Propagator study of the selvedge field in linear and nonlinear nonlocal jellium optics

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Describing matter on the basis of an inhomogeneous jellium model, a nonlocal electromagnetic propagator formalism is used to study the selvedge field in linear and nonlinear nonlocal surface optics of metals. Fundamental coupled integral equations for the divergence-free and rotational-free parts of the selvedge field are established and solved analytically in a novel way. Progress is obtained in the analysis by dividing the kernels into parts which are separable and nonseparable in the observation and source coordinates. Special emphasis is devoted to an investigation of the selvedge field associated with surface second-harmonic generation, and a detailed comparison to propagator formalisms of other authors is presented.

I. INTRODUCTION

At the outermost atomic layers of a metal surface, the density of conduction-band electrons changes from zero (in vacuum) to the bulk value of the metal.[1,2] The interaction of light with the conduction electrons in this so-called density-profile region is of fundamental interest for our understanding of the intricate linear and nonlinear coupling between electromagnetic waves and the many-particle system of inhomogeneous jellium systems. To describe the light-jellium interaction one requires a calculation of the light-induced current density caused by a prescribed electromagnetic field and, subsequently, a self-consistent determination of the local field. The links between the current density and the electric field are the linear and nonlinear response tensors which for jellium optics normally have to be calculated in a nonlocal approach. To determine *ab initio* the response tensors connected to the inhomogeneous jellium of a metal surface is in itself a formidable task. A very popular and efficient scheme for attacking the problem, conceptually, is based on the well-known and fundamental Kubo formalism.[3] The Kubo formalism for many-electron systems, however, does not allow us in any simple manner to extract details about the behavior of the light-perturbed response of the surface region. Thus, in the context of nonlocal metal optics, usually, one has to use the random-phase-approximation (RPA) theory,[4-8] or even simpler, microscopic models, e.g., the finite (FB)[9,10] or infinite-barrier (IB) model,[11] the semiclassical infinite-barrier (SCIB) model,[12,16] the Boltzmann-equation (BE) model in the relaxation-time approximation,[13] or the hydrodynamic (HY) model.[17] In the present work we shall assume that the nonlocal response tensors are known, and hence devote our study to a description of qualitative and analytical schemes for calculating the selvedge fields. We shall address the problem on the basis of an electromagnetic propagator formalism.

The analysis is organized as follows. In Sec. II the fundamental integral equation for the selvedge field is established. The integral equation is set up so that the "background" solution is that of the SCIB model. The kernel of the integral equation contains the screened, so-called nonlocal, electromagnetic propagator associated with the SCIB model.[18,19] We split the integral equation into s- and p-polarized parts which are uncoupled. The p-polarized part is further divided into two coupled integral equations for the divergence-free and the rotational-free parts of the selvedge fields. In Sec. III our analysis deviates radically from previous propagator descriptions in that we use a recent analysis[19] of the tensor-product structure of the nonlocal propagator to divide the kernels into separable and nonseparable parts. By a separable part we mean a part which can be written as a product of functions of the coordinates of the observation and source spaces. In Sec. IV, we discuss various approximate schemes for calculating the selvedge field. Thus we present an "exact" solution of the integral equations based on *brute force* neglect of the nonseparable parts of the kernels. We present a sort of first-order Born approximation where the exact solution to the separable problem is taken as the zeroth-order solution. Finally, we investigate the solution obtained for the rotational-free part of the selvedge field if it is assumed that the nonseparable parts of the divergence-free kernels are constant throughout the so-called inner and outer selvedge regions. The analyses in Secs. II–IV, which are essentially linear, can be applied in linear, nonlocal optics, of course, but also in studies of the *free fields* associated with parametric, nonlinear phenomena. In Sec. V we discuss the background field in nonlinear surface optics taking second-harmonic generation as an example, and in Sec. VI we consider the calculation of the electric field exterior to the selvedge region. In Sec. VII we compare our analysis to previous propagator theories. Thus, for second-harmonic generation we demonstrate how our formalism contains a recent theory of Guyot-Sionnest, Chen, and Shen[20] as a special case, and we discuss the progress obtained in the present work compared to the work of Guyot-Sionnest *et al.*[20] For the selvedge-field problem in linear surface optics we compare, in detail, our results to those obtained in the prominent works by Bagchi, Barrera, and Rajagopal[21] and by Sipe.[22] In the propagator formalism by Bagchi *et al.*,[21] the classical Fresnel problem with the associated *local* propagator is taken as the background problem and in the vacuum propagator work of Sipe[22] a nonretarded propagator part is separated off.

On the basis of the results presented in this paper, quantitative numerical studies of the selvedge field associated with second-harmonic generation from a metal surface are conveniently undertaken. Also, the present formalism offers an obvious possibility for incorporating lattice effects in the analysis of optical selvedge responses.

One reason for undertaking a conceptual study of the selvedge field within the framework of the jellium model is that the possibilities for using optical methods, and equally promising nonlinear methods such as second-harmonic generation[23–31] and Raman and Brillouin scattering,[32–35] as tools for studies of the dynamical and structural physical properties of various types of surfaces and interfaces in a highly reliable way, in my opinion, rely on our knowledge of the local field inside the selvedge.

II. FUNDAMENTAL INTEGRAL EQUATIONS FOR THE SELVEDGE FIELD

Let us consider the interaction of a monochromatic electromagnetic field of angular frequency Ω with a system of particles, and let us assume that the light-unperturbed state of the system is invariant against arbitrary translations in the xy plane of a Cartesian (x,y,z) coordinate system. Now, if we restrict our analysis to electric fields $\mathbf{E}(z;Q_\parallel,\Omega)$, which in a plane-wave expansion consist of only a single wave-vector component, denoted by $\mathbf{Q}_\parallel$, perpendicular to the z axis, the basic equation for the description of the field-matter interaction in the electromagnetic propagator formalism is[36]

$$\begin{aligned}\mathbf{E}(z;\mathbf{Q}_\parallel,\Omega) &= \mathbf{E}^{(0)}(z;\mathbf{Q}_\parallel,\Omega)\\ &\quad -i\mu_0\Omega\int_{-\infty}^{\infty}\overleftrightarrow{G}(z,z';\mathbf{Q}_\parallel,\Omega)\cdot\mathbf{J}_{\text{ext}}(z';\mathbf{Q}_\parallel,\Omega)dz' .\end{aligned} \tag{2.1}$$

The idea behind writing the fundamental equation in the form of Eq. (2.1) is the following. Due to the heavy difficulties in solving the basic problem in a physically appealing way, i.e., by analytic means or numerically in such a manner that the solution offers a simple interpretation, one takes as a starting point a study of a more tractable problem. The solution for this so-called background problem we denote by $\mathbf{E}^{(0)}(z;\mathbf{Q}_\parallel,\Omega)$. In *linear* optics, we choose the background field $\mathbf{E}^{(0)}$ as the solution to a "nearby" problem. Associated with this nearby problem is a dyadic electromagnetic propagator, named $\overleftrightarrow{G}(z,z';\mathbf{Q}_\parallel,\Omega)$ in Eq. (2.1). What do we mean by a nearby problem in the present context? A nearby problem is one for which (i) a simple, e.g., analytic solution can be found for $\mathbf{E}^{(0)}$ *and* $\overleftrightarrow{G}$, and (ii) the solution contains in a qualitative sense the gross features of the solution to the basic problem. In nonlocal metal optics, treated essentially in the jellium approximation, a very attractive background solution is the so-called semiclassical infinite-barrier (SCIB) solution. Many authors have studied the SCIB model[12–16] in nonlocal metal optics and investigated the $\mathbf{E}^{(0)}$ solution. Since the present author has also succeeded in constructing the associated electromagnetic propagator $\overleftrightarrow{G}$ (Ref. 18) and presented a simple, physical interpretation of its structure,[19] we shall take as the background solution that of the SCIB model. One should emphasize that the background field $\mathbf{E}^{(0)}$ in parametric second-harmonic generation studies besides the SCIB contribution contains a prescribed (if the linear field is known) contribution stemming from the *forced* nonlinear current density generated by the fundamental field inside the selvedge,[36,37] cf. Sec. VI. We note that the SCIB model is an essentially nonlocal model incorporating (i) collective polariton and plasmon excitations and electron-hole pair excitations in the jellium, and (ii) specular surface-scattering of electrons in an approximation excluding quantum interference effects. The SCIB propagator incorporates (i) the screening effects stemming from the above-mentioned excitations and (ii) the reflection and transmission properties of the field, from the inside or the outside of the metal, at the sharp metal-vacuum boundary in a way where all the vectorial properties of the field are retained.

Equation (2.1) is an integral equation for the electric field $\mathbf{E}(z;\mathbf{Q}_\parallel,\Omega)$ of the basic problem, since the so-called "external" (ext) current density $\mathbf{J}_{\text{ext}}(z';\mathbf{Q}_\parallel,\Omega)$ is related to the field $\mathbf{E}(z;\mathbf{Q}_\parallel,\Omega)$. In the present work, where we are interested in determining the electromagnetic field inside (and outside) the metal selvedge, defined here as the region where the exact, linear conductivity response function deviates from that of the SCIB model (which we take as the background model), the external current density is related linearly and nonlocally to the field as follows:

$$\mathbf{J}_{\text{ext}}(z;\mathbf{Q}_\parallel,\Omega)=\int_{\text{SE}}\overleftrightarrow{\sigma}^{\text{SE}}(z,z';\mathbf{Q}_\parallel,\Omega)\cdot\mathbf{E}(z';\mathbf{Q}_\parallel,\Omega)dz' , \tag{2.2}$$

where

$$\overleftrightarrow{\sigma}^{\text{SE}}(z,z';\mathbf{Q}_\parallel,\Omega)=\overleftrightarrow{\sigma}(z,z';\mathbf{Q}_\parallel,\Omega)-\overleftrightarrow{\sigma}^{\text{SCIB}}(z,z';\mathbf{Q}_\parallel,\Omega) \tag{2.3}$$

is the selvedge (SE) linear conductivity response tensor, given as the difference between the "exact" linear conductivity response tensor $\overleftrightarrow{\sigma}(z,z';\mathbf{Q}_\parallel,\Omega)$ [calculated for instance in the random-phase-approximation (RPA) approach] and that associated with the SCIB model, i.e., $\overleftrightarrow{\sigma}^{\text{SCIB}}(z,z';\mathbf{Q}_\parallel,\Omega)$. Due to the finite range, i.e., in practice often a few interatomic distances, of the selvedge response tensor, we have indicated in Eq. (2.2) that the integral extends over the essentially finite selvedge region (length).

Now, by combining Eqs. (2.1) and (2.2) we obtain the following basic integral equation for the field:

$$\begin{aligned}\mathbf{E}(z;\mathbf{Q}_\parallel,\Omega) &= \mathbf{E}^{(0)}(z;\mathbf{Q}_\parallel,\Omega)\\ &\quad +\int_{\text{SE}}\overleftrightarrow{K}(z,z';\mathbf{Q}_\parallel,\Omega)\cdot\mathbf{E}(z';\mathbf{Q}_\parallel,\Omega)dz' ,\end{aligned} \tag{2.4}$$

where the dyadic kernel $\overleftrightarrow{K}(z,z';\mathbf{Q}_\parallel,\Omega)$, determined via a nonlocal calculation, is given by

$$\overleftrightarrow{K}(z,z';\mathbf{Q}_{\parallel},\Omega)=-i\mu_0\Omega\int_{SE}\overleftrightarrow{G}(z,z'';\mathbf{Q}_{\parallel},\Omega)\cdot\overleftrightarrow{\sigma}^{SE}(z'',z';\mathbf{Q}_{\parallel},\Omega)dz'' . \quad (2.5)$$

In writing Eq. (2.4) we have stressed that $\mathbf{J}_{ext}$ is different from zero inside the selvedge, only.

To make progress in our analysis we split the electric field into two parts, i.e.,

$$\mathbf{E}(z;\mathbf{Q}_{\parallel},\Omega)=\mathbf{E}_T(z;\mathbf{Q}_{\parallel},\Omega)+\mathbf{E}_L(z;\mathbf{Q}_{\parallel},\Omega) , \quad (2.6)$$

which obey the conditions

$$\left[i\mathbf{Q}_{\parallel}+\mathbf{e}_z\frac{\partial}{\partial z}\right]\cdot\mathbf{E}_T(z;\mathbf{Q}_{\parallel},\Omega)=0 , \quad (2.7)$$

and

$$\left[i\mathbf{Q}_{\parallel}+\mathbf{e}_z\frac{\partial}{\partial z}\right]\times\mathbf{E}_L(z;\mathbf{Q}_{\parallel},\Omega)=\mathbf{0} , \quad (2.8)$$

respectively, $\mathbf{e}_z$ being a unit vector in the z direction. The conditions in Eqs. (2.7) and (2.8) have been chosen in such a way that the *total* field $\mathbf{E}(\mathbf{r};\omega)$ ($\mathbf{r}$ is a space coordinate), having plane-wave character parallel to the vacuum-metal surface, is divided into a divergence-free (T) and a rotational-free (L) part. The division in Eq. (2.6) implies that the basic integral equation in (2.4) can be split into the following two *coupled* integral equations for the divergence-free and rotational-free parts of the electric field:

$$\mathbf{E}_T(z)=\mathbf{E}_T^{(0)}(z)+\int_{SE}\overleftrightarrow{K}_T(z,z')\cdot[\mathbf{E}_T(z')+\mathbf{E}_L(z')]dz' , \quad (2.9)$$

and

$$\mathbf{E}_L(z)=\mathbf{E}_L^{(0)}(z)+\int_{SE}\overleftrightarrow{K}_L(z,z')\cdot[\mathbf{E}_T(z')+\mathbf{E}_L(z')]dz' , \quad (2.10)$$

in a notation where we have kept the dependence of the different quantities on $\mathbf{Q}_{\parallel}$ and Ω implicit. The vectors $\mathbf{E}_T^{(0)}$ and $\mathbf{E}_L^{(0)}$ are of course those associated with the divergence-free and rotational-free part of the background field, respectively. How to split the kernel correctly into its T and L parts, i.e.,

$$\overleftrightarrow{K}(z,z')=\overleftrightarrow{K}_T(z,z')+\overleftrightarrow{K}_L(z,z') , \quad (2.11)$$

can be inferred directly from the corresponding division of the SCIB propagator $\overleftrightarrow{G}(z,z')$, cf. Eq. (2.5). For a detailed analysis of the tensor-product structure of $\overleftrightarrow{G}(z,z')$ and of the associated division the reader is referred to Ref. 19.

