Scattering and absorption of electromagnetic radiation by a semi-infinite medium in the presence of surface roughness

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In this paper, we present a theoretical description of the scattering and absorption of electromagnetic radiation induced by roughness on the surface of a semi-infinite medium. We approach the problem by the use of scattering theory applied to the classical Maxwell equations. We obtain formulas for the roughness-induced scattering from the surface of an isotropic dielectric for both s- and p-polarized waves incident on the surface at a general angle of incidence. When the real part of the dielectric constant of the material is negative and its imaginary part small (as in a simple nearly-free-electron metal), we extract from the expressions for the total absorption rate that portion which describes roughness-induced absorption by surface polaritons (surface plasmons). We compare our results with those recently published by Ritchie and collaborators for the case of normal incidence, and we present a series of numerical studies of the roughness-induced scattering and absorption rates in aluminum.

I. INTRODUCTION

Our purpose in the present paper is to present a theoretical discussion of the effects of surface roughness on the interaction of incident electromagnetic radiation with the surface of a semi-infinite crystal. In the presence of roughness, which will be present on even the most carefully prepared sample, the incident radiation may be scattered away from the specular direction, either into the vacuum above the sample or into the material, where it is absorbed, if the sample is thick. Thus, the presence of roughness decreases the value of the measured reflection coefficient below the value appropriate to the idealized semi-infinite sample with a perfectly smooth surface. In a simple metal, for which the real part of the dielectric constant is negative and its imaginary part small, one physical process that makes an important contribution to the absorption rate is the roughness-induced coupling of the incident electromagnetic wave to surface polaritons (surface plasmons),[1] which exist in the frequency region below $\omega_p/\sqrt{2}$, where ω_p is the bulk plasma frequency.

Over the past several years, several theoretical investigations of these phenomena have appeared.[2–8] In these papers, attention is frequently confined to the case of normal incidence, and many authors have examined only the properties of the simple free-electron metal, which is described by the (real) dielectric constant $\epsilon = 1 - \omega_p^2/\omega^2$. We feel it desirable to extend these discussions to focus on the case of non-normal incidence, and to compare the relative effect of surface roughness on incident radiation of s and p polarization for situations of current experimental interest. Furthermore, even in simple metals such as aluminum, the dielectric constant may have an appreciable imaginary part in some frequency regions, and the real part of the dielectric constant need not be negative always, so it appears useful to present calculations which use the full form of the complex dielectric constant.

Also, if one examines the recent papers of Ritchie and his collaborators,[4–6] one sees that in one of them,[5] the expressions obtained for the surface-roughness-induced scattering and absorption of radiation normally incident on the sample differ substantially from the results of the other two papers.[4,6] The question of which set of results is correct remains.

The remarks of the two preceding paragraphs suggests that the theoretical description of the surface-roughness-induced scattering and absorption of electromagnetic radiation remains incomplete at the present time. It is for this reason that we have chosen to examine these questions.

In some of the papers cited earlier, the analysis proceeds by the use of the formalism of second quantization. The quanta associated with the incident and scattered waves, as well as those associated with the surface polaritons, are described by introducing appropriate annihilation and creation operators. This formalism, while elegant, is difficult in practice to generalize to the case where all of the modes have a finite lifetime as a consequence of the imaginary part of the dielectric constant.

We view the problem as a problem in classical electromagnetic theory, and we choose to work directly with Maxwell's equations. We formally expand the dielectric constant in a Taylor series in the amplitude $\zeta(x, y)$ of the surface roughness, and use a method described earlier[9] to convert Maxwell's equations to integral form, with the term proportional to $\zeta(x, y)$ treated by the methods of scattering theory. Within the first Born approximation, one obtains from this approach the contribution to the roughness-induced scattering and absorption rate proportional to δ^2, where δ is the rms deviation of the rough surface from a perfect plane.

In a recent set of papers, Kröger and Kretschmann[7] and Juranek[8] have examined this problem from the point of view of classical electromagnetic theory. While their methods differ substantially from ours, their final results appear similar in structure.

When our results at normal incidence are compared to the appropriate expressions in the recent work of Ritchie and co-workers,[4-6] we find agreement with the results of the first[4] and final[6] papers, rather than with those of the second.[5] We also believe that one assumption in Ref. 5 is not valid, and as a consequence the results there are not correct. A comment about this point may prove useful.

In Ref. 5, which confines its attention to the simple free-electron metal, the calculation proceeds by introducing a transformation to a curvilinear coordinate system within which the rough surface is mapped into a smooth plane. By transforming the field variables and coordinates, the Hamiltonian H is broken up into a part H_0, independent of the roughness amplitude $\zeta(x, y)$, and a part H_1, of first order in this parameter, with higher-order terms ignored. The part H_1 is treated via the Golden Rule of perturbation theory. Since H_0 has the form of a Hamiltonian of a semi-infinite solid with a plane interface, it is presumed that the eigenstates of H_0 are those associated with the plane-surface problem in a flat space. However, the transformation from the initial flat space to the curvilinear coordinate system is nonunitary in nature. The commutation relations between the field amplitudes and their canonically conjugate momenta are not left invariant by this transformation. The commutation relations in the new space contain contributions proportional to the roughness amplitude $\zeta(x, y)$ (or more precisely, to certain of its derivatives). Thus, while H_0 has the appearance of a Hamiltonian of a semi-infinite solid bounded by a plane surface, the equations of motion generated by it contain terms proportional to $\zeta(x, y)$, contrary to the assumption made by Elson and Ritchie. Thus, their calculation includes some terms proportional to the derivatives of $\zeta(x, y)$, but not all of them.

In their second paper,[6] Elson and Ritchie again use the transformation to a curvilinear coordinate system. However, as we do here, they work directly with the wave equation of electromagnetic theory. In this second work, we presume the method generates all terms proportional to $\zeta(x, y)$.

The transformation to curvilinear coordinates, while it yields correct results when all terms of the same order in $\zeta(x, y)$ are retained in the theory, has one cumbersome feature, in our view. When applied to the slightly rough plane interface, it converts a problem with a perturbation highly localized in the z coordinate (normal to the surface) into one which extends from $z=-\infty$ to $z=+\infty$. We use here the very simple and straightforward approach described earlier that allows us to work with a perturbation that is highly localized, and that also generates in a formal sense all contributions to the scattered fields that are of first order in $\zeta(x, y)$.

This paper is organized as follows. In Sec. II, we derive expressions for the fraction of energy scattered from the surface into the vacuum outside the crystal by the roughness, for both s- and p-polarized radiation at non-normal incidence. In Sec. III, we use the same form of scattering theory to obtain expressions for the fraction of energy scattered into the solid (absorbed) by the roughness. In Sec. IV, we examine the structure of the expressions obtained in Sec. III, and we obtain from them expressions for the contribution to absorption by roughness-induced coupling to surface polaritons, when the real part of the dielectric constant is negative and its imaginary part small. In Secs. III and IV we find that at non-normal incidence the Poynting vector has a nonzero time average parallel as well as perpendicular to the surface. To our knowledge, the properties of the component parallel to the surface have not been considered previously, and under circumstances described below, it may play a significant role in the absorption process. In Sec. V, we present a series of numerical calculations carried out for parameters characteristic of aluminum. The purpose of these calculations is to explore the predictions of the theory at non-normal incidence, and to explore to what extent the simple expressions derived in Sec. IV describe the roughness-induced absorption. Finally, in an Appendix, we derive the complete set of electromagnetic Green's functions required for the scattering theory presented in the text. These Green's functions are also useful for a variety of other problems, and it is therefore useful to present their full form.

II. SCATTERING OF ELECTROMAGNETIC RADIATION BY A ROUGH SURFACE

In this section we formulate the problem of the interaction of an incident electromagnetic wave with a rough surface, and obtain the cross sections for the scattering of s- and p-polarized incident radiation caused by the surface roughness. In Sec. III the general results obtained here will be applied to the determination of the fraction of the incident radiation absorbed by the medium bounded by the rough surface.

Let the height of the surface above the xy plane be specified by the equation

$$z=\zeta(x, y) . \tag{2.1}$$

Above this surface is vacuum, while the medium occupies the space below it, and is characterized by a (complex) frequency-dependent dielectric constant $\epsilon(\omega)$ which we assume to be isotropic. Thus, the dielectric constant of the system of medium plus adjacent vacuum can be written

$$\epsilon(z;\omega)=\Theta(z-\zeta(x,y))+\epsilon(\omega)\Theta(\zeta(x,y)-z) , \tag{2.2}$$

where $\Theta(z)$ is Heaviside's unit step function. We now expand $\epsilon(z;\omega)$ in powers of $\zeta(x,y)$:

$$\epsilon(z;\omega)=\epsilon_0(z;\omega)+[\epsilon(\omega)-1]\zeta(x,y)\delta(z)+O(\zeta^2) , \tag{2.3}$$

where

$$\epsilon_0(z;\omega)=\begin{cases}1 , & z>0\\ \epsilon(\omega) , & z<0 .\end{cases} \tag{2.4}$$

