tag{36}$$

In the limit $a\to\infty$ of an infinite quantization volume it becomes apparent that the exact same relation holds in free space, i.e., without any quantization volume, but the sum over modes then consists of an integral over traveling modes and a discrete sum over trapped modes, and the traveling modes have the plane-wave normalization constant [Eq. (22)]. Thus traveling and trapped modes are added together without any additional weighting factor, in contrast to the factor $2\pi/L$ suggested by Eq. (4.13) of [6].

In order to evaluate the right-hand side of Eq. (36) we work out the integral over k_z in the second term by closing the contour in the complex plane. As $z+z'-L>0$, we close the contour in the upper half-plane. The analytic properties of the integrand become immediately apparent once one rewrites the reflection coefficients [Eq. (19)] with Eq. (21) as

$$R_{\mathrm{TE}}=\frac{(k_z^2-k_{dz}^2)e^{-ik_zL}}{[k_z-ik_{dz}\tan(k_{dz}L/2)][k_z+ik_{dz}\cot(k_{dz}L/2)]}\tag{37}$$

$$R_{\mathrm{TM}}=\frac{\left(k_z^2-\frac{k_{dz}^2}{n^4}\right)e^{-ik_zL}}{\left[k_z-i\frac{k_{dz}}{n^2}\tan(k_{dz}L/2)\right]\left[k_z+i\frac{k_{dz}}{n^2}\cot(k_{dz}L/2)\right]}.\tag{38}$$

Thus the reflection coefficients have poles in the upper half-plane at exactly those values of $k_z=i\kappa$ where, according to the dispersion relation (31), the trapped modes occur. Closing the contour in the upper half-plane, we pick up residues from these poles. When calculating these residues we need to bear in mind that the two independent variables are k_z and $k_\parallel$ and that, according to Eq. (17), k_{dz} is a function of those. So, for example, in order to calculate the residue of the nth pole of R_{TE} at $k_z=i\kappa_n$ that corresponds to a symmetric trapped mode, we write R_{TE} as a product of the denominator that has the pole and some function $F(k_z,k_\parallel)$,

$$R_{\mathrm{TE}}=\frac{F(k_z,k_\parallel)}{k_z-ik_{dz}\tan(k_{dz}L/2)}.\tag{39}$$

Then we use L'Hospital's rule to take the limit when calculating the residue,

$$\begin{aligned}\mathrm{Res}[R_{\mathrm{TE}}]_{k_z=i\kappa_n}&=\lim_{k_z\to i\kappa_n}\frac{F(k_z,k_\parallel)}{k_z-ik_{dz}\tan(k_{dz}L/2)}(k_z-i\kappa_n)\\&=\lim_{k_z\to i\kappa_n}\frac{F(k_z,k_\parallel)}{1-i\frac{\partial}{\partial k_z}[k_{dz}\tan(k_{dz}L/2)]}.\end{aligned}\tag{40}$$

We calculate the residues around the second set of poles that correspond to the antisymmetric trapped modes in exactly the same way and obtain in total

$$\begin{aligned}&\frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}dk_zR_{\mathrm{TE}}(k_z,\mathbf{k}_\parallel)e^{ik_z(z+z')}\\&\quad=-\sum_{k_z}|M_{\mathrm{TE}}|^2|L_{\mathrm{TE}}|^2e^{-\kappa(z+z')},\end{aligned}\tag{41}$$

where the sum on the right-hand side runs over the locations of the poles, i.e., over the solutions of the dispersion relation (31) for TE modes. Exactly the same procedure works also for the TM modes, giving a result analogous to Eq. (41).

Thus we find that the term in the square brackets on the right-hand side of Eq. (36) is zero for each polarization, so that in the region $z,z'>L/2$ Eq. (36) yields the completeness relation (10), which we had set out to prove.