In the jellium approximation s- and p-polarized electromagnetic fields are uncoupled so that Eqs. (2.9) and (2.10) can be further simplified. Thus, by choosing the direction of $\mathbf{Q}_{\parallel}$ parallel to the x axis, i.e., $\mathbf{Q}_{\parallel}\|\mathbf{e}_x$, where $\mathbf{e}_x$ is a unit vector in the positive x direction, the kernels take the form

$$\overleftrightarrow{K}_I(z,z')=\begin{bmatrix}K_{I,xx} & 0 & K_{I,xz}\\ 0 & \delta_{I,T}K_{T,yy} & 0\\ K_{I,zx} & 0 & K_{I,zz}\end{bmatrix} , \quad I=T \text{ or } L \quad (2.12)$$

where $\delta_{T,T}=1$ and $\delta_{L,T}=0$. The decoupling of the s and p polarizations enables us to introduce a *truncated* coordinate representation for the fields and kernels. Thus, we employ the following notation for the fields:

$$\mathbf{e}_T^s(z)\equiv e_T^s(z)\mathbf{e}_y , \quad (2.13)$$

$$\mathbf{e}_T^p(z)\equiv e_{T,x}^p\mathbf{e}_x+e_{T,z}^p\mathbf{e}_z\equiv\begin{bmatrix}e_{T,x}^p(z)\\ e_{T,z}^p(z)\end{bmatrix} , \quad (2.14)$$

$$\mathbf{e}_L^p(z)\equiv e_{L,x}^p\mathbf{e}_x+e_{L,z}^p\mathbf{e}_z\equiv\begin{bmatrix}e_{L,x}^p(z)\\ e_{L,z}^p(z)\end{bmatrix} . \quad (2.15)$$

We note that $\mathbf{e}_L^s=\mathbf{0}$ and that $\mathbf{E}_T=\mathbf{e}_T^s+\mathbf{e}_T^p$ and $\mathbf{E}_L=\mathbf{e}_L^p$. Equations corresponding to (2.13)–(2.15) can be written down for the background field $\mathbf{E}^{(0)}$ also, cf. Eqs. (2.19)–(2.21) below. The truncated tensor notations for the kernels are

$$K_T^s\equiv K_{T,yy} , \quad (2.16)$$

and

$$\overleftrightarrow{K}_T^p\equiv\begin{bmatrix}K_{T,xx} & K_{T,xz}\\ K_{T,zx} & K_{T,zz}\end{bmatrix} , \quad (2.17)$$

$$\overleftrightarrow{K}_L^p\equiv\begin{bmatrix}K_{L,xx} & K_{L,xz}\\ K_{L,zx} & K_{L,zz}\end{bmatrix} . \quad (2.18)$$

By inserting Eqs. (2.13)–(2.18) into Eqs. (2.9) and (2.10), we obtain the results

$$e_T^s(z)=e_T^{(0)s}(z)+\int_{SE}K_T^s(z,z')e_T^s(z')dz' , \quad (2.19)$$

$$\mathbf{e}_T^p(z)=\mathbf{e}_T^{(0)p}(z)+\int_{SE}\overleftrightarrow{K}_T^p(z,z')\cdot[\mathbf{e}_T^p(z')+\mathbf{e}_L^p(z')]dz' , \quad (2.20)$$

$$\mathbf{e}_L^p(z)=\mathbf{e}_L^{(0)p}(z)+\int_{SE}\overleftrightarrow{K}_L^p(z,z')\cdot[\mathbf{e}_T^p(z')+\mathbf{e}_L^p(z')]dz' , \quad (2.21)$$

in truncated notation. The s-polarized part of the field is divergence-free and the associated basic integral equation (2.19) is a scalar one. The p-polarized field, on the other hand, consists of both a divergence-free and a rotational-free part. These parts are coupled and the basic vectorial integral equations are (2.20) and (2.21).

It appears from Eqs. (2.19)–(2.21) that once the field *inside* the selvedge is determined via the basic integral equations, the field exterior to the selvedge can be obtained by *essentially* straightforward integrations of *known* functions over the selvedge (see Sec. VI).

III. STRUCTURE OF THE KERNEL

To make progress in our analysis of the basic integral equations [(2.19)–(2.21)] for the selvedge field, we take as a starting point the result of a recent investigation[19] of the tensor-product structure of the SCIB propagator, $\overleftrightarrow{G}(z,z'')$. We assume that the sharp-boundary metal occupies the domain $z>0$, the rest of the space being vacuum. Furthermore, the following superscript notation is used: $\ll$ $(z''<0,z<0)$, $<>$ $(z''<0,z>0)$, $><$ $(z''>0,z<0)$, and $\gg$ $(z''>0,z>0)$. Thus, by denoting the Heaviside unit step function by Θ, we write

$$\begin{aligned}\overleftrightarrow{G}(z,z'')=&\Theta(-z'')\Theta(-z)\overleftrightarrow{G}^{\ll}(z,z'')\\&+\Theta(-z'')\Theta(z)\overleftrightarrow{G}^{<>}(z,z'')\\&+\Theta(z'')\Theta(-z)\overleftrightarrow{G}^{><}(z,z'')\\&+\Theta(z'')\Theta(z)\overleftrightarrow{G}^{\gg}(z,z'')\ .\end{aligned} \tag{3.1}$$

The substructure of $\overleftrightarrow{G}^{\ll}(z,z'')$ is

$$\overleftrightarrow{G}^{\ll}(z,z'')=\overleftrightarrow{D}^{\ll}_{TT}(z-z'')+\overleftrightarrow{I}^{\ll}_{TT}(z+z'')+\overleftrightarrow{g}^{\ll}_{LL}(z-z'')\ , \tag{3.2}$$

where $\overleftrightarrow{D}^{\ll}_{TT}$ and $\overleftrightarrow{I}^{\ll}_{TT}$ denote the so-called direct (D) and indirect (I) contributions to the propagator, respectively, and $\overleftrightarrow{g}^{\ll}_{LL}$ the self-field contribution. The subscripts given to the propagators are to be interpreted as follows. Multiplying the propagator in consideration with $\exp[iQ_{\parallel}(x-x'')]$, the new propagator is divergence-free (T) or rotational-free (L) in the (x,y,z) coordinates if the subscript to the right is T or L, respectively. The subscript to the left indicates whether the new propagator *transposed* is divergence-free (T) or rotational-free (L) in the (x'',y'',z'') coordinates. The dyadic Green's functions $\overleftrightarrow{G}^{<>}$ and $\overleftrightarrow{G}^{><}$ have the substructures

$$\overleftrightarrow{G}^{<>}(z,z'')=\overleftrightarrow{G}^{<>}_{TT}(z,z'')+\overleftrightarrow{G}^{<>}_{TL}(z,z'') \tag{3.3}$$

and

$$\overleftrightarrow{G}^{><}(z,z'')=\overleftrightarrow{G}^{><}_{TT}(z,z'')+\overleftrightarrow{G}^{><}_{LT}(z,z'') \tag{3.4}$$

in the above-mentioned subscript and superscript notation. The propagator $\overleftrightarrow{G}^{\gg}$ has the most complicated substructure, i.e.,

$$\begin{aligned}\overleftrightarrow{G}^{\gg}(z,z'')=&\overleftrightarrow{D}^{\gg}_{TT}(z-z'')+\overleftrightarrow{D}^{\gg}_{LL}(z-z'')\ ,\\&+\overleftrightarrow{I}^{\gg}_{TT}(z,z'')+\overleftrightarrow{I}^{\gg}_{TL}(z,z'')\\&+\overleftrightarrow{I}^{\gg}_{LT}(z,z'')+\overleftrightarrow{I}^{\gg}_{LL}(z,z'')+\overleftrightarrow{g}^{\gg}_{LL}(z-z'')\ ,\end{aligned} \tag{3.5}$$

where, as in Eq. (3.2), the direct, indirect, and self-field contributions are denoted by D, I, and g, respectively. A schematic illustration of the 14 propagator terms in Eqs. (3.2)–(3.5) is shown in Fig. 1.

Now, by substituting Eqs. (3.1)–(3.5) into Eq. (2.5), it is realized that the $\overleftrightarrow{K}_T$ and $\overleftrightarrow{K}_L$ kernels of Eq. (2.11) have the substructures

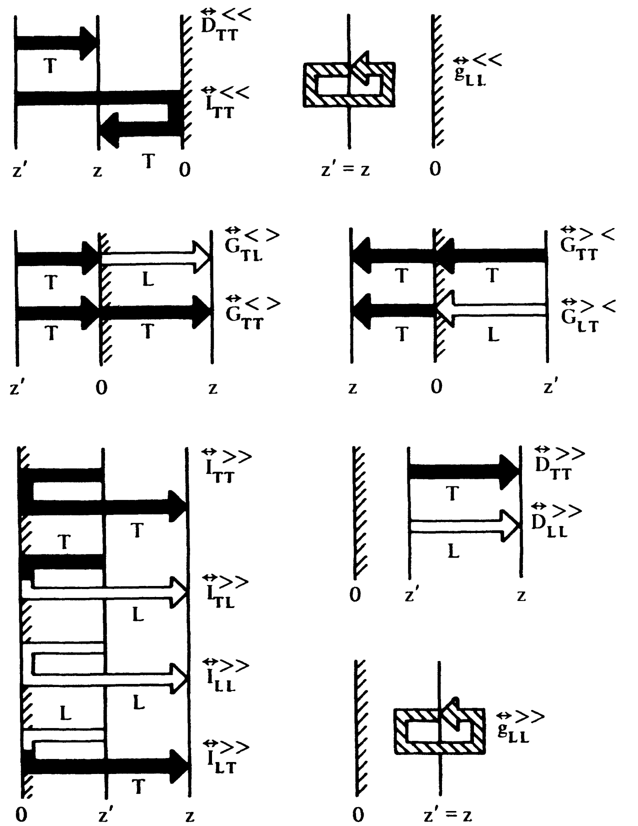

FIG. 1. Schematic illustration of the 14 terms of the screened electromagnetic propagator $\overleftrightarrow{G}(z,z')$. Within the framework of the SCIB model, this propagator describes, in a system of adjacent metal-vacuum half-spaces, the plane-wave propagation between a source plane located at z' and an observation plane at z. The boundary between the metal and vacuum domains is at $z=0$. Four of the terms, denoted by $\overleftrightarrow{G}$ (with appropriate superscripts and subscripts), describe wave propagation involving a transmission of the field at the boundary. Three terms, denoted by $\overleftrightarrow{D}$, are associated with the direct field propagation between source and observation planes located on the same side of the metal-vacuum boundary. Field propagation between a source and an observation plane located in the same medium can also take place via a so-called indirect process, i.e., a process which involves a reflection of the electromagnetic field at the metal-vacuum boundary. This possibility is described by means of the five $\overleftrightarrow{I}$ propagators. If the source and observation planes coincide $(z'=z)$ the propagator exhibits a delta-function singularity. This singularity leads to a so-called self-field contribution to the propagator. The two possible self-field terms are denoted by $\overleftrightarrow{g}$. An open arrow indicates that the coupling between source and observation planes is mediated by the rotational-free (L) part of the electromagnetic field, and a closed arrow that the coupling is caused by the divergence-free (T) component of the field. In the vacuum domain only divergence-free plane-wave contributions can occur. For the propagator terms involving a transmission or a reflection at the sharp-boundary surface a combination of L and T processes can appear. In an adequate notation, defined in the main text, superscripts and subscripts are given to the various propagator terms to locate the source and observation plane and to distinguish between rotational-free and divergence-free wave propagation.

$$\overleftrightarrow{K}_T(z,z')=-i\mu_0\Omega\int_{SE}\{\Theta(-z)\Theta(-z'')[\overleftrightarrow{D}^{<<}_{TT}(z-z'')+\overleftrightarrow{I}^{<<}_{TT}(z+z'')] +\Theta(-z)\Theta(z'')[\overleftrightarrow{G}^{><}_{TT}(z,z'')+\overleftrightarrow{G}^{><}_{LT}(z,z'')]+\Theta(z)\Theta(-z'')\overleftrightarrow{G}^{<>}_{TT}(z,z'') +\Theta(z)\Theta(z'')[\overleftrightarrow{D}^{>>}_{TT}(z-z'')+\overleftrightarrow{I}^{>>}_{TT}(z,z'')+\overleftrightarrow{I}^{>>}_{LT}(z,z'')]\}\cdot\overleftrightarrow{\sigma}^{SE}(z'',z')dz'' , \tag{3.6}$$

and

$$\overleftrightarrow{K}_L(z,z')=-i\mu_0\Omega\int_{SE}\{\Theta(-z)\Theta(-z'')\overleftrightarrow{g}^{<<}_{LL}(z-z'')+\Theta(z)\Theta(-z'')\overleftrightarrow{G}^{<>}_{TL}(z,z'') +\Theta(z)\Theta(z'')[\overleftrightarrow{D}^{>>}_{LL}(z-z'')+\overleftrightarrow{I}^{>>}_{TL}(z,z'')+\overleftrightarrow{I}^{>>}_{LL}(z,z'')+\overleftrightarrow{g}^{>>}_{LL}(z-z'')]\}\cdot\overleftrightarrow{\sigma}^{SE}(z'',z')dz'' . \tag{3.7}$$

Further progress in the analysis of the kernel structure can be obtained by investigating the tensor-product structure of the indirect propagators $\overleftrightarrow{I}^{<<}_{TT}$ $\overleftrightarrow{I}^{>>}_{TT}$, $\overleftrightarrow{I}^{>>}_{LT}$, $\overleftrightarrow{I}^{>>}_{TL}$, and $\overleftrightarrow{I}^{>>}_{LL}$ and the propagators $\overleftrightarrow{G}^{><}_{TT}$, $\overleftrightarrow{G}^{><}_{LT}$, $\overleftrightarrow{G}^{<>}_{TT}$, and $\overleftrightarrow{G}^{<>}_{TL}$. The remarkable result one finds[19] from such an investigation is that the individual tensor product is of the form $\mathbf{A}(z)\otimes\mathbf{B}(z'')$, i.e., a product of vectors which, respectively, are functions of z and z'', alone.[19] On the basis of the explicit expressions for the relevant SCIB propagator terms a straightforward calculation shows that the kernel $\overleftrightarrow{K}_L$ can be written as follows:

$$\overleftrightarrow{K}_L(z,z')=-i\mu_0\Omega\left[\Theta(z)\int_{SE}\Theta(z'')\overleftrightarrow{D}^{>>}_{LL}(z-z'')\cdot\overleftrightarrow{\sigma}^{SE}(z'',z')dz'' +\left[\frac{c_0}{\Omega}\right]^2[\Theta(-z)+\Theta(z)\epsilon^{-1}(\Omega)]\mathbf{e}_z\otimes\mathbf{e}_z\cdot\overleftrightarrow{\sigma}^{SE}(z,z')+\mathcal{H}_L(z)\otimes\int_{SE}\mathcal{L}_L(z'')\cdot\overleftrightarrow{\sigma}^{SE}(z'',z')dz''\right] , \tag{3.8}$$

where $\epsilon(\Omega)$ is the relative dielectric constant of the jellium in the long-wavelength limit, c_0 is the velocity of light in vacuum, and $\mathbf{e}_z$ is a unit vector in the z direction. The first two terms on the right-hand side of Eq. (3.8), which stem from the direct propagator part and the self-field propagator contribution, respectively, are the terms which make it so difficult to determine in explicit form the rotational-free field inside the selvedge, cf. Sec. IV C. The last term on the right-hand side of the equation is associated with the sum of the indirect propagators and the "transmission" propagator ($\overleftrightarrow{G}^{<>}_{TL}$) and is separable into a vector product of functions of z and z' alone. For the subsequent conceptual analysis, the explicit expressions for $\mathcal{H}_L(z)$ and $\mathcal{L}_L(z'')$ are not needed. For completeness, these expressions are given in Appendix A. The structure of the $\overleftrightarrow{K}_T$ kernel is a little bit more complicated. After some algebraic efforts, however, one obtains

$$\overleftrightarrow{K}_T(z,z')=-i\mu_0\Omega\left[\int_{SE}[\Theta(-z)\Theta(-z'')\overleftrightarrow{D}^{<<}_{TT}(z-z'')+\Theta(z)\Theta(z'')\overleftrightarrow{D}^{>>}_{TT}(z-z'')]\cdot\overleftrightarrow{\sigma}^{SE}(z'',z')dz'' +\sum_{i=1}^{3}\mathcal{H}^s_{T,i}(z)\mathbf{e}_y\otimes\mathbf{e}_y\cdot\int_{SE}\mathcal{L}^s_{T,i}(z'')\overleftrightarrow{\sigma}^{SE}(z'',z')dz''+\sum_{j=1}^{3}\mathcal{H}_{T,j}(z)\otimes\int_{SE}\mathcal{L}_{T,j}(z'')\cdot\overleftrightarrow{\sigma}^{SE}(z'',z')dz''\right] . \tag{3.9}$$

The explicit expressions for the functions $\mathcal{H}^s_{T,i}(z)$, $\mathcal{L}^s_{T,i}(z'')$, $\mathcal{H}_{T,j}(z)$, and $\mathcal{L}_{T,j}(z'')$ occurring in the separable kernels are given in Appendix A. One notices that the separable kernels stem from the propagators $\overleftrightarrow{G}^{><}_{TT}$, $\overleftrightarrow{G}^{><}_{LT}$, $\overleftrightarrow{G}^{<>}_{TT}$, $\overleftrightarrow{I}^{<<}_{TT}$, $\overleftrightarrow{I}^{>>}_{TT}$, and $\overleftrightarrow{I}^{>>}_{LT}$, cf. Fig. 1. The nonseparable part of the $\overleftrightarrow{K}_T$ kernel originates in the direct propagators only.