A surface, even a rough surface, represents a static scatterer of electromagnetic radiation. Thus, if in Maxwell's equation

$$\nabla\times\nabla\times\vec{E}=-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\vec{D} , \tag{2.5}$$

we substitute

$$\vec{E}(\vec{x};t)=\vec{E}(\vec{x};\omega)e^{-i\omega t} , \tag{2.6a}$$

$$\vec{D}(\vec{x};t)=\vec{D}(\vec{x};\omega)e^{-i\omega t} , \tag{2.6b}$$

and use the relation

$$\vec{D}(\vec{x};\omega)=\epsilon(z;\omega)\vec{E}(\vec{x};\omega) , \tag{2.7}$$

the equation for the Fourier coefficient of the electric field $\vec{E}(\vec{x};\omega)$ can be written in the form

$$\nabla\times\nabla\times\vec{E}(\vec{x};\omega)-\epsilon_0(z;\omega)(\omega^2/c^2)\vec{E}(\vec{x};\omega)$$
$$=(\omega^2/c^2)[\epsilon(\omega)-1]\zeta(x,y)\delta(z)\vec{E}(\vec{x};\omega) . \tag{2.8}$$

We now introduce the Green's function $D_{\mu\nu}(\vec{x},\vec{x}';\omega)$ as the solution of the equation

$$\sum_\mu\left(\epsilon_0(z;\omega)\frac{\omega^2}{c^2}\delta_{\lambda\mu}-\frac{\partial^2}{\partial x_\lambda\partial x_\mu}+\delta_{\lambda\mu}\nabla^2\right)D_{\mu\nu}(\vec{x},\vec{x}';\omega)$$
$$=4\pi\delta_{\lambda\nu}\,\delta(\vec{x}-\vec{x}') . \tag{2.9}$$

With the use of this function we can convert the partial differential equation (2.8) into an integral equation

$$E_\mu(\vec{x};\omega)=E_\mu^{(0)}(\vec{x};\omega)-(\omega^2/4\pi c^2)[\epsilon(\omega)-1]$$
$$\times\sum_\nu\int d^3x'\,D_{\mu\nu}(\vec{x},\vec{x}';\omega)\zeta(x',y')$$
$$\times\delta(z')E_\nu(\vec{x}';\omega) , \tag{2.10}$$

where $E_\mu^{(0)}(\vec{x};\omega)$ is a solution of the corresponding homogeneous equation

$$\sum_\nu\left(\epsilon_0(z;\omega)\frac{\omega^2}{c^2}\delta_{\mu\nu}-\frac{\partial^2}{\partial x_\mu\partial x_\nu}+\delta_{\mu\nu}\nabla^2\right)E_\nu^{(0)}(\vec{x};\omega)=0, \tag{2.11}$$

and describes specular reflection of the incident electromagnetic field from a plane surface. Since the right-hand side of Eq. (2.10) is already of first order in the surface-profile function $\zeta(x,y)$, the first Born approximation suffices to yield the scattered electric field

$$E_\mu^{(s)}(\vec{x};\omega)=E_\mu(\vec{x};\omega)-E_\mu^{(0)}(\vec{x};\omega) \tag{2.12}$$

to first order in $\zeta(x,y)$, and we find that

$$E_\mu^{(s)}(\vec{x};\omega)=-\frac{\omega^2}{4\pi c^2}[\epsilon(\omega)-1]\sum_\nu\int d^3x'\,D_{\mu\nu}(\vec{x},\vec{x}';\omega)$$
$$\times\zeta(x',y')\delta(z')E_\nu^{(0)}(\vec{x}';\omega) . \tag{2.13}$$

To proceed farther it is convenient to introduce the Fourier representations of $D_{\mu\nu}(\vec{x},\vec{x}';\omega)$ and $\zeta(x,y)$:

$$D_{\mu\nu}(\vec{x},\vec{x}';\omega)=\int\frac{d^2k_\parallel}{(2\pi)^2}e^{i\vec{k}_\parallel\cdot(\vec{x}_\parallel-\vec{x}_\parallel')}d_{\mu\nu}(\vec{k}_\parallel\omega\,|\,zz') , \tag{2.14}$$

$$\zeta(\vec{x}_\parallel)=\int\frac{d^2k_\parallel}{(2\pi)^2}e^{i\vec{k}_\parallel\cdot\vec{x}_\parallel}\hat{\zeta}(\vec{k}_\parallel) , \tag{2.15}$$

where $\vec{k}_\parallel$ and $\vec{x}_\parallel$ are two-dimensional vectors whose Cartesian components are $(k_x, k_y, 0)$ and $(x, y, 0)$, respectively. The form of the representation (2.14) is dictated by the fact that the system of medium plus vacuum characterized by the dielectric constant $\epsilon_0(z;\omega)$, Eq. (2.4), is invariant against an infinitesimal displacement parallel to the plane $z=0$, but not perpendicular to it. If we also write the field $E_\nu^{(0)}(\vec{x};\omega)$ in the form

$$E_\nu^{(0)}(\vec{x};\omega)=e^{i\vec{k}_\parallel^{(0)}\cdot\vec{x}_\parallel}E_\nu^{(0)}(\vec{k}_\parallel^{(0)}\omega\,|\,z) , \tag{2.16}$$

where $\vec{k}_\parallel^{(0)}$ is the component of the wave vector of the incident radiation parallel to the surface, we can express the scattered field in the following form

$$E_\mu^{(s)}(\vec{x};\omega)=-\frac{\omega^2}{16\pi^3c^2}[\epsilon(\omega)-1]\int d^2k_\parallel\,e^{i\vec{k}_\parallel\cdot\vec{x}_\parallel}\hat{\zeta}(\vec{k}_\parallel-\vec{k}_\parallel^{(0)})$$
$$\times\sum_\nu\int dz'\,d_{\mu\nu}(\vec{k}_\parallel\omega\,|\,zz')\delta(z')E_\nu^{(0)}(\vec{k}_\parallel^{(0)}\omega\,|\,z') . \tag{2.17}$$

At this point, we pause in the mathematical development to comment on the boundary conditions satisfied by the incident and the scattered field generated by our treatment. The incident field in Eq. (2.16) satisfies the electromagnetic boundary conditions across the flat plane $z=0$, by construction. The Green's function $d_{\mu\nu}(\vec{k}_\parallel\omega\,|\,zz')$, when considered a function of z for fixed z', satisfies the same boundary condition as the μth Cartesian component of the electric field. Thus, in our theory, the approximate expression for the total field $E_\mu(\vec{x};\omega)$ provided by Eqs. (2.12) and (2.17) satisfies the boundary conditions across the plane $z=0$. The exact field, of course, will satisfy the boundary conditions across the surface $z=\zeta(x,y)$ rather than the plane $z=0$. A similar feature is shared by the Born approximation of quantum mechanics, applied to a perturbed step potential.

It might be thought that the integration over z' in this expression could be carried out directly in view of the presence of the δ function in the integrand. However, as we will see explicitly below, the functions $d_{\mu\nu}(\vec{k}_\parallel\omega|zz')$ and $E_\nu^{(0)}(\vec{k}_\parallel^{(0)}\omega|z')$ can be discontinuous across the plane $z'=0$. In evaluating the integral over z' we therefore use the rule that if $F(z')$ is a function of z' that possesses a (finite) jump discontinuity at $z'=0$, then

$$\int_{-\infty}^{\infty} F(z')\delta(z')\,dz' = \tfrac{1}{2}[F(0+)+F(0-)]\,, \qquad (2.18)$$

a result which has its origin in the evenness of the δ function and its normalization to unity and which clearly reduces to the usual one if $F(z')$ is continuous across $z'=0$. The result (2.18) enables us to represent the scattered field, Eq. (2.17), as

$$E_\mu^{(s)}(\vec{x};\omega) = -\frac{\omega^2}{16\pi^3c^2}[\epsilon(\omega)-1]\int d^2k_\parallel\, e^{i\vec{k}_\parallel\cdot\vec{x}_\parallel} \times\hat{\zeta}(\vec{k}_\parallel-\vec{k}_\parallel^{(0)})\Lambda_\mu(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega|z)\,, \qquad (2.19)$$

where

$$\Lambda_\mu(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega|z) = \frac{1}{2}\sum_\nu [d_{\mu\nu}(\vec{k}_\parallel\omega|z+)E_\nu^{(0)}(\vec{k}_\parallel^{(0)}\omega|+) + d_{\mu\nu}(\vec{k}_\parallel\omega|z-)E_\nu^{(0)}(\vec{k}_\parallel^{(0)}\omega|-)]\,, \qquad (2.20)$$

and the notation + and − denotes 0+ and 0−, respectively.