While the proof of the completeness relation is an important check on the derivation of the modes, the most valuable exploit of the above calculation for practical purposes is the knowledge of how to sum such modes. A typical second-order perturbative calculation in nonrelativistic quantum electrodynamics, e.g., of the Casimir-Polder force on an atom near a dielectric slab, involves a product of mode functions and a sum over intermediate photon states. This sum again consists of an integral over traveling modes and a discrete sum over trapped modes, which is awkward to handle. Following the derivations of this paper in reverse direction,

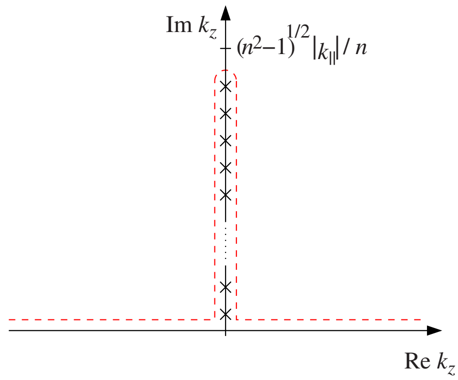

FIG. 2. (Color online) The integration path $\mathcal{C}$ in the complex k_z plane.

one can convert the sum over discrete trapped modes into a contour integral and then combine this with the integral over traveling modes. This constitutes a significant simplification of the calculation because the resulting contour integrals are easily evaluated through complex-variable techniques.

Provided the rest of the integrand $Q(k_z,\mathbf{k}_\parallel)$ is analytic in the vicinity of the poles of the reflection coefficients R_{TE} and R_{TM} on the positive imaginary k_z axis, we can evaluate such a typical sum over all modes in the region $z,z'>L/2$ by writing it as a contour integral in the complex k_z plane,

$$\int d^2\mathbf{k}_\parallel \sum_{k_z} Q(k_z,\mathbf{k}_\parallel)\sqrt{\varepsilon(z)}f_{\mathbf{k}}(\mathbf{r})\sqrt{\varepsilon(z')}f^*_{\mathbf{k}}(\mathbf{r}')\Big|_{\text{all modes}}$$
$$= \frac{1}{(2\pi)^3}\int d^3\mathbf{k}\, Q(k_z,\mathbf{k}_\parallel)e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}$$
$$+ \frac{1}{(2\pi)^3}\int d^2\mathbf{k}_\parallel \int_{\mathcal{C}} dk_z Q(k_z,\mathbf{k}_\parallel)e^{ik_z(z+z')+i\mathbf{k}_\parallel\cdot(\mathbf{r}_\parallel-\mathbf{r}'_\parallel)}$$
$$\times [R_{\text{TE}}(k_z,\mathbf{k}_\parallel)+R_{\text{TM}}(k_z,\mathbf{k}_\parallel)] \qquad (42)$$

where the integration path $\mathcal{C}$ encloses all poles of R_{TE} and R_{TM} on the positive imaginary k_z axis as shown in Fig. 2. The first term on the right-hand side of Eq. (42), corresponding to the delta function on the right-hand side of the completeness relation (10), is the free-space contribution, whereas the second term with the contour integral along $\mathcal{C}$ arises only due to the presence of the slab. Renormalization of course removes the free-space part, so that the quantity of interest comes out of the second term, and thus very conveniently from a single contour integral, greatly simplifying the calculation of such quantities.

VI. SUMMARY AND CONCLUSIONS

We have shown how one quantizes the electromagnetic field in the presence of a typical layered dielectric. The mode functions of the field are relatively easy to derive, but summing them, as is required in standard perturbation calculations, can be problematic because the spectrum of modes comprises both discrete and continuous parts and there is no *a priori* prescription on their relative weighting in a sum over all modes. For a single dielectric slab of arbitrary thickness we have shown how to get around this problem by introducing a quantization volume, which makes all modes discrete. In the limit of an infinitely large quantization volume we have recovered the modes as derived in free space and thereby we have shown unambiguously how to correctly sum continuous and discrete modes. We have demonstrated the correctness of our approach and procedure by proving the completeness of all modes. In the process we have transformed the integral over the continuous part of the spectrum into a sum over residues around the poles of the reflection coefficients. As is well known from scattering theory [12], the reflection coefficient has poles wherever there are bound states. Therefore one can apply the same procedure in reverse and express the sum over the discrete modes as a contour integral in the complex plane, which can then be combined with the integral over the continuous part of the spectrum. The resulting formula is significantly simpler than the original sum over all modes, and it is extremely useful for perturbative calculations in nonrelativistic quantum electrodynamics near layered dielectric structures.

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perpendicular to the slab, in z direction, that is being discretized by imposing boundary conditions at the edges of a quantization box in z direction.

[11] For the symmetric TE and the antisymmetric TM modes the number of solutions is given by the integer part of $[\sqrt{n^2-1}k_{\|}L/(2\pi)+1]$, and for the symmetric TM and the antisymmetric TE modes by the integer part of $[\sqrt{n^2-1}k_{\|}L/(2\pi)+1/2]$.

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