The truncated kernels can be obtained directly from Eqs. (3.8) and (3.9) by utilizing that (i) the different terms in the propagator can be written in a form equivalent to that in Eq. (2.12), and (ii) the selvedge response tensor

$$\overleftrightarrow{\sigma}^{SE}=\begin{bmatrix}\sigma^{SE}_{xx} & 0 & \sigma^{SE}_{xz}\\ 0 & \sigma^{SE}_{yy} & 0\\ \sigma^{SE}_{zx} & 0 & \sigma^{SE}_{zz}\end{bmatrix} \tag{3.10}$$

in truncated notation has the two components

$$\overleftrightarrow{\sigma}^{p,SE}\equiv\begin{bmatrix}\sigma^{SE}_{xx} & \sigma^{SE}_{xz}\\ \sigma^{SE}_{zx} & \sigma^{SE}_{zz}\end{bmatrix} \tag{3.11}$$

and

$$\sigma^{s,SE}\equiv\sigma^{SE}_{yy} . \tag{3.12}$$

By adding the appropriate superscripts p and s to the relevant propagators and to the functions appearing in the separable parts of the kernels (see Appendix A), and by introducing $\mathbf{e}^p_z\equiv(0,1)$ one gets

$$K_T^s(z,z')=-i\mu_0\Omega\left[\int_{SE}[\Theta(-z)\Theta(-z'')D_{TT}^{s,<<}(z-z'')+\Theta(z)\Theta(z'')D_{TT}^{s,>>}(z-z'')]\sigma^{s,SE}(z'',z')dz'' + \sum_{i=1}^{3}\mathcal{H}_{T,i}^s(z)\int_{SE}\mathcal{L}_{T,i}^s(z'')\sigma^{s,SE}(z'',z')dz''\right], \quad (3.13)$$

$$\vec{K}_T^p(z,z')=-i\mu_0\Omega\left[\int_{SE}[\Theta(-z)\Theta(-z'')\vec{D}_{TT}^{p,<<}(z-z'')+\Theta(z)\Theta(z'')\vec{D}_{TT}^{p,>>}(z-z'')]\cdot\vec{\sigma}^{p,SE}(z'',z')dz'' + \sum_{j=1}^{3}\mathcal{H}_{T,j}^p(z)\otimes\int_{SE}\mathcal{L}_{T,j}^p(z'')\cdot\vec{\sigma}^{p,SE}(z'',z')dz''\right] \quad (3.14)$$

and

$$\vec{K}_L^p(z,z')=-i\mu_0\Omega\left[\Theta(z)\int_{SE}\Theta(z'')\vec{D}_{LL}^{p,>>}(z-z'')\cdot\vec{\sigma}^{p,SE}(z'',z')dz'' + \left[\frac{c_0}{\Omega}\right]^2[\Theta(-z)+\Theta(z)\epsilon^{-1}(\Omega)]\mathbf{e}_z^p\otimes\mathbf{e}_z^p\cdot\vec{\sigma}^{p,SE}(z,z')+\mathcal{H}_L^p(z)\otimes\int_{SE}\mathcal{L}_L^p(z'')\cdot\vec{\sigma}^{p,SE}(z'',z')dz''\right]. \quad (3.15)$$

The integral equations in (2.19)–(2.21) with the kernels written as in Eqs. (3.13)–(3.15) constitute the basis for our calculation of the selvedge field in the following section.

IV. SCHEMES FOR CALCULATION OF THE SELVEDGE FIELD

A. Brute-force reduction of kernel

To determine the electric field inside the selvedge in the s-polarized case one has to combine Eqs. (2.19) and (3.13). To solve the resulting integral equation by analytical methods will in general not be possible. However, let us consider the integral equation obtained by brute-force omission of the nonseparable direct propagator terms, i.e.,

$$\mathcal{E}_T^s(z)=e_T^{(0)s}(z)-i\mu_0\Omega\sum_{i=1}^{3}\mathcal{H}_{T,i}^s(z)\int\int_{SE}\mathcal{L}_{T,i}^s(z'')\sigma^{s,SE}(z'',z')\mathcal{E}_T^s(z')dz''dz' , \quad (4.1)$$

where the solution for the electric field has been denoted by $\mathcal{E}_T^s(z)$. This integral equation can be solved exactly by means of the ansatz

$$\mathcal{E}_T^s(z)=e_T^{(0)s}(z)+\sum_{i=1}^{3}a_i\mathcal{H}_{T,i}^s(z) , \quad (4.2)$$

where the a_i's are as yet unknown, z-independent constants. Now, by inserting Eq. (4.2) into (4.1), and utilizing the fact that each of the factors to $\mathcal{H}_{T,i}^s(z)$, $i=1,2,3$, must vanish separately in order that the ansatz solves the integral equation, one obtains the following set of inhomogenous, linear equations among the unknown constants:

$$\sum_{j=1}^{3}(\delta_{ij}+\alpha_{ij})a_j=A_i, \quad i=1,2,3 \quad (4.3)$$

where

$$\alpha_{ij}\equiv i\mu_0\Omega\int\int_{SE}\mathcal{L}_{T,i}^s(z'')\sigma^{s,SE}(z'',z')\mathcal{H}_{T,j}^s(z')dz''dz' , \quad (4.4)$$

and

$$A_i\equiv -i\mu_0\Omega\int\int_{SE}\mathcal{L}_{T,i}^s(z'')\sigma^{s,SE}(z'',z')e_T^{(0)s}(z')dz''dz' , \quad (4.5)$$

and δ_{ij} being the Kronecker delta. Inserting the values of a_j ($j=1,2,3$) obtained via the solution of the equations in (4.3) into Eq. (4.2) our approximate solution for the s-polarized part of the field inside the selvedge has been established.

Brute-force neglect of the direct and self-field parts of the propagator leads, for the p-polarized case, to the following coupled integral equations among the divergence-free $[\mathcal{E}_T^p(z)]$ and the rotational-free $[\mathcal{E}_L^p(z)]$ parts of the field:

$$\mathcal{E}_T^p(z)=\mathbf{e}_T^{(0)p}(z)-i\mu_0\Omega\sum_{i=1}^{3}\mathcal{H}_{T,i}^p(z)\otimes\int\int_{SE}\mathcal{L}_{T,i}^p(z'')\cdot\vec{\sigma}^{p,SE}(z'',z')\cdot[\mathcal{E}_T^p(z')+\mathcal{E}_L^p(z')]dz''dz' , \quad (4.6)$$

and

$$\mathcal{E}_L^p(z)=\mathbf{e}_L^{(0)p}(z)-i\mu_0\Omega\mathcal{H}_L^p(z)\otimes\int\int_{\mathrm{SE}}\mathcal{L}_L^p(z'')\cdot\overleftrightarrow{\sigma}^{p,\mathrm{SE}}(z'',z')\cdot[\mathcal{E}_T^p(z')+\mathcal{E}_L^p(z')]dz''dz' \ . \tag{4.7}$$

The coupled integral equations above can be solved exactly, following the same procedure as for the s-polarized case. Thus, by means of the ansatz

$$\mathcal{E}_T^p(z)=\mathbf{e}_T^{(0)p}(z)+\sum_{i=1}^{3}b_i\mathcal{H}_{T,i}^p(z)\ , \tag{4.8}$$

$$\mathcal{E}_L^p(z)=\mathbf{e}_L^{(0)p}(z)+b_4\mathcal{H}_L^p(z)\ , \tag{4.9}$$

one obtains after insertion into Eqs. (4.6) and (4.7) a set of four inhomogeneous linear equations among the unknown b_i's $(i=1,2,3,4)$, namely,

$$\sum_{j=1}^{4}(\delta_{ij}+\beta_{ij})b_j=B_i,\quad i=1,2,3,4 \tag{4.10}$$

where

$$\beta_{ij}\equiv i\mu_0\Omega\int\int_{\mathrm{SE}}\mathcal{L}_{T,i}^p(z'')\cdot\overleftrightarrow{\sigma}^{p,\mathrm{SE}}(z'',z')\cdot\mathcal{H}_{T,j}^p(z')dz''dz',\quad i,j=1,2,3 \tag{4.11}$$

$$\beta_{i4}\equiv i\mu_0\Omega\int\int_{\mathrm{SE}}\mathcal{L}_{T,i}^p(z'')\cdot\overleftrightarrow{\sigma}^{p,\mathrm{SE}}(z'',z')\cdot\mathcal{H}_L^p(z')dz''dz',\quad i=1,2,3 \tag{4.12}$$

$$\beta_{4j}\equiv i\mu_0\Omega\int\int_{\mathrm{SE}}\mathcal{L}_L^p(z'')\cdot\overleftrightarrow{\sigma}^{p,\mathrm{SE}}(z'',z')\cdot\mathcal{H}_{T,j}^p(z')dz''dz',\quad j=1,2,3 \tag{4.13}$$

$$\beta_{44}\equiv i\mu_0\Omega\int\int_{\mathrm{SE}}\mathcal{L}_L^p(z'')\cdot\overleftrightarrow{\sigma}^{p,\mathrm{SE}}(z'',z')\cdot\mathcal{H}_L^p(z')dz''dz'\ , \tag{4.14}$$

and

$$B_i\equiv -i\mu_0\Omega\int\int_{\mathrm{SE}}\mathcal{L}_{T,i}^p(z'')\cdot\overleftrightarrow{\sigma}^{p,\mathrm{SE}}(z'',z')\cdot[\mathbf{e}_T^{(0)p}(z')+\mathbf{e}_L^{(0)p}(z')]dz''dz',\quad i=1,2,3 \tag{4.15}$$

$$B_4\equiv -i\mu_0\Omega\int\int_{\mathrm{SE}}\mathcal{L}_L^p(z'')\cdot\overleftrightarrow{\sigma}^{p,\mathrm{SE}}(z'',z')\cdot[\mathbf{e}_T^{(0)p}(z')+\mathbf{e}_L^{(0)p}(z')]dz''dz'\ . \tag{4.16}$$

Having calculated the unknown b_i's $(i=1,2,3,4)$ from the system of equations in (4.10) we have achieved our goal of determining the p-polarized selvedge field in the approximation where only the contributions from separable propagators are retained. In a forthcoming paper we shall compare the analytical result obtained for the selvedge field via Eqs. (4.2), (4.8), and (4.9), with that obtained from an "exact" numerical calculation based on the complete integral equations, i.e., (2.19)–(2.21) with (3.13)–(3.15). For simplicity, a simple model will be adopted for the selvedge response function $\overleftrightarrow{\sigma}^{\mathrm{SE}}$.

B. First-order Born approximation

So far, we have avoided any form of perturbative calculation in our analysis of the selvedge field. We have approached the determination of the field in two steps. In the first step, the SCIB model was adopted to give a background solution which contains many of the essential physical ingredients of nonlocal optics. In the second step, part of the selvedge response was incorporated into an "exact" solution based on the separable parts of the SCIB kernel. To proceed from here, it seems difficult to avoid a perturbative description. Hence, it is natural to take $\mathcal{E}_T^s(z)$, $\mathcal{E}_T^p(z)$, and $\mathcal{E}_L^p(z)$ as zeroth-order fields in an iterative (eventually numerical) calculation of the fields throughout the selvedge. Thus, in first-order Born approximation the s-polarized selvedge field is given by

$$e_T^s(z)=\mathcal{E}_T^s(z)+\int_{\mathrm{SE}}\Psi_T^s(z,z')\mathcal{E}_T^s(z')dz'\ , \tag{4.17}$$

where the kernel Ψ_T^s, associated with the nonseparable parts of the SCIB propagator, is

$$\Psi_T^s(z,z')=-i\mu_0\Omega\times\int_{\mathrm{SE}}[\Theta(-z)\Theta(-z'')D_{TT}^{s,<<}(z-z'')+\Theta(z)\Theta(z'')D_{TT}^{s,>>}(z-z'')]\times\sigma^{s,\mathrm{SE}}(z'',z')dz''\ . \tag{4.18}$$

In truncated notation, one obtains in a first-order Born approximation the following results for the p-polarized divergence-free and rotational-free parts of the selvedge field:

$$\mathbf{e}_T^p(z)=\mathcal{E}_T^p(z)+\int_{\mathrm{SE}}\overleftrightarrow{\Psi}_T^p(z,z')\cdot[\mathcal{E}_T^p(z')+\mathcal{E}_L^p(z')]dz'\ , \tag{4.19}$$

and

$$\mathbf{e}_L^p(z)=\mathcal{E}_L^p(z)+\int_{\mathrm{SE}}\overleftrightarrow{\Psi}_L^p(z,z')\cdot[\mathcal{E}_T^p(z')+\mathcal{E}_L^p(z')]dz'\ , \tag{4.20}$$

where the kernels $\overleftrightarrow{\Psi}_T^p$ and $\overleftrightarrow{\Psi}_L^p$ are given by

$$\overleftrightarrow{\Psi}{}^{p}_{T}(z,z')=-i\mu_0\Omega\int_{\rm SE}[\Theta(-z)\Theta(-z'')\overleftrightarrow{\mathbf{D}}{}^{p,<<}_{TT}(z-z'')+\Theta(z)\Theta(z'')\overleftrightarrow{\mathbf{D}}{}^{p,>>}_{TT}(z-z'')]\cdot\overleftrightarrow{\sigma}{}^{p,\rm SE}(z'',z')dz'' , \quad (4.21)$$

and

$$\overleftrightarrow{\Psi}{}^{p}_{L}(z,z')=-i\mu_0\Omega\left[\Theta(z)\int_{\rm SE}\Theta(z'')\overleftrightarrow{\mathbf{D}}{}^{p,>>}_{LL}(z-z'')\cdot\overleftrightarrow{\sigma}{}^{p,\rm SE}(z'',z')dz'' + \left[\frac{c_0}{\Omega}\right]^2[\Theta(-z)+\Theta(z)\epsilon^{-1}(\Omega)]\mathbf{e}^p_z\otimes\mathbf{e}^p_z\cdot\overleftrightarrow{\sigma}{}^{p,\rm SE}(z,z')\right] . \quad (4.22)$$

C. Long-wavelength approximation for the divergence-free direct propagators

In the previous subsection the contributions from the direct propagator terms to the selvedge field were determined by a first-order Born approximation, i.e., by integrating products of the *exact* kernels $[\Psi^s_T(z,z'), \overleftrightarrow{\Psi}{}^p_T(z,z'), \overleftrightarrow{\Psi}{}^p_L(z,z')]$ and the *approximate* fields $[\mathcal{E}^s_T(z'), \mathcal{E}^p_T(z'), \mathcal{E}^p_L(z')]$ over the selvedge. An alternative scheme would be to calculate the divergence-free parts of the direct propagators (kernels) *approximatively* and then solve the appearing integral equations *exactly*.