It is shown in the Appendix that the function $d_{\mu\nu}(\vec{k}_\parallel\omega|zz')$ can be expressed in terms of a simpler function $g_{\mu\nu}(k_\parallel\omega|zz')$ according to

$$d_{\mu\nu}(\vec{k}_\parallel\omega|zz') = \sum_{\mu'\nu'} S_{\mu'\mu}(\vec{k}_\parallel)S_{\nu'\nu}(\vec{k}_\parallel)\,g_{\mu'\nu'}(k_\parallel\omega|zz')\,, \qquad (2.21)$$

where the 3×3 real orthogonal matrix $\underline{S}(\vec{k}_\parallel)$ is given by

$$\underline{S}(\vec{k}_\parallel) = \frac{1}{k_\parallel}\begin{pmatrix} k_x & k_y & 0\\ -k_y & k_x & 0\\ 0 & 0 & k_\parallel\end{pmatrix},\qquad \underline{S}^{-1}(\vec{k}_\parallel) = \frac{1}{k_\parallel}\begin{pmatrix} k_x & -k_y & 0\\ k_y & k_x & 0\\ 0 & 0 & k_\parallel\end{pmatrix}. \qquad (2.22)$$

In calculating both the scattering and absorption of electromagnetic radiation by a rough surface, we assume that the plane of incidence is the xz plane. The vector $\vec{k}_\parallel^{(0)}$ is then given by

$$\vec{k}_\parallel^{(0)} = (k^{(0)}, 0, 0)\,. \qquad (2.23)$$

We will consider only incident radiation which is polarized either parallel to the plane of incidence (p polarization) or perpendicular to it (s polarization). It is then a straightforward matter to find the electric field $\vec{E}^{(0)}(\vec{x};\omega)e^{-i\omega t}$ in the vacuum and in the medium. The results are for $z>0$:

$$E_x^{(0)}(\vec{x};t) = e^{i(k^{(0)}x-\omega t)}\left(e^{-ik_z^{(0)}z} + \frac{k_z^{(i)}+\epsilon(\omega)k_z^{(0)}}{k_z^{(i)}-\epsilon(\omega)k_z^{(0)}}e^{ik_z^{(0)}z}\right)E_x^{(1)}\,, \qquad (2.24a)$$

$$E_y^{(0)}(\vec{x};t) = e^{i(k^{(0)}x-\omega t)}\left(e^{-ik_z^{(0)}z} + \frac{k_z^{(0)}+k_z^{(i)}}{k_z^{(0)}-k_z^{(i)}}e^{ik_z^{(0)}z}\right)E_y^{(1)}\,, \qquad (2.24b)$$

$$E_z^{(0)}(\vec{x};t) = e^{i(k^{(0)}x-\omega t)}\,\frac{k^{(0)}}{k_z^{(0)}}\left(e^{-ik_z^{(0)}z} - \frac{k_z^{(i)}+\epsilon(\omega)k_z^{(0)}}{k_z^{(i)}-\epsilon(\omega)k_z^{(0)}}e^{ik_z^{(0)}z}\right)E_x^{(1)}\,, \qquad (2.24c)$$

and for $z<0$:

$$E_x^{(0)}(\vec{x};t) = e^{i(k^{(0)}x-\omega t)}e^{ik_z^{(i)}z}\,\frac{2k_z^{(i)}}{k_z^{(i)}-\epsilon(\omega)k_z^{(0)}}E_x^{(1)}\,, \qquad (2.25a)$$

$$E_y^{(0)}(\vec{x};t) = e^{i(k^{(0)}x-\omega t)}e^{ik_z^{(i)}z}\,\frac{2k_z^{(0)}}{k_z^{(0)}-k_z^{(i)}}E_y^{(1)}\,, \qquad (2.25b)$$

$$E_z^{(0)}(\vec{x};t) = e^{i(k^{(0)}x-\omega t)}e^{ik_z^{(i)}z}\,\frac{-2k^{(0)}}{k_z^{(i)}-\epsilon(\omega)k_z^{(0)}}E_x^{(1)}\,. \qquad (2.25c)$$

The quantities $k_z^{(0)}$ and $k_z^{(i)}$ appearing in these expressions are defined by

$$k_z^{(0)} = (\omega^2/c^2 - k^{(0)2})^{1/2}\,, \qquad (2.26)$$

$$k_z^{(i)} = -(\epsilon(\omega)\,\omega^2/c^2 - k^{(0)2})^{1/2}\,, \qquad (2.27)$$

where the negative sign for the square root in Eq. (2.27), together with the fact that $\mathrm{Im}\,\epsilon(\omega)>0$, leads to the result that $\mathrm{Im}\,k_z^{(i)}<0$. (We take the branch cut for the square root along the negative real axis.) In each of Eqs. (2.24) the first term on the right-hand side represents the incident electric field, while the second represents the reflected field. The vector $\vec{E}^{(1)}$ gives the amplitude of the incident field, and in writing Eqs. (2.24) and (2.25) we have used the fact that

$$E_z^{(1)} = \frac{k^{(0)}}{k_z^{(0)}} E_x^{(1)} , \tag{2.28a}$$

$$E_z^{(1)} = -\frac{k^{(0)}}{k_z^{(0)}} E_x^{(1)} \tag{2.28b}$$

for the incident and reflected fields, respectively.

It follows from Eqs. (2.24) and (2.25) and the definitions (2.6), (2.16), and (2.23) that the amplitudes $E_\nu^{(0)}(\vec{k}_\parallel^{(0)}\omega \mid \pm)$ are given by

$$E_x^{(0)}(\vec{k}_\parallel^{(0)}\omega \mid +) = E_x^{(0)}(\vec{k}_\parallel^{(0)}\omega \mid -) = \frac{2k_z^{(i)}}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}} E_x^{(1)} , \tag{2.29}$$

$$E_y^{(0)}(\vec{k}_\parallel^{(0)}\omega \mid +) = E_y^{(0)}(\vec{k}_\parallel^{(0)}\omega \mid -) = \frac{-2k_z^{(0)}}{k_z^{(i)} - k_z^{(0)}} E_y^{(1)} , \tag{2.30}$$

$$E_z^{(0)}(\vec{k}_\parallel^{(0)}\omega \mid +) = \frac{-2\epsilon(\omega)k^{(0)}}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}} E_x^{(1)} , \tag{2.31a}$$

$$E_z^{(0)}(\vec{k}_\parallel^{(0)}\omega \mid -) = \frac{-2k^{(0)}}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}} E_x^{(1)} . \tag{2.31b}$$

The results obtained so far apply equally to the scattering and absorption of light by a rough surface. In the remainder of this section we confine our attention to the scattering problem.

In the scattering problem the coordinate z in Eqs. (2.19)–(2.21) must be positive. The results of the Appendix show us that for $z > 0$ the function $g_{\mu\nu}(k_\parallel\omega \mid z\pm)$ has the form

$$g_{\mu\nu}(k_\parallel\omega \mid z\pm) = e^{ik_z z}\hat{g}_{\mu\nu}(k_\parallel\omega \mid \pm) , \tag{2.32}$$

where

$$k_z = \begin{cases} (\omega^2/c^2 - k_\parallel^2)^{1/2}, & \omega^2/c^2 > k_\parallel^2 \quad (2.33a) \\ i(k_\parallel^2 - \omega^2/c^2)^{1/2}, & \omega^2/c^2 < k_\parallel^2 . \quad (2.33b) \end{cases}$$

The function $g_{\mu\nu}(k_\parallel\omega \mid z\pm)$ clearly satisfies the outgoing wave condition at infinity for $\omega^2/c^2 > k_\parallel^2$, and describes exponentially decaying waves for $\omega^2/c^2 < k_\parallel^2$. The nonvanishing functions $\hat{g}_{\mu\nu}(k_\parallel\omega \mid \pm)$ are given explicitly by

$$\hat{g}_{xx}(k_\parallel\omega \mid +) = \hat{g}_{xx}(k_\parallel\omega \mid -) = -\frac{4\pi i c^2}{\omega^2}\frac{k_1 k_z}{k_1 - \epsilon(\omega)k_z} , \tag{2.34}$$

$$\hat{g}_{zx}(k_\parallel\omega \mid +) = \hat{g}_{zx}(k_\parallel\omega \mid -) = \frac{4\pi i c^2}{\omega^2}\frac{k_\parallel k_1}{k_1 - \epsilon(\omega)k_z} , \tag{2.35}$$

$$\hat{g}_{yy}(k_\parallel\omega \mid +) = \hat{g}_{yy}(k_\parallel\omega \mid -) = \frac{4\pi i}{k_1 - k_z} , \tag{2.36}$$

$$\hat{g}_{xz}(k_\parallel\omega \mid +) = -\frac{4\pi i c^2}{\omega^2}\frac{\epsilon(\omega)k_\parallel k_z}{k_1 - \epsilon(\omega)k_z} , \tag{2.37a}$$

$$\hat{g}_{xz}(k_\parallel\omega \mid -) = -\frac{4\pi i c^2}{\omega^2}\frac{k_\parallel k_z}{k_1 - \epsilon(\omega)k_z} , \tag{2.37b}$$

$$\hat{g}_{zz}(k_\parallel\omega \mid +) = \frac{4\pi i c^2}{\omega^2}\frac{\epsilon(\omega)k_\parallel^2}{k_1 - \epsilon(\omega)k_z} , \tag{2.38a}$$

$$\hat{g}_{zz}(k_\parallel\omega \mid -) = \frac{4\pi i c^2}{\omega^2}\frac{k_\parallel^2}{k_1 - \epsilon(\omega)k_z} . \tag{2.38b}$$

The quantity k_1 appearing in these equations is

$$k_1 = -\left(\epsilon(\omega)\frac{\omega^2}{c^2} - k_\parallel^2\right)^{1/2} , \tag{2.39}$$

and $\mathrm{Im}\, k_1 < 0$.

Combining Eqs. (2.20), (2.21), and (2.32), we can express $\Lambda_\mu(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega \mid z)$ conveniently as

$$\Lambda_\mu(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega \mid z) = e^{ik_z z}\bar{\lambda}_\mu(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega) , \tag{2.40}$$

where

$$\bar{\lambda}_\mu(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega) = \sum_{\mu'} \lambda_{\mu'}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega)S_{\mu'\mu}(\vec{k}_\parallel) , \tag{2.41}$$

with

$$\lambda_\mu(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega) = \frac{1}{2}\sum_\nu [\hat{g}_{\mu\nu}(k_\parallel\omega \mid +)\,\mathcal{E}_\nu^{(0)}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega \mid +) + \hat{g}_{\mu\nu}(k_\parallel\omega \mid -)\,\mathcal{E}_\nu^{(0)}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega \mid -)] \tag{2.42}$$

and

$$\mathcal{E}_\mu^{(0)}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega \mid \pm) = \sum_\nu S_{\mu\nu}(\vec{k}_\parallel)E_\nu^{(0)}(\vec{k}_\parallel^{(0)}\omega \mid \pm) . \tag{2.43}$$

The scattered field amplitude (2.19) can now be written

$$\vec{E}^{(s)}(\vec{x};\omega) = \frac{-\omega^2}{16\pi^3 c^2}[\epsilon(\omega) - 1]\int d^2k_\parallel\, e^{i\vec{k}\cdot\vec{x}} \times \xi(\vec{k}_\parallel - \vec{k}_\parallel^{(0)})\,\vec{\bar{\lambda}}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega) , \tag{2.44}$$

where $\vec{k}$ is the three-dimensional vector

$$\vec{k} = \vec{k}_\parallel + \hat{z}k_z . \tag{2.45}$$

It must be kept in mind that k_z is a function of $\vec{k}_\parallel$ given by Eq. (2.33).