Let us consider now such an approach for the s-polarized selvedge field. Since the propagator $D^{s,>>}_{TT}(z-z'')$, given in explicit form by[18]

$$D^{s,>>}_{TT}(z-z'')=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{iq_\perp(z-z'')}}{N_T(q)}dq_\perp , \quad (4.23)$$

is normally dominated by its contribution from the collective polariton mode, we take

$$D^{s,>>}_{TT}(z-z'')\cong\frac{e^{i\kappa^T_\perp|z-z''|}}{2i\kappa^T_\perp} , \quad (4.24)$$

where $\kappa^T_\perp=\kappa^T_\perp(Q_\parallel,\Omega)$ is determined by the well-known[34] polariton dispersion relation $N_T(Q_\parallel,\kappa^T_\perp,\Omega)=0$. The direct propagator in vacuum, $D^{s,<<}_{TT}(z-z'')$, is given by an expression similar in form to that of Eq. (4.24), namely

$$D^{s,<<}_{TT}(z-z'')=\frac{e^{iq^0_\perp|z-z''|}}{2iq^0_\perp} , \quad (4.25)$$

with $q^0_\perp=[(\Omega/c_0)^2-Q^2_\parallel]^{1/2}$. Since for optical frequencies $q^0_\perp|z-z''|\ll 1$ and $\kappa^T_\perp|z-z''|\ll 1$ for points z and z'' inside the selvedge, it follows that $D^{s,<<}_{TT}\cong(2iq^0_\perp)^{-1}$ and $D^{s,>>}_{TT}\cong(2i\kappa^T_\perp)^{-1}$ in lowest order in the long-wavelength limit. In turn, this implies that

$$\Psi^s_T(z,z')\cong-\frac{\mu_0\Omega}{2}\left[\frac{\Theta(-z)}{q^0_\perp}\int_{\rm SE}\Theta(-z'')\sigma^{s,\rm SE}(z'',z')dz''+\frac{\Theta(z)}{\kappa^T_\perp}\int_{\rm SE}\Theta(z'')\sigma^{s,\rm SE}(z'',z')dz''\right] , \quad (4.26)$$

which means that the kernel is constant in the inner ($z>0$) and outer ($z<0$) selvedge region, the constants being in general different in the two regions. It appears from Eq. (4.26) that the two terms in $\Psi^s_T(z,z')$ each can be separated into functions of z and z'. This has the consequence that $K^s_T(z,z')$ of Eq. (3.13) is totally separable. The corresponding integral equation in (2.19) can now be solved exactly by means of the ansatz

$$e^s_T(z)=e^{(0)s}_T(z)+\sum_{i=1}^{3}c_i\mathcal{H}^s_{T,i}(z)+c_4\Theta(-z)+c_5\Theta(z) , \quad (4.27)$$

where the c_i's ($i=1-5$) are determined by the following set of inhomogeneous linear equations:

$$\sum_{j=1}^{5}(\delta_{ij}+\alpha_{ij})c_j=A_i,\quad i=1,2,3,4,5 . \quad (4.28)$$

The explicit expressions for α_{ij} and A_i of Eq. (4.28) are for $i,j=1,2,3$ given by Eqs. (4.4) and (4.5), and as far as the new elements are concerned given by

$$\left.\begin{matrix}\alpha_{i4}\\ \alpha_{i5}\end{matrix}\right\}=i\mu_0\Omega\int\int_{\rm SE}\mathcal{L}^s_{T,i}(z'')\sigma^{s,\rm SE}(z'',z')\Theta(\mp z')dz''dz' ,\quad i=1,2,3 \quad (4.29)$$

$$\alpha_{4i}=\frac{\mu_0\Omega}{2q^0_\perp}\int\int_{\rm SE}\Theta(-z'')\sigma^{s,\rm SE}(z'',z')\mathcal{H}^s_{T,i}(z')dz''dz' ,\quad i=1,2,3 \quad (4.30)$$

$$\alpha_{5i}=\frac{\mu_0\Omega}{2\kappa^T_\perp}\int\int_{\rm SE}\Theta(z'')\sigma^{s,\rm SE}(z'',z')\mathcal{H}^s_{T,i}(z')dz''dz' ,\quad i=1,2,3 \quad (4.31)$$

$$\left.\begin{matrix}\alpha_{44}\\ \alpha_{45}\end{matrix}\right\}=\frac{\mu_0\Omega}{2q^0_\perp}\int\int_{\rm SE}\Theta(-z'')\sigma^{s,\rm SE}(z'',z')\Theta(\mp z')dz''dz' , \quad (4.32)$$

$$\left.\begin{matrix}\alpha_{54}\\ \alpha_{55}\end{matrix}\right\}=\frac{\mu_0\Omega}{2\kappa_\perp^T}\int\int_{\rm SE}\Theta(\mp z'')\sigma^{s,\rm SE}(z'',z')\Theta(z')dz''dz' , \tag{4.33}$$

and

$$A_4=-\frac{\mu_0\Omega}{2q_\perp^0}\int\int_{\rm SE}\Theta(-z'')\sigma^{s,\rm SE}(z'',z')e_T^{(0)s}(z')dz''dz' , \tag{4.34}$$

$$A_5=-\frac{\mu_0\Omega}{2\kappa_\perp^T}\int\int_{\rm SE}\Theta(z'')\sigma^{s,\rm SE}(z'',z')e_T^{(0)s}(z')dz''dz' . \tag{4.35}$$

In Eqs. (4.29), (4.32), and (4.33) the upper and lower element on the left-hand side are associated with the minus and plus sign in the step function, respectively.

Let me emphasize here that the result in Eq. (4.27) is only partially a long-wavelength result because the indirect contributions are treated nonperturbatively. For many purposes it will be sufficient to calculate also the indirect terms in the long-wavelength limit. The result appearing from such a treatment will of course be a self-consistent long-wavelength result, cf. Ref. 21.

Let us close this section by deriving an integral equation for the rotational-free selvedge field alone, based on the assumption that the divergence-free selvedge field can be adequately described by its value in the long-wavelength limit.

Utilizing the explicit expressions for $\overleftrightarrow{\rm D}_{TT}^{p,<<}$ and $\overleftrightarrow{\rm D}_{TT}^{p,>>}$ given in Ref. 19 and Eqs. (A7), (A9), and (A11), one obtains, taking the long-wavelength limit in the z dependence of the kernel $\overleftrightarrow{\rm K}_T^p$,

$$\overleftrightarrow{\rm K}_T^p(z,z')\cong\Theta(-z)\overleftrightarrow{\rm K}_T^p(z\to0-,z')+\Theta(z)\overleftrightarrow{\rm K}_T^p(z\to0+,z') . \tag{4.36}$$

Furthermore, also for the background field we neglect the field variations in the vacuum and metal domains, i.e.,

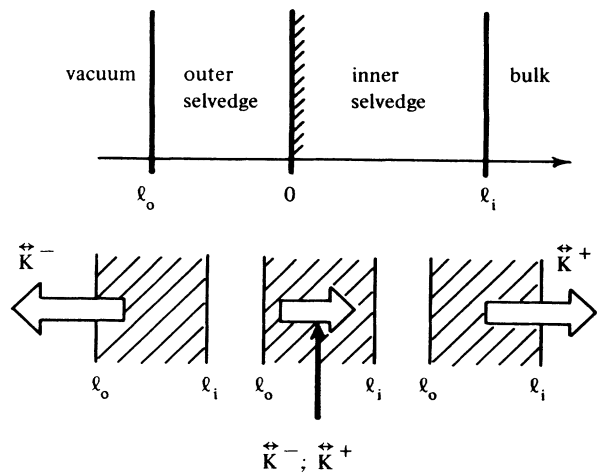

FIG. 2. Schematic diagram (upper part of the figure) showing the division of space into four domains: vacuum, outer selvedge, inner selvedge, and bulk. In the lower part of the figure is shown which of the propagators ($\overleftrightarrow{\rm K}-,\overleftrightarrow{\rm K}+$) one has to use when calculating the field, stemming from the selvedge sources, in vacuum, inside the selvedge, and in the bulk.

$$\mathbf{e}_T^{(0)p}(z)\cong\Theta(-z)\mathbf{e}_T^{(0)p}(z\to0-)+\Theta(z)\mathbf{e}_T^{(0)p}(z\to0+) . \tag{4.37}$$

For the following conceptual discussion we do not need the explicit expressions for $\overleftrightarrow{\rm K}_T^p(z\to0-,z')$, $\overleftrightarrow{\rm K}_T^p(z\to0+,z')$, $\mathbf{e}_T^{(0)p}(z\to0-)$, and $\mathbf{e}_T^{(0)p}(z\to0+)$. By inserting Eqs. (4.36) and (4.37) into Eq. (2.20) it becomes obvious that the divergence-free selvedge field is of the form

$$\mathbf{e}_T^p(z)=\Theta(-z)\mathbf{e}_T^{p,-}+\Theta(z)\mathbf{e}_T^{p,+} , \tag{4.38}$$

where the outer (−) and inner (+) (see Fig. 2) selvedge fields $\mathbf{e}_T^{p,-}$ and $\mathbf{e}_T^{p,+}$ are independent of z. By combining Eqs. (2.20) and (4.36)–(4.38) one obtains the following two linear and inhomogeneous equations among the unknown quantities $\mathbf{e}_T^{p,-}$ and $\mathbf{e}_T^{p,+}$:

$$\left[\overleftrightarrow{\rm U}-\int_{\rm SE}\Theta(-z')\overleftrightarrow{\rm K}_T^p(z\to0-,z')dz'\right]\cdot\mathbf{e}_T^{p,-}-\left[\int_{\rm SE}\Theta(z')\overleftrightarrow{\rm K}_T^p(z\to0-,z')dz'\right]\cdot\mathbf{e}_T^{p,+}=\mathbf{e}_T^{(0)p}(z\to0-)+\int_{\rm SE}\overleftrightarrow{\rm K}_T^p(z\to0-,z')\cdot\mathbf{e}_L^p(z')dz' , \tag{4.39}$$

and

$$-\left[\int_{\rm SE}\Theta(-z')\overleftrightarrow{\rm K}_T^p(z\to0+,z')dz'\right]\cdot\mathbf{e}_T^{p,-}+\left[\overleftrightarrow{\rm U}-\int_{\rm SE}\Theta(z')\overleftrightarrow{\rm K}_T^p(z\to0+,z')dz'\right]\cdot\mathbf{e}_T^{p,+}=\mathbf{e}_T^{(0)p}(z\to0+)+\int_{\rm SE}\overleftrightarrow{\rm K}_T^p(z\to0+,z')\cdot\mathbf{e}_L^p(z')dz' , \tag{4.40}$$

where $\overleftrightarrow{\rm U}$ is the unit tensor of dimension 2×2. Solving Eqs. (4.39) and (4.40) one gets

$$\mathbf{e}_T^{p,-}=\mathbf{A}^-+\int_{\rm SE}\overleftrightarrow{\rm B}^-(z')\cdot\mathbf{e}_L^p(z')dz' , \tag{4.41}$$

$$\mathbf{e}_T^{p,+}=\mathbf{A}^++\int_{\rm SE}\overleftrightarrow{\rm B}^+(z')\cdot\mathbf{e}_L^p(z')dz' , \tag{4.42}$$

where $\mathbf{A}^-$, $\mathbf{A}^+$, $\overleftrightarrow{\rm B}^-$, and $\overleftrightarrow{\rm B}^+$ are known quantities. The somewhat lengthy explicit expressions for these quantities are not needed for our purpose. To establish the desired integral equation for the rotational-free part of the selvedge field we insert Eq. (4.38) [with Eqs. (4.41) and (4.42)] into Eq. (2.21) and make use of the expression in Eq. (3.15) [with Eq. (4.22)]. Hereby, one obtains

$$\begin{aligned}\mathbf{e}^p_L(z)=\mathbf{e}^{(0)}_{\mathrm{eff}}(z)&+\left[\int_{\mathrm{SE}}\Theta(-z')\overleftrightarrow{\mathbf{K}}^p_L(z,z')dz'\right]\cdot\left[\int_{\mathrm{SE}}\overleftrightarrow{\mathbf{B}}^-(z')\cdot\mathbf{e}^p_L(z')dz'\right]\\&+\left[\int_{\mathrm{SE}}\Theta(z')\overleftrightarrow{\mathbf{K}}^p_L(z,z')dz'\right]\cdot\left[\int_{\mathrm{SE}}\overleftrightarrow{\mathbf{B}}^+(z')\cdot\mathbf{e}^p_L(z')dz'\right]\\&-i\mu_0\Omega\mathcal{H}^p_L(z)\otimes\int_{\mathrm{SE}}\left[\int_{\mathrm{SE}}\mathcal{L}^p_L(z'')\cdot\overleftrightarrow{\sigma}^{p,\mathrm{SE}}(z'',z')dz''\right]\cdot\mathbf{e}^p_L(z')dz'+\int_{\mathrm{SE}}\overleftrightarrow{\Psi}^p_L(z,z')\cdot\mathbf{e}^p_L(z')dz'\ ,\end{aligned}\tag{4.43}$$

where, for brevity, we have introduced

$$\mathbf{e}^{(0)}_{\mathrm{eff}}(z)=\mathbf{e}^{(0)p}_L(z)+\left[\int_{\mathrm{SE}}\Theta(-z')\overleftrightarrow{\mathbf{K}}^p_L(z,z')dz'\right]\cdot\mathbf{A}^-+\left[\int_{\mathrm{SE}}\Theta(z')\overleftrightarrow{\mathbf{K}}^p_L(z,z')dz'\right]\cdot\mathbf{A}^+\ .\tag{4.44}$$

The integral equation in (4.43) is the fundamental one for the irrotational part of the selvedge field in the case where a decoupling from the solenoidal field, via a long-wavelength treatment of the divergence-free selvedge field, can be justified.

As a starting point for an iterative solution of Eq. (4.43) one neglects the term containing the nonseparable kernel $\overleftrightarrow{\Psi}^p_L$. The reduced integral equation has the exact solution

$$\begin{aligned}\mathcal{E}^p_L(z)=\mathbf{e}^{(0)}_{\mathrm{eff}}(z)&+\left[\int_{\mathrm{SE}}\Theta(-z')\overleftrightarrow{\mathbf{K}}^p_L(z,z')dz'\right]\cdot\mathbf{\Lambda}^-\\&+\left[\int_{\mathrm{SE}}\Theta(z')\overleftrightarrow{\mathbf{K}}^p_L(z,z')dz'\right]\cdot\mathbf{\Lambda}^++\Lambda\mathcal{H}^p_L(z)\ ,\end{aligned}\tag{4.45}$$

where the five z-independent constants Λ, $\mathbf{\Lambda}^-=(\Lambda^-_x,\Lambda^-_z)$, and $\mathbf{\Lambda}^+=(\Lambda^+_x,\Lambda^+_z)$ are determined by the usual procedure. By using Eq. (4.45) as the zeroth-order solution, one obtains in first-order Born approximation

$$\mathbf{e}^p_L(z)=\mathcal{E}^p_L(z)+\int_{\mathrm{SE}}\overleftrightarrow{\Psi}^p_L(z,z')\cdot\mathcal{E}^p_L(z')dz'\ .\tag{4.46}$$

One should stress at this point that even though part of the rapid variation of the rotational-free field through the selvedge has been taken into account in $\mathcal{E}^p_L(z)$, one cannot expect a first-order Born approximation to be sufficient for the quantitative determination of $\mathbf{e}^p_L(z)$ since also the contributions from the direct kernel and from the self-field kernel vary rapidly across the selvedge (see also Fig. 3).

V. BACKGROUND FIELD IN SECOND-HARMONIC GENERATION

The analyses in Secs. II–IV can be applied to studies in linear and parametrically nonlinear, nonlocal jellium optics provided that the appropriate values of $\mathbf{Q}_\parallel$ and Ω are inserted into the conductivity response tensors $\overleftrightarrow{\sigma}^{\mathrm{SCIB}}(z,z';\mathbf{Q}_\parallel,\Omega)$ and $\overleftrightarrow{\sigma}^{\mathrm{SE}}(z,z';\mathbf{Q}_\parallel,\Omega)$, the propagator $\overleftrightarrow{\mathbf{G}}(z,z';\mathbf{Q}_\parallel,\Omega)$, and the background field $\mathbf{E}^{(0)}(z;\mathbf{Q}_\parallel,\Omega)$. For linear-field problems we shall take $(\mathbf{Q}_\parallel,\Omega)=(\mathbf{q}_\parallel,\omega)$,

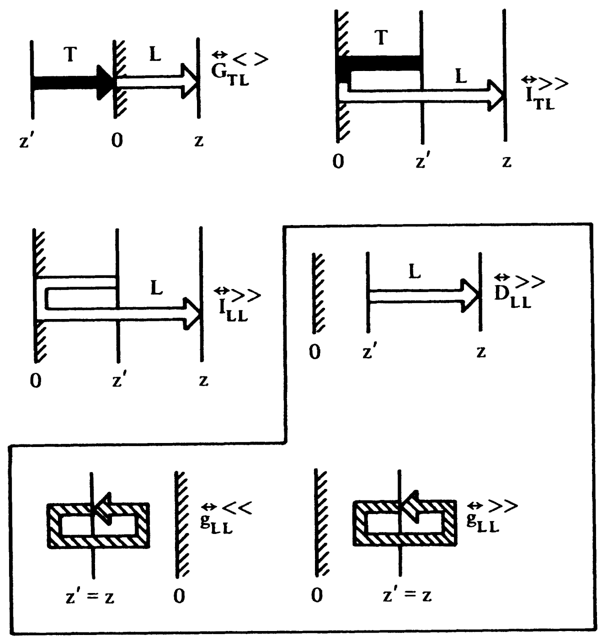

FIG. 3. Schematic diagrams showing the contributions to the screened electromagnetic propagator which are irrotational in the observation coordinates. For an explanation of the graphic symbols and the notation used for the various propagator terms the reader is referred to the text accompanying Fig. 1. In the calculations of the electromagnetic field inside the selvedge, the contributions from the diagrams outside the frame shown can be treated in a nonperturbative way by separation of the respective kernels. Since the kernels associated with the diagrams inside the frame cannot be separated into products of functions depending on either the source or observation coordinates alone, the contributions to the selvedge field stemming from these diagrams have to be treated within the framework of an iterative approach. Due to the singular structure of the self-field propagators, denoted by $\overleftrightarrow{g}^{<<}_{LL}$ and $\overleftrightarrow{g}^{>>}_{LL}$, the contribution to the rotational-free kernel in Eq. (3.8) from these has a functional dependence on z' and z which essentially is given by the linear and nonlocal conductivity response function of the selvedge. From a calculational point of view the most difficult field propagation is associated with $\overleftrightarrow{\mathbf{D}}^{>>}_{LL}$ since this propagator term relates the conductivity response tensor of the selvedge and the rotational-free kernel [Eq. (3.8)] nonlocally.

and for parametric second-harmonic generation investigations, $(\mathbf{Q}_{\|},\Omega)=(2\mathbf{q}_{\|},2\omega)$.

In linear jellium optics, the background field $\mathbf{E}^{(0)}(z;\mathbf{q}_{\|},\omega)$ is identical to the field $\mathbf{E}^{\rm SCIB}(z;\mathbf{q}_{\|},\omega)$, obtained by means of the well known and extensively studied semiclassical infinite-barrier model. In parametric, second-harmonic generation investigations on jellium, the background field has the following form:[36]

$$\mathbf{E}^{(0)}(z;2\mathbf{q}_{\|},2\omega)=\mathbf{E}_{*}^{\rm SCIB}(z;2\mathbf{q}_{\|},2\omega)-2i\mu_0\omega\int_{\rm SE}\overleftrightarrow{G}(z,z';2\mathbf{q}_{\|},2\omega)\cdot\mathbf{J}_d^{\rm SE}(z';2\mathbf{q}_{\|},2\omega)dz' \ . \tag{5.1}$$

The first term on the right-hand side of Eq. (5.1) is closely related to the second-harmonic field obtained within the framework of a consistent SCIB model. To realize this, we write it in the form

$$\mathbf{E}_{*}^{\rm SCIB}(z;2\mathbf{q}_{\|},2\omega)=-2i\mu_0\omega\int_0^{\infty}\overleftrightarrow{G}(z,z';2\mathbf{q}_{\|},2\omega)\cdot\mathbf{J}_{d,*}^{\rm SCIB}(z';2\mathbf{q}_{\|},2\omega)dz' \ , \tag{5.2}$$

where the driven (d), nonlinear, current density $\mathbf{J}_{d,*}^{\rm SCIB}$ is given by

$$\mathbf{J}_{d,*}^{\rm SCIB}(z';2\mathbf{q}_{\|},2\omega)=\int_0^{\infty}\int_0^{\infty}\overleftrightarrow{\Sigma}^{\rm SCIB}(z',z'',z''';\mathbf{q}_{\|}\to2\mathbf{q}_{\|},\omega\to2\omega):\mathbf{E}(z''';\mathbf{q}_{\|},\omega)\mathbf{E}(z'';\mathbf{q}_{\|},\omega)dz'''dz'' \ , \tag{5.3}$$

$\overleftrightarrow{\Sigma}^{\rm SCIB}$ being the nonlinear conductivity response tensor in the SCIB model. The driven, nonlinear, current density in Eq. (5.3) deviates from that of the pure SCIB model due to the fact that it is the self-consistently determined linear electric field $\mathbf{E}$ obtained on the basis of the complete model including selvedge effects which occurs under the integral sign of the equation. The asterisk ($*$) added as subscript to the field and current density in the equations above indicates that in order to obtain the zeroth-order field in parametric, second-harmonic generation, *in principle,* one needs the full solution, i.e., a solution incorporating selvedge response effects consistently, to the linear-field problem. Now, the relation between $\mathbf{J}_{d,*}^{\rm SCIB}$ and the consistent driven current density $\mathbf{J}_d^{\rm SCIB}$ in the SCIB model is obtained by writing the fundamental field in the form

$$\mathbf{E}(z;\mathbf{q}_{\|},\omega)=\mathbf{E}^{\rm SCIB}(z;\mathbf{q}_{\|},\omega)+\Delta\mathbf{E}(z;\mathbf{q}_{\|},\omega) \ , \tag{5.4}$$

where $\Delta\mathbf{E}$ gives the deviation of the field from that, $\mathbf{E}^{\rm SCIB}$, obtained within the framework of the SCIB model. By inserting Eq. (5.4) into (5.3), and this equation in turn into (5.2), we get

$$\mathbf{E}_{*}^{\rm SCIB}(z;2\mathbf{q}_{\|},2\omega)=\mathbf{E}^{\rm SCIB}(z;2\mathbf{q}_{\|},2\omega)+\delta\mathbf{E}(z;2\mathbf{q}_{\|},2\omega) \ , \tag{5.5}$$

where

$$\mathbf{E}^{\rm SCIB}(z;2\mathbf{q}_{\|},2\omega)=-2i\mu_0\omega\int_0^{\infty}\overleftrightarrow{G}(z,z';2\mathbf{q}_{\|};2\omega)\cdot\mathbf{J}_d^{\rm SCIB}(z';2\mathbf{q}_{\|},2\omega)dz' \tag{5.6}$$

is the genuine sharp-boundary, nonlinear field with the expression

$$\mathbf{J}_d^{\rm SCIB}(z';2\mathbf{q}_{\|},2\omega)=\int_0^{\infty}\int_0^{\infty}\overleftrightarrow{\Sigma}^{\rm SCIB}(z',z'',z''';\mathbf{q}_{\|}\to2\mathbf{q}_{\|},\omega\to2\omega):\mathbf{E}^{\rm SCIB}(z''';\mathbf{q}_{\|},\omega)\mathbf{E}^{\rm SCIB}(z'';\mathbf{q}_{\|},\omega)dz'''dz'' \tag{5.7}$$

for the true driven, nonlinear current density in the SCIB model. The contribution $\delta\mathbf{E}$ is given by

$$\delta\mathbf{E}(z;2\mathbf{q}_{\|},2\omega)=-2i\mu_0\omega\int_0^{\infty}\overleftrightarrow{G}(z,z';2\mathbf{q}_{\|},2\omega)\cdot\Delta\mathbf{J}_d^{\rm SCIB}(z';2\mathbf{q}_{\|},2\omega)dz' \ , \tag{5.8}$$

with

$$\begin{aligned}\Delta\mathbf{J}_d^{\rm SCIB}(z';2\mathbf{q}_{\|},2\omega)=\int_0^{\infty}\int_0^{\infty}\overleftrightarrow{\Sigma}^{\rm SCIB}(z',z'',z''';\mathbf{q}_{\|}\to2\mathbf{q}_{\|},\omega\to2\omega):[\Delta\mathbf{E}(z''';\mathbf{q}_{\|},\omega)\mathbf{E}^{\rm SCIB}(z'';\mathbf{q}_{\|},\omega)\\ +\mathbf{E}^{\rm SCIB}(z''';\mathbf{q}_{\|},\omega)\Delta\mathbf{E}(z'';\mathbf{q}_{\|},\omega)+\Delta\mathbf{E}(z''';\mathbf{q}_{\|},\omega)\Delta\mathbf{E}(z'';\mathbf{q}_{\|},\omega)]dz'''dz'' \ .\end{aligned} \tag{5.9}$$

The second term on the right-hand side of Eq. (5.1) involves the so-called nonlinear, driven selvedge current density given by

$$\mathbf{J}_d^{\rm SE}(z';2\mathbf{q}_{\|},2\omega)=\int\int_{\rm SE}\overleftrightarrow{\Sigma}^{\rm SE}(z',z'',z''';\mathbf{q}_{\|}\to2\mathbf{q}_{\|},\omega\to2\omega):\mathbf{E}(z''';\mathbf{q}_{\|},\omega)\mathbf{E}(z'';\mathbf{q}_{\|},\omega)dz'''dz'' \ , \tag{5.10}$$

where $\overleftrightarrow{\Sigma}^{\rm SE}$ is the nonlinear conductivity response tensor of the selvedge. The tensor $\overleftrightarrow{\Sigma}^{\rm SE}$ is obtained as the difference between the "exact" nonlinear response tensor $\overleftrightarrow{\Sigma}$, calculated eventually by the RPA method, and the semiclassical infinite-barrier model response tensor, i.e.,

$$\overleftrightarrow{\Sigma}^{\rm SE}(z,z',z'';\mathbf{q}_{\|}\to2\mathbf{q}_{\|},\omega\to2\omega)=\overleftrightarrow{\Sigma}(z,z',z'';\mathbf{q}_{\|}\to2\mathbf{q}_{\|},\omega\to2\omega)-\overleftrightarrow{\Sigma}^{\rm SCIB}(z,z',z'';\mathbf{q}_{\|}\to2\mathbf{q}_{\|},\omega\to2\omega) \ . \tag{5.11}$$

The contribution to the background field from the second term on the right-hand side of Eq. (5.1), *in principle,* also requires a self-consistent solution of the complete linear-field problem.

According to the discussion in Secs. II–IV, it is convenient for the analysis of the field inside the selvedge to write the background field in terms of its s- and p-polarized components using the adequate truncated notation. Thus, by inserting the appropriate expressions for the propagator, taken from Eqs. (3.1)–(3.5), into Eqs. (5.1) and (5.2), one obtains (see also Ref. 36) for the s-polarized divergence-free (T) field

$$e_T^{(0)s}(z;2)=e_{*,T}^{\mathrm{SCIB},s}(z;2)-2i\mu_0\omega\int_{\mathrm{SE}}\{\Theta(-z')\Theta(-z)[D_{TT}^{s,<<}(z-z';2)+I_{TT}^{s,<<}(z+z';2)]$$
$$+\Theta(-z')\Theta(z)G_{TT}^{s,<>}(z,z';2)+\Theta(z')\Theta(-z)G_{TT}^{s,><}(z,z';2)$$
$$+\Theta(z')\Theta(z)[D_{TT}^{s,>>}(z-z';2)+I_{TT}^{s,>>}(z,z';2)]\}J_d^{\mathrm{SE},s}(z';2)dz' \tag{5.12}$$

with

$$e_{*,T}^{\mathrm{SCIB},s}(z;2)=-2i\mu_0\omega\int_0^\infty\{\Theta(-z)G_{TT}^{s,><}(z,z';2)+\Theta(z)[D_{TT}^{s,>>}(z-z';2)+I_{TT}^{s,>>}(z,z';2)]\}J_{d,*}^{\mathrm{SCIB},s}(z';2)dz' . \tag{5.13}$$

In agreement with the notation of the previous sections, we have added superscript s and subscript T to the appropriate quantities. For brevity, and to stress that the field, the current density, and the propagator parts are those belonging to the second-harmonic frequency, the number 2 has been added to the various arguments. For the p-polarized case the explicit truncated expression for the divergence-free part of the field takes the form

$$\mathbf{e}_T^{(0)p}(z;2)=\mathbf{e}_{*,T}^{\mathrm{SCIB},p}(z;2)-2i\mu_0\omega\int_{\mathrm{SE}}\{\Theta(-z')\Theta(-z)[\overleftrightarrow{\mathbf{D}}_{TT}^{p,<<}(z-z';2)+\overleftrightarrow{\mathbf{I}}_{TT}^{p,<<}(z+z';2)]$$
$$+\Theta(-z')\Theta(z)\overleftrightarrow{\mathbf{G}}_{TT}^{p,<>}(z,z';2)+\Theta(z')\Theta(-z)[\overleftrightarrow{\mathbf{G}}_{TT}^{p,><}(z,z';2)+\overleftrightarrow{\mathbf{G}}_{LT}^{p,><}(z,z';2)]$$
$$+\Theta(z')\Theta(z)[\overleftrightarrow{\mathbf{D}}_{TT}^{p,>>}(z-z';2)+\overleftrightarrow{\mathbf{I}}_{TT}^{p,>>}(z,z';2)+\overleftrightarrow{\mathbf{I}}_{LT}^{p,>>}(z,z';2)]\}\cdot\mathbf{J}_d^{\mathrm{SE},p}(z';2)dz' , \tag{5.14}$$

where

$$\mathbf{e}_{*,T}^{\mathrm{SCIB},p}(z;2)=-2i\mu_0\omega\int_0^\infty\{\Theta(-z)[\overleftrightarrow{\mathbf{G}}_{TT}^{p,><}(z,z';2)+\overleftrightarrow{\mathbf{G}}_{LT}^{p,><}(z,z';2)]$$
$$+\Theta(z)[\overleftrightarrow{\mathbf{D}}_{TT}^{p,>>}(z-z';2)+\overleftrightarrow{\mathbf{I}}_{TT}^{p,>>}(z,z';2)+\overleftrightarrow{\mathbf{I}}_{LT}^{p,>>}(z,z';2)]\}\cdot\mathbf{J}_{d,*}^{\mathrm{SCIB},p}(z';2)dz' \tag{5.15}$$

in usual notation. Finally, one obtains for the rotational-free part of the p-polarized background field the result

$$\mathbf{e}_L^{(0)p}(z;2)=\mathbf{e}_{*,L}^{\mathrm{SCIB},p}(z;2)+\frac{1}{2i\epsilon_0\omega}[\Theta(-z)+\epsilon^{-1}(2\omega)\Theta(z)]\mathbf{e}_z^p\otimes\mathbf{e}_z^p\cdot\mathbf{J}_d^{\mathrm{SE},p}(z;2)$$
$$-2i\mu_0\omega\int_{\mathrm{SE}}\{\Theta(-z')\Theta(z)\overleftrightarrow{\mathbf{G}}_{TL}^{p,<>}(z,z';2)+\Theta(z')\Theta(z)[\overleftrightarrow{\mathbf{D}}_{LL}^{p,>>}(z-z';2)+\overleftrightarrow{\mathbf{I}}_{TL}^{p,>>}(z,z',2)$$
$$+\overleftrightarrow{\mathbf{I}}_{LL}^{p,>>}(z,z';2)]\}\cdot\mathbf{J}_d^{\mathrm{SE},p}(z';2)dz' \tag{5.16}$$

with

$$\mathbf{e}_{*,L}^{\mathrm{SCIB},p}(z;2)=\frac{1}{2i\epsilon_0\epsilon(2\omega)\omega}\mathbf{e}_z^p\otimes\mathbf{e}_z^p\cdot\mathbf{J}_{d,*}^{\mathrm{SCIB},p}(z;2)-2i\mu_0\omega\Theta(z)\int_0^\infty[\overleftrightarrow{\mathbf{D}}_{LL}^{p,>>}(z-z';2)+\overleftrightarrow{\mathbf{I}}_{TL}^{p,>>}(z,z';2)$$
$$+\overleftrightarrow{\mathbf{I}}_{LL}^{p,>>}(z,z';2)]\cdot\mathbf{J}_{d,*}^{\mathrm{SCIB},p}(z';2)dz' . \tag{5.17}$$

In parametric, second-harmonic generation studies the s- and p-polarized selvedge fields can be analyzed independently of each other once the driven, nonlinear current densities $J_{d,*}^{\mathrm{SCIB},s}, J_d^{\mathrm{SE},s}, \mathbf{J}_{d,*}^{\mathrm{SCIB},p}=(J_{d,*,x}^{\mathrm{SCIB},p}, J_{d,*,z}^{\mathrm{SCIB},p})$, and $\mathbf{J}_d^{\mathrm{SE},p}=(J_{d,x}^{\mathrm{SE},p}, J_{d,z}^{\mathrm{SE},p})$, are known. Thus, in a sense the nonlinear s- and p-polarized selvedge fields are uncoupled. However, due to the general form of the nonlinear response tensors $\overleftrightarrow{\Sigma}^{\mathrm{SCIB}}$ and $\overleftrightarrow{\Sigma}^{\mathrm{SE}}$ (see Refs. 38 and 39), the fields are *indirectly* coupled via the fundamental field if this consists of a superposition of s-and p-polarized components.