If we write the scattered magnetic field in the form

$$\vec{H}^{(s)}(\vec{x};t) = \vec{H}^{(s)}(\vec{x};\omega)\,e^{-i\omega t} , \tag{2.46}$$

then from the Maxwell equation $\nabla\times\vec{E} = -c^{-1}(\partial\vec{H}/\partial t)$ we find directly that

$$\vec{H}^{(s)}(\vec{x};\omega) = -\frac{\omega}{16\pi^3 c}[\epsilon(\omega) - 1]\int d^2k_\parallel\, e^{i\vec{k}\cdot\vec{x}} \times \xi(\vec{k}_\parallel - \vec{k}_\parallel^{(0)})\,\vec{k}\times\vec{\bar{\lambda}}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega) . \tag{2.47}$$

We next turn our attention to the form of the Poynting vector associated with the scattered radiation, in the vacuum above the crystal. We are concerned here with the energy radiated into the vacuum above the surface, away from the crystal surface. Thus, in the formulas displayed in the remainder of this section, we confine our attention to the region $k_\parallel < \omega/c$, where k_z is real, and the fields propagate away from the surface. When $k_\parallel > \omega/c$, k_z is pure imaginary, and the scattered fields associated with these values of $k_\parallel$ decay to zero exponentially as one moves away from the crystal into the vacuum. We shall return to discuss these exponentially decaying fields in Sec. IV, where we will see they have a real physical effect; they set up an energy flux that is localized near the surface and flows parallel to it. For the moment, we confine our attention to the region $k_\parallel < \omega/c$, and we append the symbol < to the integral sign where necessary to remind the reader of this restriction in the expressions that follow. The complex Poynting vector for the scattered radiation is therefore given by

$$\vec{S} = \frac{c}{8\pi}\vec{E}^{(s)}(\vec{x};t)^* \times \vec{H}^{(s)}(\vec{x};t)$$
$$= \frac{\omega^3}{2048\pi^7 c^2}|\epsilon(\omega)-1|^2 \int_< d^2k_\parallel \int_< d^2k'_\parallel e^{-i(\vec{k}-\vec{k}')\cdot\vec{x}}$$
$$\times \hat{\xi}(\vec{k}_\parallel - \vec{k}_\parallel^{(0)})^* \hat{\xi}(\vec{k}'_\parallel - \vec{k}_\parallel^{(0)}) \vec{\lambda}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)^* \times [\vec{k}' \times \vec{\vec{\lambda}}(\vec{k}'_\parallel \vec{k}_\parallel^{(0)\prime}\omega)] . \qquad (2.48)$$

In order that we can compare our results with experimental data for a metal surface it is reasonable to assume that the surface-profile function $\xi(x,y)$ is a stationary stochastic process, and that our result (2.48) for the Poynting vector should be averaged over the probability distribution function for this process. In fact we have to average the product $\hat{\xi}(\vec{k}_\parallel)\hat{\xi}(\vec{k}'_\parallel)$. The averaging restores infinitesimal translational invariance parallel to the plane $z=0$, and we have that

$$\langle \hat{\xi}(\vec{k}_\parallel)\hat{\xi}(\vec{k}'_\parallel)\rangle = [(2\pi)^2/A]\,\delta(\vec{k}_\parallel + \vec{k}'_\parallel)\langle|\hat{\xi}(\vec{k}_\parallel)|^2\rangle , \qquad (2.49)$$

where A is the area of the metal surface, and use has been made of the reality condition $\hat{\xi}(-\vec{k}_\parallel) = \hat{\xi}(\vec{k}_\parallel)^*$. Following Elson and Ritchie[5] we make the replacement

$$A^{-1}\langle|\hat{\xi}(\vec{k}_\parallel)|^2\rangle = \delta^2 g(k_\parallel) , \qquad (2.50)$$

where δ^2 is the mean-square surface-height variation, and the surface scattering factor $g(k_\parallel)$ is assumed to depend only on the magnitude of $\vec{k}_\parallel$, but not on its direction. With the use of Eqs. (2.49) and (2.50) the spatial average of the Poynting vector (2.48) can be written

$$\langle\vec{S}\rangle = \delta^2 \frac{\omega^3|\epsilon(\omega)-1|^2}{512\pi^5 c^2}\int_< d^2k_\parallel g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)$$
$$\times\{\vec{k}|\vec{\vec{\lambda}}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega)|^2 - \vec{\vec{\lambda}}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega)$$
$$\times[\vec{k}\cdot\vec{\lambda}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega^*)]\} , \qquad (2.51)$$

where we have expanded the triple vector product. With the aid of the definitions (2.41)–(2.43), and the results given by Eqs. (2.34)–(2.38), it is straightforward to establish the two useful results

$$\vec{k}\cdot\vec{\vec{\lambda}}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega)^* = 0 , \qquad (2.52a)$$

$$|\vec{\vec{\lambda}}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega)|^2 = |\vec{\lambda}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega)|^2 . \qquad (2.52b)$$

The first of these is a consequence of the transverse nature of the scattered electric field. Thus the spatial average of the Poynting vector takes the simple form

$$\langle\vec{S}\rangle = \delta^2 \frac{\omega^3|\epsilon(\omega)-1|^2}{512\pi^5 c^2}\int_< d^2k_\parallel g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)$$
$$\times\vec{k}|\vec{\lambda}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega)|^2 , \qquad (2.53)$$

which is manifestly real. The magnitude of the real part of the averaged Poynting vector describing radiation associated with wave vector components parallel to the surface between $\vec{k}_\parallel$ and $\vec{k}_\parallel + d\vec{k}_\parallel$ is therefore

$$\langle S(\vec{k}_\parallel)\rangle\, d^2k_\parallel = \delta^2 \frac{\omega^4|\epsilon(\omega)-1|^2}{512\pi^5 c^3} g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)$$
$$\times|\vec{\lambda}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega)|^2\, d^2k_\parallel , \qquad (2.54)$$

where we have used the result that $k = (k_\parallel^2 + k_z^2)^{1/2} = \omega/c$.

To proceed farther, we require the $\lambda_\mu(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega)$. We first record the expressions for the quantities $\mathcal{E}_\mu^{(0)}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega|\pm)$. Combining Eqs. (2.22), (2.29)–(2.31), and (2.43) we obtain

$$\mathcal{E}_x^{(0)}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega|\pm) = \frac{1}{k_\parallel}\left(\frac{2k_x k_z^{(i)}}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}} E_x^{(1)} - \frac{2k_y k_z^{(0)}}{k_z^{(i)} - k_z^{(0)}} E_y^{(1)}\right) , \qquad (2.55)$$

$$\mathcal{E}_y^{(0)}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega|\pm) = \frac{1}{k_\parallel}\left(\frac{-2k_y k_z^{(i)}}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}} E_x^{(1)} - \frac{2k_x k_z^{(0)}}{k_z^{(i)} - k_z^{(0)}} E_y^{(1)}\right) , \qquad (2.56)$$

$$\mathcal{E}_z^{(0)}(\vec{k}_\parallel\vec{k}_\parallel^{(0)}\omega|+) = \frac{-2\epsilon(\omega)k^{(0)}}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}} E_x^{(1)} , \qquad (2.57a)$$

$$\mathcal{E}_z^{(0)}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega|-) = \frac{-2k^{(0)}}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}} E_x^{(1)} . \tag{2.57b}$$

Substitution of these results, together with Eqs. (2.34)–(2.38), into Eq. (2.42) yields the results

$$\lambda_x(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) = -(k_z/k_\parallel)\lambda_z(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) , \tag{2.58}$$

$$\lambda_y(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) = \frac{-4\pi i}{k_1 - k_z}\frac{1}{k_\parallel} \times \left(\frac{2k_y k_z^{(i)}}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}} E_x^{(1)} + \frac{2k_x k_z^{(0)}}{k_z^{(i)} - k_z^{(0)}} E_y^{(1)}\right) , \tag{2.59}$$

$$\lambda_z(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) = \frac{4\pi i c^2}{\omega^2}\frac{1}{k_1 - \epsilon(\omega)k_z}\frac{1}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}} \times \{2k_x k_1 k_z^{(i)} - k_\parallel^2 k^{(0)}[\epsilon^2(\omega)+1]\} E_x^{(1)} - \frac{4\pi i c^2}{\omega^2}\frac{k_1}{k_1 - \epsilon(\omega)k_z}\frac{2k_y k_z^{(0)}}{k_z^{(i)} - k_z^{(0)}} E_y^{(1)} . \tag{2.60}$$