It was pointed out in Sec. IV C that a long-wavelength approximation for the divergence-free part of the selvedge field often can be adopted, provided that the field variation of the background field across the inner and outer selvedge is negligible. It appears from Eqs. (5.12)–(5.15) that the criterion for this is tantamount to the requirement that the parts of the propagator which are divergence-free in the unmarked coordinates (x,z), cf. Eqs. (2.7) and (2.8), vary slowly across the selvedge. A slow variation in the divergence-free field in the selvedge region also allows us to take the $\mathbf{E}_T$-field components of Eq. (5.10) outside the integral sign, thus simplifying the calculation of the driven nonlinear selvedge current density. As an example, if the fundamental field is s polarized, one obtains by writting the fundamental field in the form

$$e_T^s(z;1)=e_T^{s,-}\Theta(-z)+e_T^{s,+}\Theta(z) , \tag{5.18}$$

where $e_T^{s,-}$ and $e_T^{s,+}$ are the outer ($-$) and inner ($+$) selvedge fields, respectively, the following expression for the p-polarized selvedge current density:

$$\mathbf{J}_d^{\mathrm{SE},p}(z';2)=\Bigg[(e_T^{s_i-})^2\int_{l_0}^{0}\int_{l_0}^{0}\overleftrightarrow{\Sigma}^{\mathrm{SE}}(z',z'',z''';1\to 2)dz'''dz'' + e_T^{s_i-}e_T^{s_i+}\int_0^{l_i}\int_{l_0}^{0}[\overleftrightarrow{\Sigma}^{\mathrm{SE}}(z',z'',z''';1\to 2)+\overleftrightarrow{\Sigma}^{\mathrm{SE}}(z',z''',z'';1\to 2)]dz'''dz'' + (e_T^{s_i+})^2\int_0^{l_i}\int_0^{l_i}\overleftrightarrow{\Sigma}^{\mathrm{SE}}(z',z'',z''';1\to 2)dz'''dz''\Bigg]:\mathbf{e}_y\mathbf{e}_y\ . \tag{5.19}$$

The form of $\overleftrightarrow{\Sigma}^{\mathrm{SE}}$ implies that the nonlinear current density has only x and z components in the present case.[39] The limits of the integrals in Eq. (5.19) are those illustrated in Fig. 2. Note that the nonlinear response function *effectively* is a sum of local response functions in this example.

VI. ELECTRIC FIELD EXTERIOR TO THE SELVEDGE

Once the field inside the selvedge has been determined via self-consistent solutions to the appropriate integral equations, the field exterior to the selvedge can be obtained directly from the knowledge of the relevant propagator parts. Let us denote the divergence-free and rotational-free fields inside the selvedge by $\mathbf{E}_T^{\mathcal{S}}(z)$ and $\mathbf{E}_L^{\mathcal{S}}(z)$, respectively. Thus, the field in vacuum, $\mathbf{E}_T^{\mathcal{V}}(z)$, which will be divergence-free, is given by

$$\mathbf{E}_T^{\mathcal{V}}(z)=\mathbf{E}_T^{\mathcal{V}(0)}(z)+\int_{\mathrm{SE}}\overleftrightarrow{\mathbf{K}}_T^{-}(z,z')\cdot[\mathbf{E}_T^{\mathcal{S}}(z')+\mathbf{E}_L^{\mathcal{S}}(z')]dz',\quad z<l_0 \tag{6.1}$$

where $\mathbf{E}_T^{\mathcal{V}(0)}(z)$ is the background field in vacuum. The appropriate kernel $\overleftrightarrow{\mathbf{K}}_T^{-}$ in this case has the explicit form (cf. Fig. 2)

$$\overleftrightarrow{\mathbf{K}}_T^{-}(z,z')=-i\mu_0\Omega\int_{\mathrm{SE}}\{\Theta(-z'')[\overleftrightarrow{\mathbf{D}}_{TT}^{<<}(z-z'')+\overleftrightarrow{\mathbf{I}}_{TT}^{<<}(z+z'')]+\Theta(z'')[\overleftrightarrow{\mathbf{G}}_{TT}^{><}(z,z'')+\overleftrightarrow{\mathbf{G}}_{LT}^{><}(z,z'')]\}\cdot\overleftrightarrow{\sigma}^{\mathrm{SE}}(z'',z')dz''\ , \tag{6.2}$$

as one readily verifies. Inside the metal surface in the bulk the electric field has both a divergence-free $\mathbf{E}_T^{\mathcal{B}}(z)$, and a rotational-free, $\mathbf{E}_L^{\mathcal{B}}(z)$, component. The two components are determined by the equations

$$\mathbf{E}_T^{\mathcal{B}}(z)=\mathbf{E}_T^{\mathcal{B}(0)}(z)+\int_{\mathrm{SE}}\overleftrightarrow{\mathbf{K}}_T^{+}(z,z')\cdot[\mathbf{E}_T^{\mathcal{S}}(z')+\mathbf{E}_L^{\mathcal{S}}(z')]dz',\quad z>l_i \tag{6.3}$$

and

$$\mathbf{E}_L^{\mathcal{B}}(z)=\mathbf{E}_L^{\mathcal{B}(0)}(z)+\int_{\mathrm{SE}}\overleftrightarrow{\mathbf{K}}_L^{+}(z,z')\cdot[\mathbf{E}_T^{\mathcal{S}}(z')+\mathbf{E}_L^{\mathcal{S}}(z')]dz',\quad z>l_i \tag{6.4}$$

where the kernels, cf. Fig. 2, are given by

$$\overleftrightarrow{\mathbf{K}}_T^{+}(z,z')=-i\mu_0\Omega\int_{\mathrm{SE}}\{\Theta(-z'')\overleftrightarrow{\mathbf{G}}_{TT}^{<>}(z,z'')+\Theta(z'')[\overleftrightarrow{\mathbf{D}}_{TT}^{>>}(z-z'')+\overleftrightarrow{\mathbf{I}}_{TT}^{>>}(z,z'')+\overleftrightarrow{\mathbf{I}}_{LT}^{>>}(z,z'')]\}\cdot\overleftrightarrow{\sigma}^{\mathrm{SE}}(z'',z')dz''\ , \tag{6.5}$$

and

$$\overleftrightarrow{\mathbf{K}}_L^{+}(z,z')=-i\mu_0\Omega\int_{\mathrm{SE}}\{\Theta(-z'')\overleftrightarrow{\mathbf{G}}_{TL}^{<>}(z,z'')+\Theta(z'')[\overleftrightarrow{\mathbf{D}}_{LL}^{>>}(z-z'')+\overleftrightarrow{\mathbf{I}}_{TL}^{>>}(z,z'')+\overleftrightarrow{\mathbf{I}}_{LL}^{>>}(z,z'')]\}\cdot\overleftrightarrow{\sigma}^{\mathrm{SE}}(z'',z')dz''\ . \tag{6.6}$$

The background fields in the bulk, i.e., $\mathbf{E}_T^{\mathcal{B}(0)}$ and $\mathbf{E}_L^{\mathcal{B}(0)}$, and in vacuum are for linear-field problems determined by the SCIB model. For nonlinear-field problems these fields can be obtained by combining Eqs. (3.1)–(3.5), (5.1), and (5.2). Hence,

$$\mathbf{E}_T^{\mathcal{V}(0)}(z;2)=-2i\mu_0\omega\int_0^{\infty}[\overleftrightarrow{\mathbf{G}}_{TT}^{><}(z,z';2)+\overleftrightarrow{\mathbf{G}}_{LT}^{><}(z,z';2)]\cdot\mathbf{J}_{d,*}^{\mathrm{SCIB}}(z';2)dz' -2i\mu_0\omega\int_{\mathrm{SE}}\{\Theta(-z')[\overleftrightarrow{\mathbf{D}}_{TT}^{<<}(z-z';2)+\overleftrightarrow{\mathbf{I}}_{TT}^{<<}(z+z';2)]+\Theta(z')[\overleftrightarrow{\mathbf{G}}_{TT}^{><}(z,z';2)+\overleftrightarrow{\mathbf{G}}_{LT}^{><}(z,z';2)]\}\cdot\mathbf{J}_d^{\mathrm{SE}}(z';2)dz'\ , \tag{6.7}$$

$$\mathbf{E}_T^{\mathcal{B}(0)}(z;2)=-2i\mu_0\omega\int_0^{\infty}[\overleftrightarrow{\mathbf{D}}_{TT}^{>>}(z-z';2)+\overleftrightarrow{\mathbf{I}}_{TT}^{>>}(z,z';2)+\overleftrightarrow{\mathbf{I}}_{LT}^{>>}(z,z';2)]\cdot\mathbf{J}_{d,*}^{\mathrm{SCIB}}(z';2)dz' -2i\mu_0\omega\int_{\mathrm{SE}}\{\Theta(-z')\overleftrightarrow{\mathbf{G}}_{TT}^{<>}(z,z';2)+\Theta(z')[\overleftrightarrow{\mathbf{D}}_{TT}^{>>}(z-z',2)+\overleftrightarrow{\mathbf{I}}_{TT}^{>>}(z,z';2)+\overleftrightarrow{\mathbf{I}}_{LT}^{>>}(z,z';2)]\}\cdot\mathbf{J}_d^{\mathrm{SE}}(z';2)dz'\ , \tag{6.8}$$

and

$$\mathbf{E}_L^{\mathcal{B}(0)}(z;2)=\frac{1}{2i\epsilon_0\epsilon(2\omega)\omega}\mathbf{e}_z\otimes\mathbf{e}_z\cdot\mathbf{J}_{d,*}^{\mathrm{SCIB}}(z;2)-2i\mu_0\omega\int_0^\infty[\overleftrightarrow{\mathbf{D}}_{LL}^{\gg}(z-z';2)+\overleftrightarrow{\mathbf{I}}_{TL}^{\gg}(z,z';2)+\overleftrightarrow{\mathbf{I}}_{LL}^{\gg}(z,z';2)]\cdot\mathbf{J}_{d,*}^{\mathrm{SCIB}}(z';2)dz'$$
$$-2i\mu_0\omega\int_{\mathrm{SE}}\{\Theta(-z')\overleftrightarrow{\mathbf{G}}_{TL}^{<>}(z,z';2)+\Theta(z')[\overleftrightarrow{\mathbf{D}}_{LL}^{\gg}(z-z';2)+\overleftrightarrow{\mathbf{I}}_{TL}^{\gg}(z,z';2)+\overleftrightarrow{\mathbf{I}}_{LL}^{\gg}(z,z';2)]\}\cdot\mathbf{J}_d^{\mathrm{SE}}(z';2)dz' \;. \tag{6.9}$$

VII. COMPARISON TO PREVIOUS PROPAGATOR THEORIES

Within the context of nonlocal, second-harmonic generation, the basic framework for an electromagnetic propagator description incorporating nonlocal screening effects was established some years ago by the present author,[37] and recently some preliminary steps were taken in the study of the nonlinear, selvedge field.[40] To my knowledge, the only other propagator formalism dealing with nonlocal phenomena in second-harmonic generation is that presented recently by Guyot-Sionnest, Chen, and Shen.[20] The work of Guyot-Sionnest *et al.*,[20] which emphasizes an analysis of interface nonlinearities stemming from both structural asymmetries and field discontinuities, deviates from the present work in many ways as I shall demonstrate below. A minor difference is due to the fact that Guyot-Sionnest *et al.*[20] consider an interface between two media having complex dielectric constants of the bulk which are local whereas I consider a metal-vacuum surface and incorporate nonlocal effects in the bulk response of the metal. A more important difference, however, stems from the fact that Guyot-Sionnest *et al.*[20] use a local Green's function formalism whereas the present work is based on a nonlocal formalism. This, for instance, means that the background solution of the present theory can incorporate effects stemming from single-particle excitations and from the rotational-free collective response of the medium which usually has a very short penetration depth. In both nonlinear optics of metals and semiconductors, these effects can be of extreme importance. Of course also for a self-consistent treatment of the nonlinear radiation from the selvedge region it is essential to incorporate screening effects associated with these mechanisms. Guyot-Sionnest *et al.*[20] do not try to make progress in the study of the solution to the basic integral equation [see for instance Eq. (2.4)]. Being interested only in the field generated by nonlinear wave mixing in the bulk of the two media, they claim that the effect arising from the external selvedge current density is of no importance. This is hard to believe from (i) what is known from studies of linear, nonlocal optics, especially with p-polarized incident light and from (ii) the fact that electron-hole pairs and plasmons are excited in the surface region also in nonlinear optics. For a description of the nonlinear field *inside* the selvedge, a consideration of the background solution alone is, of course, incorrect.