When we substitute Eqs. (2.58)–(2.60) into Eq. (2.54), the contribution from $|\lambda_x|^2 + |\lambda_z|^2$ corresponds to scattered radiation that is p polarized; the contribution from $|\lambda_y|^2$ corresponds to scattered radiation that is s polarized. Within each category the contribution containing $|E_x^{(1)}|^2$ corresponds to incident radiation which is p polarized, while the contribution containing $|E_y^{(1)}|^2$ corresponds to incident radiation which is s polarized. We can therefore decompose the differential Poynting vector (2.54) into contributions associated with the scattering of incident radiation of a given polarization into radiation with prescribed polarization. Thus, in an obvious notation

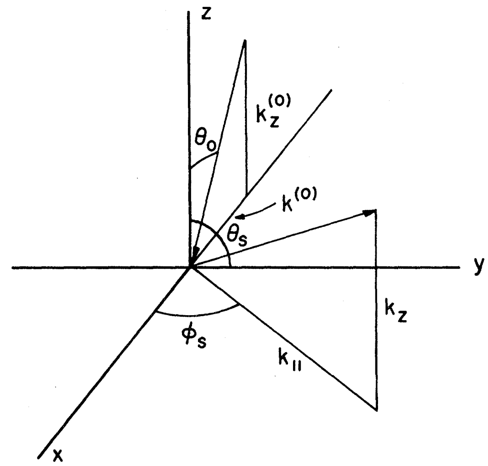

FIG. 1. Scattering geometry employed in this paper.

$$\langle S(\vec{k}_\parallel|s\to p)\rangle d^2k_\parallel = \delta^2 \frac{\omega^2|\epsilon(\omega)-1|^2}{8\pi^3 c} g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)\frac{k_y^2 k_z^{(0)2}}{k_\parallel^2} \times \frac{|k_1|^2}{|k_1 - \epsilon(\omega)k_z|^2|k_z^{(i)} - k_z^{(0)}|^2}|E_y^{(1)}|^2 d^2k_\parallel , \tag{2.61}$$

$$\langle S(\vec{k}_\parallel|s\to s)\rangle d^2k_\parallel = \delta^2 \frac{\omega^4|\epsilon(\omega)-1|^2}{8\pi^3 c^3} g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)\frac{k_x^2 k_z^{(0)}}{k_\parallel^2}\frac{|E_y^{(1)}|^2}{|k_1 - k_z|^2|k_z^{(i)} - k_z^{(0)}|^2} d^2k_\parallel , \tag{2.62}$$

$$\langle S(\vec{k}_\parallel|p\to s)\rangle d^2k_\parallel = \delta^2 \frac{\omega^4|\epsilon(\omega)-1|^2}{8\pi^3 c^3} g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)\frac{k_y^2|k_z^{(i)}|^2}{k_\parallel^2}\frac{|E_x^{(1)}|^2}{|k_1 - k_z|^2|k_z^{(i)} - \epsilon(\omega)k_z^{(0)}|^2} d^2k_\parallel , \tag{2.63}$$

$$\langle S(\vec{k}_\parallel|p\to p)\rangle d^2k_\parallel = \delta^2 \frac{\omega^2|\epsilon(\omega)-1|^2}{8\pi^3 c} g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)\frac{1}{k_\parallel^2} \times \frac{|k_x k_1 k_z^{(i)} - \frac{1}{2}k_\parallel^2 k^{(0)}[\epsilon^2(\omega)+1]|^2}{|k_1 - \epsilon(\omega)k_z|^2|k_z^{(i)} - \epsilon(\omega)k_z^{(0)}|^2}|E_x^{(1)}|^2 d^2k_\parallel . \tag{2.64}$$

We can simplify these results somewhat. We note first from Eqs. (2.24) and the scattering geometry depicted in Fig. 1, that the incident flux per unit area of the *surface* is

$$S_s^{(0)} = (c/8\pi)\cos\theta_0 |E_y^{(1)}|^2 , \tag{2.65}$$

for s-polarized incident radiation, where θ_0 is the angle of incidence, and

$$S_p^{(0)} = \frac{c}{8\pi}\frac{1}{\cos\theta_0}|E_x^{(1)}|^2 , \tag{2.66}$$

for p-polarized incident radiation. We will normalize the expressions (2.61)–(2.64) by dividing Eqs. (2.61) and (2.62) by Eq. (2.65) and Eqs. (2.63) and (2.64) by Eq. (2.66). We also note that Eqs. (2.61)–(2.64) give the energy crossing unit area normal to the direction of $\vec{k}$ per unit time. We normalize the scattered flux to unit surface area by multiplying each of Eqs. (2.61)–(2.64) by $\cos\theta_s$, where θ_s is the polar scattering angle. We next note that when $k_\parallel < \omega/c$, we may write

$$d^2k_\parallel = k_\parallel dk_\parallel d\varphi_s = (\omega^2/c^2)\cos\theta_s d\Omega_s , \tag{2.67}$$

where $d\Omega_s = \sin\theta_s\, d\theta_s\, d\varphi_s$ is the element of solid angle about the scattering direction (θ_s, φ_s). Finally, we note the geometrical relations valid in the radiation region $k_\parallel < \omega/c$.

$$k_x = (\omega/c)\sin\theta_s\cos\varphi_s\,, \qquad k = \omega/c$$
$$k_y = (\omega/c)\sin\theta_s\sin\varphi_s\,, \qquad k^{(0)} = (\omega/c)\sin\theta_0$$
$$k_z = (\omega/c)\cos\theta_s\,, \qquad k_z^{(0)} = (\omega/c)\cos\theta_0 \qquad (2.68)$$
$$k_1 = -(\omega/c)[\epsilon(\omega) - \sin^2\theta_s]^{1/2}\,,$$
$$k_z^{(i)} = -(\omega/c)[\epsilon(\omega) - \sin^2\theta_0]^{1/2}\,.$$

Again, we point out that the negative signs attached to the square roots in the expressions for k_1 and $k_z^{(i)}$ lead to the results $\mathrm{Im}\, k_1 < 0$ and $\mathrm{Im}\, k_z^{(i)} < 0$, required by the boundary conditions at infinity.

Combining the normalizations described above and the results given by Eqs. (2.67) and (2.68), with the results expressed by Eqs. (2.61)–(2.64), we obtain finally the cross sections for the scattering of radiation into unit solid angle about (θ_s, φ_s):

$$\frac{df(\vec{k}_\parallel | s\to p)}{d\Omega_s} = \delta^2 \frac{\omega^4|\epsilon(\omega)-1|^2}{\pi^2 c^4} g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)\cos\theta_0\cos^2\theta_s\sin^2\varphi_s \times \frac{|\epsilon(\omega) - \sin^2\theta_s|}{|\epsilon(\omega)\cos\theta_s + [\epsilon(\omega)-\sin^2\theta_s]^{1/2}|^2 |\cos\theta_0 + [\epsilon(\omega) - \sin^2\theta_0]^{1/2}|^2} \qquad (2.69)$$

$$\frac{df(\vec{k}_\parallel | s\to s)}{d\Omega_s} = \delta^2 \frac{\omega^4|\epsilon(\omega)-1|^2}{\pi^2 c^4} g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)\cos\theta_0\cos^2\theta_s\cos^2\varphi_s \times \frac{1}{|\cos\theta_s + [\epsilon(\omega)-\sin^2\theta_s]^{1/2}|^2 |\cos\theta_0 + [\epsilon(\omega) - \sin^2\theta_0]^{1/2}|^2}\,, \qquad (2.70)$$

$$\frac{df(\vec{k}_\parallel | p\to s)}{d\Omega_s} = \delta^2 \frac{\omega^4|\epsilon(\omega)-1|^2}{\pi^2 c^4} g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)\cos\theta_0\cos^2\theta_s\sin^2\varphi_s \times \frac{|\epsilon(\omega) - \sin^2\theta_0|}{|\cos\theta_s + [\epsilon(\omega)-\sin^2\theta_s]^{1/2}|^2 |\epsilon(\omega)\cos\theta_0 + [\epsilon(\omega) - \sin^2\theta_0]^{1/2}|^2}\,, \qquad (2.71)$$

$$\frac{df(\vec{k}_\parallel | p\to p)}{d\Omega_s} = \delta^2 \frac{\omega^4|\epsilon(\omega)-1|^2}{\pi^2 c^4} g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|)\cos\theta_0\cos^2\theta_s \times \frac{|\cos\varphi_s[\epsilon(\omega)-\sin^2\theta_s]^{1/2}[\epsilon(\omega)-\sin^2\theta_0]^{1/2} - \frac{1}{2}\sin\theta_0\sin\theta_s[\epsilon^2(\omega)+1]|^2}{|\epsilon(\omega)\cos\theta_s + [\epsilon(\omega)-\sin^2\theta_s]^{1/2}|^2 |\epsilon(\omega)\cos\theta_0 + [\epsilon(\omega) - \sin^2\theta_0]^{1/2}|^2}\,. \qquad (2.72)$$

III. ABSORPTION OF ELECTROMAGNETIC RADIATION BY A ROUGH SURFACE

In Sec. II we have developed a formalism for treating the interaction of an electromagnetic wave with the rough surface of some medium, and applied it to the determination of the cross sections for the scattering of the electromagnetic wave by the surface roughness. In this section we apply the same formalism to the determination of the absorption of the electromagnetic wave by the medium arising from the surface roughness.