Let us now compare the background solution from the work of Sionnest *et al.*[20] with that presented in Sec. V of the present paper. The quite simple result for the background field given by Sionnest *et al.* is obtained, essentially, by utilizing the continuity properties of the Green's function across the plane $z'=0$. The derivation (see Ref. 18) of the nonlocal Green's function used in the present work was based on the following continuity equations:

$$G_{yy}(z,z'\to 0-)=G_{yy}(z,z'\to 0+) \;, \tag{7.1}$$

$$\frac{\partial G_{yy}(z,z'\to 0-)}{\partial z'}=\frac{\partial G_{yy}(z,z'\to 0+)}{\partial z'} \;, \tag{7.2}$$

and

$$G_{xx}(z,z'\to 0-)=G_{xx}(z,z'\to 0+) \;, \tag{7.3}$$

$$G_{zx}(z,z'\to 0-)=G_{zx}(z,z'\to 0+) \;, \tag{7.4}$$

$$\frac{\partial G_{xx}(z,z'\to 0-)}{\partial z'}+iQ_\parallel G_{xz}(z,z'\to 0-)=\frac{\partial G_{xx}(z,z'\to 0+)}{\partial z'}+iQ_\parallel G_{xz}(z,z'\to 0+) \;, \tag{7.5}$$

$$\frac{\partial G_{zx}(z,z'\to 0-)}{\partial z'}+iQ_\parallel G_{zz}(z,z'\to 0-)=\frac{\partial G_{zx}(z,z'\to 0+)}{\partial z'}+iQ_\parallel G_{zz}(z,z'\to 0+) \;, \tag{7.6}$$

where those of Eqs. (7.1) and (7.2) are appropriate for s-polarized propagation and the remaining ones for p-polarized propagation. To facilitate the comparison with the results of Sionnest *et al.*,[20] we use the fact that the continuity conditions in Eqs. (7.5) and (7.6) can be replaced by the equivalent, vectorial relation

$$\left[\lim_{z'\to 0-}\int_{-\infty}^{\infty}\overleftrightarrow{\mathbf{G}}(z,z'')\cdot\overleftrightarrow{\epsilon}^{\mathrm{SCIB}}(z'',z')dz''\right]\cdot\mathbf{e}_z=\left[\lim_{z'\to 0+}\int_{-\infty}^{\infty}\overleftrightarrow{\mathbf{G}}(z,z'')\cdot\overleftrightarrow{\epsilon}^{\mathrm{SCIB}}(z'',z')dz''\right]\cdot\mathbf{e}_z \;, \tag{7.7}$$

as demonstrated in Appendix B. The appropriate linear and nonlocal, dielectric tensor of the SCIB model is given by

$$\overleftrightarrow{\epsilon}^{\mathrm{SCIB}}(z'',z')=\delta(z''-z')\overleftrightarrow{\mathrm{U}}+\frac{i}{\epsilon_0\Omega}\overleftrightarrow{\sigma}^{\mathrm{SCIB}}(z'',z') , \quad (7.8)$$

where δ and $\overleftrightarrow{\mathrm{U}}$ are the Dirac delta function and the unit tensor, respectively. As in previous sections, we have omitted the superfluous quantities $\mathbf{Q}_\parallel$ and Ω from the notation. If the dielectric response is local (loc) and isotropic, i.e.,

$$\overleftrightarrow{\epsilon}^{\mathrm{SCIB}}(z'',z')\Longrightarrow\epsilon^{\mathrm{loc}}(z')\delta(z''-z')\overleftrightarrow{\mathrm{U}} , \quad (7.9)$$

the continuity condition in Eq. (7.7) is reduced to

$$\lim_{z'\to 0-}\left[\begin{pmatrix} G_{xz}^{\mathrm{loc}}(z,z') \\ 0 \\ G_{zz}^{\mathrm{loc}}(z,z')\end{pmatrix}\epsilon^{\mathrm{loc}}(z')\right] = \lim_{z'\to 0+}\left[\begin{pmatrix} G_{xz}^{\mathrm{loc}}(z,z') \\ 0 \\ G_{zz}^{\mathrm{loc}}(z,z')\end{pmatrix}\epsilon^{\mathrm{loc}}(z')\right] , \quad (7.10)$$

which is precisely the form given by Sionnest *et al.*[20] To stress that there is a local propagator associated with the local dielectric response, we have added the superscript loc to the Green's function in Eq. (7.10). By writing the background field in Eq. (5.1) in the form

$$\mathbf{E}^{(0)}(z;2\mathbf{q}_\parallel,2\omega)=-2i\mu_0\omega\int_{\mathrm{SE+B}}\overleftrightarrow{\mathrm{G}}(z,z';2\mathbf{q}_\parallel,2\omega)\cdot\boldsymbol{\Upsilon}(z';2\mathbf{q}_\parallel,2\omega)dz' , \quad (7.11)$$

where

$$\boldsymbol{\Upsilon}(z';2\mathbf{q}_\parallel,2\omega)=\int\int_{\mathrm{SE+B}}\overleftrightarrow{\Sigma}(z',z'',z''';\mathbf{q}_\parallel\to 2\mathbf{q}_\parallel,\omega\to 2\omega):\mathbf{E}(z''';\mathbf{q}_\parallel,\omega)\mathbf{E}(z'';\mathbf{q}_\parallel,\omega)dz'''dz'' \quad (7.12)$$

in a notation where SE + B means that the integrations extend over the selvedge (SE) plus bulk (B), it is readily realized that the contribution to the ith component of the background field from the selvedge region in the local regime for the dielectric response is given by

$$-2i\mu_0\omega\left[\int_{\mathrm{SE}}\overleftrightarrow{\mathrm{G}}(z,z';2\mathbf{q}_\parallel,2\omega)\cdot\boldsymbol{\Upsilon}(z';2\mathbf{q}_\parallel,2\omega)dz'\right]_i$$
$$\cong -2i\mu_0\omega\left[\sum_{j=x,y}G_{ij}^{\mathrm{loc}}(z,z'=0;2\mathbf{q}_\parallel,2\omega)\Upsilon_j^S(2\mathbf{q}_\parallel,2\omega)+\lim_{z'\to 0}[G_{iz}^{\mathrm{loc}}(z,z';2\mathbf{q}_\parallel,2\omega)\epsilon^{\mathrm{loc}}(z';2\omega)]\Upsilon_z^S(2\mathbf{q}_\parallel,2\omega)\right] , \quad (7.13)$$

where we have defined the surface (S) current density $\boldsymbol{\Upsilon}^S$ via

$$\Upsilon_j^S\equiv\begin{cases}\sum_{k,l}\int\int\int_{\mathrm{SE}}\Sigma_{jkl}(z',z'',z''')E_l(z''';\mathbf{q}_\parallel,\omega)E_k(z'';\mathbf{q}_\parallel,\omega)dz'''dz''dz', & j=x,y\\ \sum_{k,l}\int\int\int_{\mathrm{SE}}[\epsilon^{\mathrm{loc}}(z';2\omega)]^{-1}\Sigma_{jkl}(z',z'',z''')E_l(z''';\mathbf{q}_\parallel,\omega)E_k(z'';\mathbf{q}_\parallel,\omega)dz'''dz''dz', & j=z .\end{cases} \quad (7.14)$$

To obtain the result in Eq. (7.13) with (7.14), which is precisely equivalent to that of Sionnest *et al.*,[20] it has been assumed that $G_{ij}^{\mathrm{loc}}(j=x,y)$ and $G_{iz}^{\mathrm{loc}}\epsilon^{\mathrm{loc}}$ assume, in the entire selvedge region, essentially their values at $z'=0$. By insertion of $\overleftrightarrow{\mathrm{G}}^{\mathrm{loc}}$ into Eq. (7.11) it readily follows that also the bulk (B) contribution to the background field in Eq. (7.11) is identical to that given by Sionnest *et al.*[20] The nonlinear surface susceptibility introduced by Sionnest *et al.*[20] in Eqs. (10) and (11) of their paper is readily obtained from Eq. (7.14) utilizing that for the *fundamental* field E_x, E_y, and $\epsilon^{\mathrm{loc}}E_z$ is almost constant across the selvedge region. With this remark the contact to the propagator work of Sionnest, Chen, and Shen[20] has been established. For a discussion of the relation of the theory of Sionnest *et al.*[20] to those derived by other authors the reader is referred to Ref. 20.

A perturbative Green's-function approach was developed some years ago by Bagchi, Barrera, and Rajagopal[21] to investigate in linear optics the electric field near a metal surface with a smooth electron-density profile. This propagator formalism of Bagchi *et al.*, which among other things led to new and potentially useful expressions for the changes in the reflection coefficients for s- and p-polarized light from the standard Fresnel coefficients, can easily be obtained from the present propagator theory if one makes a number of additional approximations. Thus, Bagchi *et al.*[21] use a local Green's-function formalism taking the classical Fresnel problem for an isotropic metal as the background problem and assume that the bulk response is local. Furthermore, they make the long-wavelength approximation $\mathbf{q}_\parallel\to\mathbf{0}$ in the dielectric response tensor. In this long-wavelength limit the conductivity response tensor

$$\overleftrightarrow{\sigma}(z,z';\mathbf{0},\omega)\equiv\sigma^{\mathrm{Fresn}}(z;\omega)\overleftrightarrow{\mathrm{U}}\delta(z-z')+\overleftrightarrow{\sigma}^{\mathrm{SE}}(z,z';\mathbf{0},\omega) \quad (7.15)$$

is diagonal. Since the Fresnel (Fresn) response tensor is proportional to the unit tensor, $\overleftrightarrow{\sigma}^{\text{SE}}$ is also diagonal. Now, by assuming that the expression in Eq. (7.10), with

$$\epsilon^{\text{loc}}(z';\omega)=1+\frac{i}{\epsilon_0\omega}\sigma^{\text{Fresn}}(z';\omega) , \quad (7.16)$$

is constant throughout the selvedge region, the truncated kernels in Eqs. (2.16) and (2.17) are given by

$$K_T^s(z,z';0,\omega)=-i\mu_0\omega G_{yy}^{\text{loc}}(z,z'=0)\int_{\text{SE}}\sigma_{yy}^{\text{SE}}(z'',z')dz'' \quad (7.17)$$

and

$$\overleftrightarrow{\mathbf{K}}_T^p(z,z';0,\omega)=-i\mu_0\omega\begin{bmatrix} G_{xx}^{\text{loc}}(z,z'=0)\int_{\text{SE}}\sigma_{xx}^{\text{SE}}(z'',z')dz'' & \lim_{z''\to 0}[\epsilon^{\text{loc}}(z'')G_{xz}^{\text{loc}}(z,z'')] \times\int_{\text{SE}}[\epsilon^{\text{loc}}(z'')]^{-1}\sigma_{zz}^{\text{SE}}(z'',z')dz'' \\ G_{zx}^{\text{loc}}(z,z'=0)\int_{\text{SE}}\sigma_{xx}^{\text{SE}}(z'',z')dz'' & \lim_{z''\to 0}[\epsilon^{\text{loc}}(z'')G_{zz}^{\text{loc}}(z,z'')] \times\int_{\text{SE}}[\epsilon^{\text{loc}}(z'')]^{-1}\sigma_{zz}^{\text{SE}}(z'',z')dz'' \end{bmatrix} , \quad (7.18)$$

leaving out the parameters $\mathbf{Q}_\parallel\to\mathbf{0}$ and ω from the terms on the right-hand side of the equations. Since only the self-field part of the rotational-free propagator survives in the local limit, it follows immediately that

$$\overleftrightarrow{\mathbf{K}}_L^p(z,z';0,\omega)=\frac{1}{\epsilon_0\omega}[\Theta(-z)+\epsilon^{-1}(\omega)\Theta(z)]\mathbf{e}_z^p\otimes\mathbf{e}_z^p\sigma_{zz}^{\text{SE}}(z,z') \quad (7.19)$$

for the Fresnel-background problem. Furthermore, as it is known[19,41] that the Fresnel-background field is divergence-free so that $\mathbf{e}_L^{(0)p}(z)$ of Eq. (2.21) is zero, the calculations of Bagchi *et al.*[21] are described within the framework of Eqs. (2.19)–(2.21) setting $\mathbf{e}_L^{(0)p}(z)=0$ and utilizing Eqs. (7.17)–(7.19). By assuming that $e_T^s(z')$ is constant across the selvedge one obtains by combining Eqs. (2.19) and (7.17)

$$e_T^s(z)=e_T^{(0)s}(z)-i\mu_0\omega e_T^s(z=0)G_{yy}^{\text{loc}}(z,z'=0)\int\int_{\text{SE}}\sigma_{yy}^{\text{SE}}(z'',z')dz''dz' , \quad (7.20)$$

with

$$e_T^s(z=0)=\frac{e_T^{(0)s}(z=0)}{1+i\mu_0\omega G_{yy}^{\text{loc}}(z=0,z'=0)\int\int_{\text{SE}}\sigma_{yy}^{\text{SE}}(z'',z')dz''dz'} , \quad (7.21)$$

i.e., precisely the result of Bagchi *et al.*[21] To determine the p-polarized field $\mathbf{e}_T^p(z)$, following Bagchi *et al.*,[21] one introduces the inverse, dielectric response function ϵ_{zz}^{-1} via

$$E_z(z)=\int_{-\infty}^{\infty}\epsilon_{zz}^{-1}(z,z';0,\omega)D_z(z')dz' \quad (7.22)$$

and assumes that the normal component of the $\mathbf{D}$ field, i.e., $D_z(z)$, and the tangential component of the electric field, are constant across the selvedge. This procedure, after adding Eqs. (2.20) and (2.21), reproduces immediately the results of Bagchi *et al.*[21] which we desist from writing down here.

A Green's function formalism has also been used by Sipe[22] to study the coupling between the bulk and the selvedge in linear, nonlocal optics. Sipe's approach deviates basically from the present one due to his use of the dyadic vacuum propagator in all space. In the notation of this work, the vacuum propagator has the following tensor-product ($\otimes$) structure:[19]

$$\overleftrightarrow{\mathbf{D}}_{TT}^{\ll}(z-z')=\frac{e^{iq_\perp^0|z-z'|}}{2iq_\perp^0}[\mathbf{e}_y\otimes\mathbf{e}_y+\Theta(z-z')\mathbf{e}_i\otimes\mathbf{e}_i +\Theta(z'-z)\mathbf{e}_r\otimes\mathbf{e}_r] , \quad (7.23)$$

where $\mathbf{e}_i=c_0(q_\perp^0,0,-q_\parallel)/\omega$ and $\mathbf{e}_r=c_0(-q_\perp^0,0,-q_\parallel)/\omega$, cf. Appendix A. Sipe[22] divides the vacuum propagator into two pieces, i.e.,

$$\overleftrightarrow{\mathbf{D}}_{TT}^{\ll}(z-z')=\overleftrightarrow{\mathbf{G}}_0^T(z-z')+\overleftrightarrow{\mathbf{G}}_0^{\text{NR}}(z-z') , \quad (7.24)$$

where

$$\overleftrightarrow{G}_0^{NR}(z-z') \equiv \overleftrightarrow{D}_{TT}^{\ll}(z-z';c_0\to\infty) = \frac{q_\parallel}{2}\left[\frac{c_0}{\omega}\right]^2 e^{-q_\parallel|z-z'|}\{\mathbf{e}_x\otimes\mathbf{e}_x-\mathbf{e}_z\otimes\mathbf{e}_z+i[\Theta(z-z')-\Theta(z'-z)](\mathbf{e}_x\otimes\mathbf{e}_z+\mathbf{e}_z\otimes\mathbf{e}_x)\}\ , \tag{7.25}$$

is the form of the vacuum propagator in the nonretarded (NR) limit, that is for $c_0\to\infty$. Since $q_\perp^0=iq_\parallel$ in this limit, it is easy to demonstrate that $\overleftrightarrow{G}_0^{NR}(z-z')\exp[iq_\parallel(x-x')]$ and its transpose is rotational-free in the $\mathbf{r}$ and $\mathbf{r}'$ coordinates, respectively. One should note that $\overleftrightarrow{G}_0^{NR}(z-z')\exp[iq_\parallel(x-x')]$ is also divergence-free, because $\overleftrightarrow{D}_{TT}^{\ll}(z-z')\exp[iq_\parallel(x-x')]$ is. The explicit expression for $\overleftrightarrow{G}_0^T$ is obtained by subtracting $\overleftrightarrow{G}_0^{NR}$ from $\overleftrightarrow{D}_{TT}^{\ll}$. We have added a superscript T to $\overleftrightarrow{G}_0^T$ to indicate that $\overleftrightarrow{G}_0^T(z-z')\exp[iq_\parallel(x-x')]$ and its transposition are divergence-free in $\mathbf{r}$ and $\mathbf{r}'$, respectively. Inside the selvedge Sipe uses the long-wavelength limit expressions for $\overleftrightarrow{G}_0^T$ and $\overleftrightarrow{G}_0^{NR}$, i.e., he sets $\exp(iq_\perp^0|z-z'|)\approx\exp(-q_\parallel|z-z'|)\approx 1$. In this approximation $\overleftrightarrow{G}_0^T$, given by

$$\overleftrightarrow{G}_0^T\approx\frac{1}{2iq_\perp^0}\mathbf{e}_y\otimes\mathbf{e}_y+\frac{1}{2}\left[\frac{c_0}{\omega}\right]^2\left[-(q_\parallel+iq_\perp^0)\mathbf{e}_x\otimes\mathbf{e}_x+\left[q_\parallel-i\frac{q_\parallel^2}{q_\perp^0}\right]\mathbf{e}_z\otimes\mathbf{e}_z\right]\ , \tag{7.26}$$

becomes independent of z and z', and in on-diagonal form. In the long-wavelength limit $\overleftrightarrow{G}_0^{NR}$ is still a function of $z-z'$, via the Heaviside step functions [see Eq. (7.25)]. Utilizing also the vacuum self-field contribution $\overleftrightarrow{g}_{LL}^{\ll}(z-z')=(c_0/\omega)^2\delta(z-z')\mathbf{e}_z\otimes\mathbf{e}_z$ to the propagator, the results of Sipe[22] are easily established starting from Eqs. (2.1)–(2.3) assuming the bulk response to be isotropic and local.