Our starting point is the expression for the scattered electric field given by Eqs. (2.19)–(2.21). In contrast with the scattering problem, in which it is the values of $g_{\mu\nu}(k_\parallel\omega|zz')$ for $z > 0$ that are required, in the absorption problem it is their values for $z < 0$, i.e., in the medium, that are required. From the results of the Appendix we find that for $z < 0$ we can write

$$g_{\mu\nu}(k_\parallel\omega|z\pm) = e^{ik_1 z}\hat{g}_{\mu\nu}(k_\parallel\omega|\pm)\,, \qquad (3.1)$$

where the coefficient functions $\hat{g}_{\mu\nu}(k_\parallel\omega|\pm)$ are given explicitly by

$$\hat{g}_{xx}(k_\parallel\omega|+) = \hat{g}_{xx}(k_\parallel\omega|-) = -\frac{4\pi i c^2}{\omega^2}\frac{k_1 k_z}{k_1 - \epsilon(\omega)k_z}\,, \qquad (3.2)$$

$$\hat{g}_{zx}(k_\parallel\omega|+) = \hat{g}_{zx}(k_\parallel\omega|-) = \frac{4\pi i c^2}{\omega^2}\frac{k_\parallel k_z}{k_1 - \epsilon(\omega)k_z}\,, \qquad (3.3)$$

$$\hat{g}_{yy}(k_\parallel\omega|+) = \hat{g}_{yy}(k_\parallel\omega|-) = \frac{4\pi i}{k_1 - k_z}\,, \qquad (3.4)$$

$$\hat{g}_{xz}(k_\parallel\omega|+) = -\frac{4\pi i c^2}{\omega^2}\frac{k_\parallel k_1}{k_1 - \epsilon(\omega)k_z}\,, \qquad (3.5a)$$

$$\hat{g}_{xz}(k_\parallel\omega|-) = -\frac{4\pi i c^2}{\omega^2\epsilon(\omega)}\frac{k_\parallel k_1}{k_1 - \epsilon(\omega)k_z}\,, \qquad (3.5b)$$

$$\hat{g}_{zz}(k_\parallel\omega|+) = \frac{4\pi i c^2}{\omega^2}\frac{k_\parallel^2}{k_1 - \epsilon(\omega)k_z}\,, \qquad (3.6a)$$

$$\hat{g}_{zz}(k_\parallel\omega|-) = \frac{4\pi i c^2}{\omega^2\epsilon(\omega)}\frac{k_\parallel^2}{k_1 - \epsilon(\omega)k_z}\,. \qquad (3.6b)$$

Thus we can write the function $\Lambda_\mu(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega | z)$ entering Eq. (2.19) in the form

$$\Lambda_\mu(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega | z) = e^{ik_1 z}\bar{\lambda}_\mu(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) , \qquad (3.7)$$

where $\bar{\lambda}_\mu(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)$ is again defined by Eqs. (2.41)–(2.43), with the only difference being that the functions $\hat{g}_{\mu\nu}(k_\parallel \omega | \pm)$ appearing in Eq. (2.42) are now those given by Eqs. (3.2)–(3.6).

The scattered electric and magnetic fields are now given by

$$\vec{E}^{(s)}(\vec{x}; t) = -e^{-i\omega t} \frac{\omega^2}{16\pi^3 c^2}[\epsilon(\omega) - 1] \int d^2k_\parallel e^{i\vec{k}\cdot\vec{x}} \times \hat{\xi}(\vec{k}_\parallel - \vec{k}_\parallel^{(0)}) \vec{\bar{\lambda}}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) , \qquad (3.8)$$

$$\vec{H}^{(s)}(\vec{x}; t) = -e^{-i\omega t} \frac{\omega}{16\pi^3 c}[\epsilon(\omega) - 1] \int d^2k_\parallel e^{i\vec{k}\cdot\vec{x}} \times \hat{\xi}(\vec{k}_\parallel - \vec{k}_\parallel^{(0)})[\vec{k}\times \vec{\bar{\lambda}}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega] , \qquad (3.9)$$

where the three-dimensional wave vector $\vec{k}$ is now given by

$$\vec{k} = \vec{k}_\parallel + \hat{z}k_1 . \qquad (3.10)$$

It should be kept in mind that k_1 is a function of $\vec{k}_\parallel$ through Eq. (2.39), and is complex,

$$k_1 = k_1^{(1)} - ik_1^{(2)} , \quad k_1^{(2)} > 0 . \qquad (3.11)$$

The vector $\vec{k}$, therefore, is also complex.

The complex Poynting vector obtained by substituting Eqs. (3.8) and (3.9) into Eq. (2.48), and averaging the result with respect to the distribution function for the surface profile function $\xi(x, y)$, now takes the form

$$\langle \vec{S}(z)\rangle = \delta^2 \frac{\omega^3 |\epsilon(\omega) - 1|^2}{512\pi^5 c^2} \int d^2k_\parallel e^{2k_1^{(2)}z} g(|\vec{k}_\parallel - \vec{k}_\parallel^{(0)}|) \times\{\vec{k}|\vec{\bar{\lambda}}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)|^2 - \vec{\bar{\lambda}}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) \times[\vec{k}\cdot\vec{\bar{\lambda}}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)^*]\} . \qquad (3.12)$$

However, in the present case the scalar product $\vec{k}\cdot\vec{\bar{\lambda}}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)^*$ does not vanish, and both terms in braces contribute to $\langle \vec{S}(z)\rangle$. It is therefore convenient to define two vectors $\vec{A}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)$ and $\vec{B}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)$ by

$$\vec{A}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) = \vec{k}|\vec{\bar{\lambda}}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)|^2 , \qquad (3.13)$$

$$\vec{B}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) = \vec{\bar{\lambda}}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)[\vec{k}\cdot\vec{\bar{\lambda}}(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)^*] . \qquad (3.14)$$

With the aid of Eqs. (2.22) and (2.41) we can rewrite these vectors in terms of the functions λ_μ, $(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)$ as

$$A_x = k_x|\vec{\lambda}|^2 , \quad A_y = k_y|\vec{\lambda}|^2 , \quad A_z = k_1|\vec{\lambda}|^2 , \qquad (3.15)$$

$$B_x = (1/k_\parallel)(k_x\lambda_x - k_y\lambda_y)(k_\parallel\lambda_x^* + k_1\lambda_z^*) , \qquad (3.16a)$$

$$B_y = (1/k_\parallel)(k_y\lambda_x + k_x\lambda_y)(k_\parallel\lambda_x^* + k_1\lambda_z^*) , \qquad (3.16b)$$

$$B_z = \lambda_z(k_\parallel\lambda_x^* + k_1\lambda_z^*) . \qquad (3.16c)$$

We now require explicit expressions for the functions $\lambda_\mu(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega)$ appearing in Eqs. (3.15) and (3.16). Combining Eqs. (2.42), (2.55)–(2.57), and (3.2)–(3.6), we find that

$$\lambda_x(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) = -\frac{k_1}{k_\parallel}\lambda_z(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) , \qquad (3.17)$$

$$\lambda_y(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) = \frac{-4\pi i}{k_1 - k_z}\frac{1}{k_\parallel}\left(\frac{2k_y k_z^{(i)}}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}}E_x^{(1)} + \frac{2k_x k_z^{(0)}}{k_z^{(i)} - k_z^{(0)}}E_y^{(1)}\right) , \qquad (3.18)$$

$$\lambda_z(\vec{k}_\parallel \vec{k}_\parallel^{(0)}\omega) = \frac{4\pi i c^2}{\omega^2}\frac{1}{k_1 - \epsilon(\omega)k_z}\frac{1}{k_z^{(i)} - \epsilon(\omega)k_z^{(0)}} \times\{2k_x k_z k_z^{(i)} - k^{(0)}k_\parallel^2[\epsilon(\omega) + \epsilon^{-1}(\omega)]\}E_x^{(1)} - \frac{4\pi i c^2}{\omega^2}\frac{k_z}{k_1 - \epsilon(\omega)k_z}\frac{2k_y k_z^{(0)}}{k_z^{(i)} - k_z^{(0)}}E_y^{(1)} . \qquad (3.19)$$

To obtain the power absorbed by the medium we need the real part of the complex Poynting vector (3.12). If we combine Eqs. (3.17)–(3.19) with Eqs. (3.15) and (3.16) we find that the real part of $\langle \vec{S}(z)\rangle$ depends on the following quantities:

$$\mathrm{Re}(A_x - B_x) = k_x\left(\frac{k_\parallel^2 + \mathrm{Re}(k_1)^2}{k_\parallel^2}|\lambda_z|^2 + |\lambda_y|^2\right) - 2k_y\left(\frac{k_1^{(2)}}{k_\parallel}\right)\mathrm{Re}(i\lambda_y\lambda_z^*) , \qquad (3.20)$$

$$\mathrm{Re}(A_y - B_y) = k_y\left(\frac{k_\parallel^2 + \mathrm{Re}(k_1)^2}{k_\parallel^2}|\lambda_z|^2 + |\lambda_y|^2\right) + 2k_x\left(\frac{k_1^{(2)}}{k_\parallel}\right)\mathrm{Re}(i\lambda_y\lambda_z^*) , \qquad (3.21)$$

$$\mathrm{Re}(A_z - B_z) = k_1^{(1)}\left(\frac{k_\parallel^2 + |k_1|^2}{k_\parallel^2}|\lambda_z|^2 + |\lambda_y|^2\right) . \qquad (3.22)$$

With these results we can now write down the components of the real part of $\langle \vec{S}(z)\rangle$ in the case that the incident light is s polarized. We have that

$$\mathrm{Re}\langle S_x(z)\rangle_s=\delta^2\,\frac{\omega^3|\epsilon(\omega)-1|^2}{8\pi^3c^2}\,\frac{k_z^{(0)2}|E_y^{(1)}|^2}{|k_z^{(i)}-k_z^{(0)}|^2}\int d^2k_\parallel e^{2k_1^{(2)}z}g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)$$
$$\times\frac{k_x}{k_\parallel^2}\left\{\frac{k_y^2}{|k_1-\epsilon(\omega)k_z|^2}\left[\frac{c^4}{\omega^4}\,[k_\parallel^2+\mathrm{Re}(k_1^2)]|k_z|^2-2\,\frac{c^2}{\omega^2}\,k_1^{(2)}\,\mathrm{Re}\;ik_z^*\left(\frac{k_1-\epsilon(\omega)k_z}{k_1-k_z}\right)\right]+\frac{k_x^2}{|k_1-k_z|^2}\right\},\tag{3.23}$$

$$\mathrm{Re}\langle S_y(z)\rangle_s=0\;,\tag{3.24}$$

$$\mathrm{Re}\langle S_z(z)\rangle_s=\delta^2\,\frac{\omega^3|\epsilon(\omega)-1|^2}{8\pi^3c^2}\,\frac{k_z^{(0)2}|E_y^{(1)}|^2}{|k_z^{(i)}-k_z^{(0)}|^2}\int d^2k_\parallel e^{2k_1^{(2)}z}\,g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)$$
$$\times\frac{k_1^{(1)}}{k_\parallel^2}\left(\frac{c^4}{\omega^4}\,\frac{(k_\parallel^2+|k_1|^2)k_y^2|k_z|^2}{|k_1-\epsilon(\omega)k_z|^2}+\frac{k_x^2}{|k_1-k_z|^2}\right)\;.\tag{3.25}$$

The vanishing of $\mathrm{Re}\langle S_y(z)\rangle_s$ is due to the fact that the integrand of the expression for it is an odd function of k_y.

We can simplify Eqs. (3.23)–(3.25) by going to polar coordinates and setting

$$k_x=k_\parallel\cos\varphi_s\;,\quad k_y=k_\parallel\sin\varphi_s\;.\tag{3.26}$$

In this way we obtain

$$\mathrm{Re}\langle S_x(z)\rangle_s=\delta^2\,\frac{\omega^3|\epsilon(\omega)-1|^2}{8\pi^3c^2}\,\cos^2\theta_0\,\frac{|E_y^{(1)}|^2}{|k_z^{(i)}-k_z^{(0)}|^2}\int d^2k_\parallel e^{2k_1^{(2)}z}\,g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)k_\parallel\cos\varphi_s$$
$$\times\left\{\frac{c^2}{\omega^2}\,\frac{\sin^2\varphi_s}{|k_1-\epsilon(\omega)k_z|^2}\left[(k_\parallel^2+|k_1|^2)|k_z|^2-2k_1^{(2)}k_z^{(2)}k_\parallel^2\,\Theta\!\left(k_\parallel^2-\frac{\omega^2}{c^2}\right)\right]+\frac{\omega^2}{c^2}\,\frac{\cos^2\varphi_s}{|k_1-k_z|^2}\right\}\;,\tag{3.27}$$

$$\mathrm{Re}\langle S_z(z)\rangle_s=\delta^2\,\frac{\omega^3|\epsilon(\omega)-1|^2}{8\pi^3c^2}\,\cos^2\theta_0\,\frac{|E_y^{(1)}|^2}{|k_z^{(i)}-k_z^{(0)}|^2}\int d^2k_\parallel e^{2k_1^{(2)}z}$$
$$\times g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)\,k_1^{(1)}\left(\frac{c^2}{\omega^2}\,\sin^2\varphi_s\,\frac{(k_\parallel^2+|k_1|^2)|k_z|^2}{|k_1-\epsilon(\omega)k_z|^2}+\frac{\omega^2}{c^2}\,\frac{\cos^2\varphi_s}{|k_1-k_z|^2}\right).\tag{3.28}$$

In Eq. (3.27), $k_z^{(2)}=(k_\parallel^2-\omega^2/c^2)^{1/2}$, and the term in which it appears contributes only when $k_\parallel^2>\omega^2/c^2$, as the presence of the Heaviside unit step function indicates.

Turning now to the case of p-polarized incident light we find that

$$\mathrm{Re}\langle S_x(z)\rangle_p=\delta^2\,\frac{\omega^3|\epsilon(\omega)-1|^2}{8\pi^3c^2}\,\frac{|E_x^{(1)}|^2}{|k_z^{(i)}-\epsilon(\omega)k_z^{(0)}|^2}\int d^2k_\parallel e^{2k_1^{(2)}z}\,g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)$$
$$\times\frac{1}{k_\parallel^2}\left\{\frac{1}{|k_1-\epsilon(\omega)k_z|^2}\left[\frac{c^4}{\omega^4}\,[k_\parallel^2+\mathrm{Re}(k_1^2)]k_x|k_xk_zk_z^{(i)}-\tfrac{1}{2}k^{(0)}k_\parallel^2[\epsilon(\omega)+\epsilon^{-1}(\omega)]|^2+2\,\frac{c^2}{\omega^2}\,k_y^2k_1^{(2)}\right.\right.$$
$$\left.\left.\times\mathrm{Re}\left(ik_z^{(i)}\,\frac{k_1-\epsilon(\omega)k_z}{k_1-k_z}\,\{k_xk_z^*k_z^{(i)*}-\tfrac{1}{2}k^{(0)}k_\parallel^2[\epsilon^*(\omega)+\epsilon^{-1}(\omega)^*]\}\right)\right]+\frac{k_xk_y^2|k_z^{(i)}|^2}{|k_1-k_z|^2}\right\}\;,\tag{3.29}$$

$$\mathrm{Re}\langle S_y(z)\rangle_p=0\;,\tag{3.30}$$

$$\mathrm{Re}\langle S_z(z)\rangle_p=\delta^2\,\frac{\omega^3|\epsilon(\omega)-1|^2}{8\pi^3c^2}\,\frac{|E_x^{(1)}|^2}{|k_z^{(i)}-\epsilon(\omega)k_z^{(0)}|^2}\int d^2k_\parallel e^{2k_1^{(2)}z}\,g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)$$
$$\times\frac{k_1^{(1)}}{k_\parallel^2}\left(\frac{c^4}{\omega^4}\,(k_\parallel^2+|k_1|^2)\,\frac{|k_xk_zk_z^{(i)}-\tfrac{1}{2}k^{(0)}k_\parallel^2[\epsilon(\omega)+\epsilon^{-1}(\omega)]|^2}{|k_1-\epsilon(\omega)k_z|^2}+\frac{k_y^2|k_z^{(i)}|^2}{|k_1-k_z|^2}\right)\;.\tag{3.31}$$

The function $\mathrm{Re}\langle S_y(z)\rangle_p$ vanishes for this geometry also, because the integrand in the expression for it is an odd function of k_y.

We have recorded here the expression for $\mathrm{Re}\langle S_x(z)\rangle_p$ associated with p-polarized incident radiation for completeness. However, in what follows we will consider explicitly only the component $\mathrm{Re}\langle S_z(z)\rangle_p$ induced by p-polarized incident radiation. With the use of Eqs. (3.26) we can write it as

$$\mathrm{Re}\langle S_z(z)\rangle_p=\delta^2\,\frac{\omega^3|\epsilon(\omega)-1|^2}{32\pi^3c^2}\,\frac{|E_x^{(1)}|^2}{|k_z^{(i)}-\epsilon(\omega)k_z^{(0)}|^2}\left[4\,\frac{c^2}{\omega^2}\,|k_z^{(i)}|^2\int d^2k_\parallel e^{2k_1^{(2)}z}g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)k_1^{(1)}\right.$$
$$\times\left(\frac{c^2}{\omega^2}\,\cos^2\varphi_s\,\frac{(k_\parallel^2+|k_1|^2)|k_z|^2}{|k_1-\epsilon(\omega)k_z|^2}+\frac{\omega^2}{c^2}\,\frac{\sin^2\varphi_s}{|k_1-k_z|^2}\right)$$

$$+\frac{c^2}{\omega^2}\sin^2\theta_0|\epsilon(\omega)+\epsilon^{-1}(\omega)|^2\int d^2k_{\parallel}e^{2k_1^{(2)}z}g(|\vec{k}_{\parallel}-\vec{k}_{\parallel}^{(0)}|)\frac{(k_{\parallel}^2+|k_1|^2)k_{\parallel}^2k_1^{(1)}}{|k_1-\epsilon(\omega)k_z|^2}$$

$$-4\frac{c^3}{\omega^3}\sin\theta_0\int d^2k_{\parallel}e^{2k_1^{(2)}z}g(|\vec{k}_{\parallel}-\vec{k}_{\parallel}^{(0)}|)$$

$$\times\frac{(k_{\parallel}^2+|k_1|^2)k_{\parallel}k_1^{(1)}}{|k_1-\epsilon(\omega)k_z|^2}\cos\varphi_s\,\mathrm{Re}\left\{k_z^*k_z^{(i)*}[\epsilon(\omega)+\epsilon^{-1}(\omega)]\right\}\Bigg]\ . \tag{3.32}$$

Having obtained the real part of the complex Poynting vector, averaged over the surface roughness, inside the medium, for both s- and p-polarized incident radiation, we now turn to a discussion of the physical significance of these quantities.