APPENDIX A: THE FUNCTIONS APPEARING IN THE SEPARABLE KERNELS

On the basis of the explicit expressions for the SCIB-propagator terms given in Ref. 19, the unknown functions in Eqs. (3.13)–(3.15) can be obtained. Since the functions always appear as products, i.e., $\mathcal{H}_{T,i}^s(z)\mathcal{L}_{T,i}^s(z'')$, $\mathcal{H}_{T,j}^p(z)\otimes\mathcal{L}_{T,j}^p(z'')$, and $\mathcal{H}_L^p(z)\otimes\mathcal{L}_L^p(z'')$, z and z'' independent factors of course can be attached to either the first or the second function in a given product, depending on what one chooses. With this freedom of choice in mind, the calculated functions are

$$\mathcal{H}_{T,1}^s(z)=\Theta(-z)e^{-iq_\perp^0 z}\ , \tag{A1}$$

$$\mathcal{L}_{T,1}^s(z'')=\frac{r^s}{2iq_\perp^0}\Theta(-z'')e^{-iq_\perp^0 z''}+(1-r^s)\frac{\Theta(z'')}{2\pi}\int_{-\infty}^{\infty}\frac{e^{iq_\perp z''}}{N_T(q)}dq_\perp\ , \tag{A2}$$

$$\mathcal{H}_{T,2}^s(z)=\frac{\Theta(z)}{4\pi}\int_{-\infty}^{\infty}\frac{1+L(Q_\parallel,\Omega)q_\perp}{N_T(q)}e^{iq_\perp z}dq_\perp\ , \tag{A3}$$

$$\mathcal{L}_{T,2}^s(z'')=(1-r^s)\Theta(-z'')e^{-iq_\perp^0 z''}\ , \tag{A4}$$

$$\mathcal{H}_{T,3}^s(z)=\frac{\Theta(z)}{2\pi}\int_{-\infty}^{\infty}\frac{q_\perp^0-q_\perp}{N_T(q)}e^{iq_\perp z}dq_\perp\ , \tag{A5}$$

$$\mathcal{L}_{T,3}^s(z'')=i^{-1}(1-r^s)\frac{\Theta(z'')}{2\pi}\int_{-\infty}^{\infty}\frac{e^{iq_\perp z''}}{N_T(q)}dq_\perp\ , \tag{A6}$$

and

$$\mathcal{H}_{T,1}^p(z)=\Theta(-z)e^{-iq_\perp^0 z}\mathbf{e}_r\ , \tag{A7}$$

$$\mathcal{L}_{T,1}^p(z'')=\frac{r^p}{2iq_\perp^0}\Theta(-z'')e^{-iq_\perp^0 z''}\mathbf{e}_i-\frac{\Omega}{c_0q_\perp^0}(1+r^p)\frac{\Theta(z'')}{2\pi}\int_{-\infty}^{\infty}\left[\frac{Q_\parallel}{N_L(q)}\mathbf{e}_I^L(Q_\parallel,q_\perp)-\frac{q_\perp}{N_T(q)}\mathbf{e}_I^T(Q_\parallel,q_\perp)\right]\frac{e^{iq_\perp z''}}{q}dq_\perp\ , \tag{A8}$$

$$\mathcal{H}_{T,2}^p(z)=\frac{\Theta(z)}{2\pi}\int_{-\infty}^{\infty}\frac{q_\perp+M(Q_\parallel,\Omega)q^2}{qN_T(q)}\mathbf{e}_R^T(Q_\parallel,q_\perp)e^{iq_\perp z}dq_\perp\ , \tag{A9}$$

$$\mathcal{L}_{T,2}^p(z'')=\frac{\Omega}{c_0q_\perp^0}(1+r^p)\Theta(-z'')e^{-iq_\perp^0 z''}\mathbf{e}_i\ , \tag{A10}$$

$$\mathcal{H}_{T,3}^p(z)=\frac{\Theta(z)}{2\pi}\int_{-\infty}^{\infty}\frac{q_\perp-\left[\frac{c_0q}{\Omega}\right]^2q_\perp^0}{qN_T(q)}\mathbf{e}_R^T(Q_\parallel,q_\perp)e^{iq_\perp z}dq_\perp\ , \tag{A11}$$

$$\mathcal{L}_{T,3}^p(z'')=\left[\frac{\Omega}{c_0}\right]^2\frac{1+r^p}{iq_\perp^0}\frac{\Theta(z'')}{2\pi}\int_{-\infty}^{\infty}\left[\frac{Q_\parallel}{N_L(q)}\mathbf{e}_I^L(Q_\parallel,q_\perp)-\frac{q_\perp}{N_T(q)}\mathbf{e}_I^T(Q_\parallel,q_\perp)\right]\frac{e^{iq_\perp z''}}{q}dq_\perp\ , \tag{A12}$$

and

$$\mathcal{H}_L^p(z)=\frac{\Theta(z)}{2\pi}\int_{-\infty}^{\infty}\mathbf{e}_R^L(Q_\parallel,q_\perp)\frac{Q_\parallel}{qN_L(q)}e^{iq_\perp z}dq_\perp\;, \tag{A13}$$

$$\mathcal{L}_L^p(z'')=\left[\frac{\Omega}{c_0}\right]^2\frac{1+r^p}{iq_\perp^0}\left[\frac{ic_0}{2\Omega}\Theta(-z'')e^{-iq_\perp^0 z''}\mathbf{e}_i+\frac{\Theta(z'')}{2\pi}\int_{-\infty}^{\infty}\left[\frac{Q_\parallel}{N_L(q)}\mathbf{e}_I^L(Q_\parallel,q_\perp)-\frac{q_\perp}{N_T(q)}\mathbf{e}_I^T(Q_\parallel,q_\perp)\right]\frac{e^{iq_\perp z''}}{q}dq_\perp\right]\;. \tag{A14}$$

In the equations above we have introduced the abbreviations $q_\perp^0=[(\Omega/c_0)^2-Q_\parallel^2]^{1/2}$ and $q=(Q_\parallel^2+q_\perp^2)^{1/2}$ and the following unit vectors in truncated notation $\mathbf{e}_i=c_0(q_\perp^0,-Q_\parallel)/\Omega$, $\mathbf{e}_r=c_0(-q_\perp^0,-Q_\parallel)/\Omega$, $\mathbf{e}_I^T=(-q_\perp,-Q_\parallel)/q$, $\mathbf{e}_I^L=(Q_\parallel,-q_\perp)/q$, $\mathbf{e}_R^T=(q_\perp,-Q_\parallel)/q$, and $\mathbf{e}_R^L=(Q_\parallel,q_\perp)/q$. Furthermore, $r^s=r^s(Q_\parallel,\Omega)$ and $r^p=r^p(Q_\parallel,\Omega)$ denote the amplitude reflection coefficients (from the vacuum side) for s- and p-polarized light, respectively. The functions $N_T=N_T(q,\Omega)$ and $N_L=N_L(q,\Omega)$ describing collective and single-particle excitations associated with the divergence-free (T) and the rotational-free (L) parts of the electromagnetic field are well known from previous studies in the field. The explicit expressions for r^s, r^p, N_T, N_L, and the functions $L=L(Q_\parallel,\Omega)$ and $M=M(Q_\parallel,\Omega)$ can be found in Ref. 19, but are not needed here. A detailed discussion of the physical interpretation of the structure of the separable propagator terms forming the basis for the equations of this Appendix is also presented in Ref. 19. One should note that an unimportant (for the present work) factor $\exp(-iq_\perp 0+)$ has been omitted from some of the equations in this Appendix, cf. Ref. 19.

APPENDIX B: NEW FORMULATION OF THE BOUNDARY CONDITIONS FOR THE NONLOCAL PROPAGATOR

To reformulate the boundary conditions in Eqs. (7.5) and (7.6) in a physically transparent manner, we take as a starting point the integrodifferential equation for the propagator $\overleftrightarrow{G}^{\text{old}}(z',z;\mathbf{Q}_\parallel,\Omega)$ of Ref. 18, i.e.,

$$\left\{\overleftrightarrow{U}\left[\left[\frac{\Omega}{c_0}\right]^2-Q_\parallel^2\right]+Q_\parallel^2\mathbf{e}_x\otimes\mathbf{e}_x-iQ_\parallel(\mathbf{e}_x\otimes\mathbf{e}_z+\mathbf{e}_z\otimes\mathbf{e}_x)\frac{\partial}{\partial z'}+(\overleftrightarrow{U}-\mathbf{e}_z\otimes\mathbf{e}_z)\frac{\partial^2}{(\partial z')^2}\right\}\cdot\overleftrightarrow{G}^{\text{old}}(z',z)$$
$$+i\mu_0\Omega\int_{-\infty}^{\infty}\overleftrightarrow{\sigma}^{\text{SCIB}}(z',z'')\cdot\overleftrightarrow{G}^{\text{old}}(z'',z)dz''=\delta(z'-z)\overleftrightarrow{U}\;. \tag{B1}$$

Among the nine equations of (B1) the following two are of relevance for our purpose:

$$iQ_\parallel\frac{\partial G_{xx}^{\text{old}}(z',z)}{\partial z'}+Q_\parallel^2G_{zx}^{\text{old}}(z',z)$$
$$=\left[\frac{\Omega}{c_0}\right]^2G_{zx}^{\text{old}}(z',z)+i\mu_0\Omega\int_{-\infty}^{\infty}[\sigma_{zx}^{\text{SCIB}}(z',z'')G_{xx}^{\text{old}}(z'',z)+\sigma_{zz}^{\text{SCIB}}(z',z'')G_{zx}^{\text{old}}(z'',z)]dz''\;, \tag{B2}$$

and

$$iQ_\parallel\frac{\partial G_{xz}^{\text{old}}(z',z)}{\partial z'}+Q_\parallel^2G_{zz}^{\text{old}}(z',z)=-\delta(z'-z)+\left[\frac{\Omega}{c_0}\right]^2G_{zz}^{\text{old}}(z',z)$$
$$+i\mu_0\Omega\int_{-\infty}^{\infty}[\sigma_{zx}^{\text{SCIB}}(z',z'')G_{xz}^{\text{old}}(z'',z)+\sigma_{zz}^{\text{SCIB}}(z',z'')G_{zz}^{\text{old}}(z'',z)]dz''\;. \tag{B3}$$

By introducing the nonlocal, dielectric response tensor $\overleftrightarrow{\epsilon}^{\text{SCIB}}(z',z'';\mathbf{Q}_\parallel,\Omega)$ given in Eq. (7.8), Eqs. (B2) and (B3) can be written in the form

$$iQ_\parallel\left[\frac{\partial G_{xx}^{\text{old}}(z',z)}{\partial z'}-iQ_\parallel G_{zx}^{\text{old}}(z',z)\right]=\left[\frac{\Omega}{c_0}\right]^2\int_{-\infty}^{\infty}[\overleftrightarrow{\epsilon}^{\text{SCIB}}(z',z'')\cdot\overleftrightarrow{G}^{\text{old}}(z'',z)]_{zx}dz''\;, \tag{B4}$$

and

$$iQ_\parallel\left[\frac{\partial G_{xz}^{\text{old}}(z',z)}{\partial z'}-iQ_\parallel G_{zz}^{\text{old}}(z',z)\right]=\left[\frac{\Omega}{c_0}\right]^2\int_{-\infty}^{\infty}[\overleftrightarrow{\epsilon}^{\text{SCIB}}(z',z'')\cdot\overleftrightarrow{G}^{\text{old}}(z'',z)]_{zz}dz''-\delta(z'-z)\;. \tag{B5}$$

Now, since we know, cf. Ref. 18, that the left-hand sides of Eqs. (B4) and (B5) are continuous at $z'=0$, the continuity of the expressions

$$\int_{-\infty}^{\infty}[\overleftrightarrow{\epsilon}^{\,\mathrm{SCIB}}(z',z'')\cdot\overleftrightarrow{\mathrm{G}}^{\,\mathrm{old}}(z'',z)]_{zx}dz''$$

and

$$\int_{-\infty}^{\infty}[\overleftrightarrow{\epsilon}^{\,\mathrm{SCIB}}(z',z'')\cdot\overleftrightarrow{\mathrm{G}}^{\,\mathrm{old}}(z'',z)]_{zz}dz''$$

at $z'=0$ (for $z\neq 0$) follows readily. The propagator $\overleftrightarrow{\mathrm{G}}(z,z';\mathbf{Q}_\parallel,\Omega)$ of the present work is related to $\overleftrightarrow{\mathrm{G}}^{\,\mathrm{old}}$ via[19]

$$\overleftrightarrow{\mathrm{G}}(z,z'')=\begin{bmatrix} G_{xx}^{\mathrm{old}}(z'',z) & 0 & -G_{zx}^{\mathrm{old}}(z'',z) \\ 0 & G_{yy}^{\mathrm{old}}(z'',z) & 0 \\ -G_{xz}^{\mathrm{old}}(z'',z) & 0 & G_{zz}^{\mathrm{old}}(z'',z) \end{bmatrix} . \tag{B6}$$

To rewrite the continuity conditions above in terms of $\overleftrightarrow{\mathrm{G}}(z,z'')$ one makes use of the explicit expression for $\overleftrightarrow{\sigma}^{\,\mathrm{SCIB}}(z',z'')$ given by[19]

$$[\overleftrightarrow{\sigma}^{\,\mathrm{SCIB}}(z',z'')]_{ij}=\Theta(z')\Theta(z'')[\sigma_{ij}^{\infty}(z'-z'') + \xi_j\sigma_{ij}^{\infty}(z'+z'')] , \tag{B7}$$

where $\overleftrightarrow{\sigma}^{\,\infty}$ is the conductivity tensor of a homogeneous and infinitely extended jellium. The quantity ξ_j is given by $\xi_j=1$ for $j=x$ or y and $\xi_j=-1$ for $j=z$. Since $\overleftrightarrow{\sigma}^{\,\infty}(z)$ is symmetric,[42] i.e.,

$$\sigma_{xz}^{\infty}(z)=\sigma_{zx}^{\infty}(z) , \tag{B8}$$

and the diagonal and off-diagonal elements of $\overleftrightarrow{\sigma}^{\,\infty}(z)$ are even and uneven functions of z, respectively, one has

$$\sigma_{xz}^{\infty}(z)=-\sigma_{xz}^{\infty}(-z) , \tag{B9}$$

and

$$\sigma_{zz}^{\infty}(z)=\sigma_{zz}^{\infty}(-z) . \tag{B10}$$

By combining Eqs. (7.8) and (B7)–(B10) one can show

$$\epsilon_{xz}^{\mathrm{SCIB}}(z',z'')=-\epsilon_{zx}^{\mathrm{SCIB}}(z'',z') , \tag{B11}$$

and

$$\epsilon_{zz}^{\mathrm{SCIB}}(z',z'')=\epsilon_{zz}^{\mathrm{SCIB}}(z'',z') . \tag{B12}$$

Finally, by inserting Eqs. (B6), (B11), and (B12) into the continuity conditions written between Eqs. (B5) and (B6), one readily establishes the vectorial relation in Eq. (7.7).

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