Let us denote by P_0 the energy incident per unit time on unit area of the surface. Explicit expressions for this quantity are given by Eqs. (2.65) and (2.66), for s- and p-polarized incident radiation, respectively. We then define the vector $\vec{\mathcal{S}}(z)$ by

$$\vec{\mathcal{S}}(z)=(1/P_0)\,\mathrm{Re}\langle\vec{S}(z)\rangle\ , \tag{3.33}$$

where it should be kept in mind that in this section z is negative.

The z component of the Poynting vector gives the energy crossing unit area perpendicular to the z axis per unit time. To obtain the portion of the incident flux entering the medium we clearly require the z component of the Poynting vector evaluated at $z=0-$. If the incident beam strikes a rectangular area of the surface of linear dimensions L_x and L_y, then the total energy carried into the medium per unit time by the scattered waves is

$$\frac{dE_z}{dt}=\mathcal{S}_z(0-)E_0\ , \tag{3.34}$$

where

$$E_0=L_xL_yP_0 \tag{3.35}$$

is the energy per unit time that strikes the area L_xL_y. Thus if we denote by $f_z^<$ the fraction of the energy carried off by the scattered waves in the direction of the normal to the surface and into the crystal, we have

$$f_z^<=\mathcal{S}_z(0-)\ . \tag{3.36}$$

Combining Eqs. (3.28) and (2.65) and Eqs. (3.32) and (2.66) according to Eqs. (3.33) and (3.36), we find that this fraction $f_z^<$ is given by

$$f_z^{(s<)}=\delta^2\frac{\omega^3|\epsilon(\omega)-1|^2}{\pi^2c^3}\frac{\cos\theta_0}{|k_z^{(i)}-k_z^{(0)}|^2}\int d^2k_{\parallel}g(|\vec{k}_{\parallel}-\vec{k}_{\parallel}^{(0)}|)k_1^{(1)}$$

$$\times\left(\frac{c^2}{\omega^2}\sin^2\varphi_s\frac{(k_{\parallel}^2+|k_1|^2)|k_z|^2}{|k_1-\epsilon(\omega)k_z|^2}+\frac{\omega^2}{c^2}\frac{\cos^2\varphi_s}{|k_1-k_z|^2}\right)\ , \tag{3.37}$$

for s-polarized incident radiation, and

$$f_z^{(p<)}=\delta^2\frac{\omega^3|\epsilon(\omega)-1|^2}{4\pi^2c^3}\frac{\cos\theta_0}{|k_z^{(i)}-\epsilon(\omega)k_z^{(0)}|^2}\left[4\frac{c^2}{\omega^2}|k_z^{(i)}|^2\int d^2k_{\parallel}g(|\vec{k}_{\parallel}-\vec{k}_{\parallel}^{(0)}|)k_1^{(1)}\right.$$

$$\times\left(\frac{c^2}{\omega^2}\cos^2\varphi_s\frac{(k_{\parallel}^2+|k_1|^2)|k_z|^2}{|k_1-\epsilon(\omega)k_z|^2}+\frac{\omega^2}{c^2}\frac{\sin^2\varphi_s}{|k_1-k_z|^2}\right)+\frac{c^2}{\omega^2}\sin^2\theta_0|\epsilon(\omega)+\epsilon^{-1}(\omega)|^2\int d^2k_{\parallel}g(|\vec{k}_{\parallel}-\vec{k}_{\parallel}^{(0)}|)$$

$$\times\frac{(k_{\parallel}^2+|k_1|^2)k_{\parallel}^2k_1^{(1)}}{|k_1-\epsilon(\omega)k_z|^2}-4\frac{c^3}{\omega^3}\sin\theta_0\int d^2k_{\parallel}g(|\vec{k}_{\parallel}-\vec{k}_{\parallel}^{(0)}|)\frac{(k_{\parallel}^2+|k_1|^2)k_{\parallel}k_1^{(1)}}{|k_1-\epsilon(\omega)k_z|^2}\cos\varphi_s$$

$$\left.\times\mathrm{Re}\left\{k_z^*k_z^{(i)*}[\epsilon(\omega)+\epsilon^{-1}(\omega)]\right\}\right]\ , \tag{3.38}$$

for p-polarized incident radiation.

Turning now to the x component of the Poynting vector, and consequently of the vector $\vec{\mathcal{S}}(z)$, we see that $\mathrm{Re}\langle S_x(z)\rangle$ gives the energy traveling parallel to the surface which crosses unit area at a depth z per unit time. The total energy per unit time carried by the wave is therefore

$$\frac{dE_x}{dt}=L_y\int_{-\infty}^{0}dz\,\mathrm{Re}\langle S_x(z)\rangle=L_yP_0\int_{-\infty}^{0}dz\,\mathcal{S}_x(z)\ . \tag{3.39}$$

We divide this expression by E_0 to obtain the fraction f_x of the incident energy absorbed by the medium and carried off in the x direction,

$$f_x^< = \frac{1}{L_x}\int_{-\infty}^{0} dz\, \mathcal{S}_x(z)\ . \tag{3.40}$$

Thus the quantity $\mathcal{S}_x(z)$ itself has no direct physical meaning. The physically meaningful quantity is f_x, which is obtained from $\mathcal{S}_x(z)$. Combining Eqs. (3.27) and (2.65) with Eq. (3.40), we find for f_x the result

$$f_x^{(s<)} = \frac{\delta^2}{L_x}\,\frac{\omega^3|\epsilon(\omega)-1|^2}{\pi^2c^3}\,\frac{\cos\theta_0}{|k_z^{(i)}-k_z^{(0)}|^2}\int d^2k_\parallel g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)\,\frac{k_\parallel\cos\varphi_s}{2k_1^{(2)}}$$
$$\times\left\{\frac{c^2}{\omega^2}\,\frac{\sin^2\varphi_s}{|k_1-\epsilon(\omega)k_z|^2}\left[(k_\parallel^2+|k_1|^2)|k_z|^2-2k_1^{(2)}k_z^{(2)}k_\parallel^2\,\theta\left(k_\parallel^2-\frac{\omega^2}{c^2}\right)\right]+\frac{\omega^2}{c^2}\,\frac{\cos^2\varphi_s}{|k_1-k_z|^2}\right\}\ , \tag{3.41}$$

for s-polarized incident radiation.

The numerical evaluation of the results of this and Sec. II will be carried out in Secs. IV and V.

IV. CONTRIBUTION TO THE ROUGHNESS-INDUCED ABSORPTION FROM COUPLING TO SURFACE POLARITONS

Many of the earlier theoretical studies[1–6] of the roughness-induced absorption confine their attention to the simple free-electron metal, which is described by the dielectric constant $\epsilon(\omega)=1-\omega_p^2/\omega^2$. In the frequency region where $\epsilon(\omega)\le -1$, surface polaritons may propagate along the interface between the crystal and the vacuum.[10] The waves are described by the dispersion relation

$$\frac{c^2k_\parallel^2}{\omega^2}=\frac{\epsilon(\omega)}{\epsilon(\omega)+1}\ . \tag{4.1}$$

Note that for the surface polariton $ck_\parallel>\omega$, a condition that must be satisfied if the surface wave is not to radiate its energy into the vacuum. Then in some of the earlier papers, the roughness-induced absorption is presumed to arise from the roughness-induced coupling of the incident wave to the surface polariton.

The purpose of the present section is to examine the general results of Sec. III when the real part $\epsilon^{(1)}(\omega)$ of $\epsilon(\omega)$ is negative and the imaginary part $\epsilon^{(2)}(\omega)$ is small. In this case, we find contributions to the absorption rate that may be identified with roughness-induced coupling to surface polaritons. For small $\epsilon^{(2)}(\omega)$, we extract from the general expressions simple expressions for the contribution described above. We do this for the cases of s and p polarization at non-normal incidence. In Sec. V we shall make a quantitative comparison between the results obtained in the present section and numerical computations of the total absorption rate calculated from the general expressions given above. We do this for the case of aluminum metal, the material for which the approximate results should hold best. In their most recent paper,[6] Elson and Ritchie carried out an analysis similar to the one presented here, although they confined their attention to the case of normal incidence, and they have not carried out numerical studies of the sort reported in Sec. V.

We begin with the general expression for the quantity $f_z^{(s<)}$, the fraction of the energy of an incident wave with s polarization absorbed by the roughness-induced energy flow in the direction normal to the surface. We saw earlier that this quantity is given by

$$f_z^{(s<)}=\mathrm{Re}\langle S_z(0-)\rangle_s/P_0\ , \tag{4.2a}$$

where

$$P_0=c|E_y^{(1)}|^2\cos\theta_0/8\pi\ . \tag{4.2b}$$

We have the explicit form from Eq. (3.37):

$$f_z^{(s<)}=\frac{\delta^3\omega^3|\epsilon(\omega)-1|^2\cos\theta_0}{\pi^2c^3|k_z^{(i)}-k_z^{(0)}|^2}$$
$$\times\int d^2k_\parallel g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)k_1^{(1)}$$
$$\times\left(\frac{c^2}{\omega^2}\sin^2\varphi_s\,\frac{(k_\parallel^2+|k_1|^2)|k_z|^2}{|k_1-\epsilon(\omega)k_z|^2}+\frac{\omega^2}{c^2}\,\frac{\cos^2\varphi_s}{|k_1-k_z|^2}\right). \tag{4.3}$$

The first term in the large parentheses arises from scattering processes which transform the incident wave of s polarization to a scattered wave with p polarization, while the second term describes scattering of the initial wave into a scattered wave of s polarization. It is the first term which contains a description of the roughness-induced absorption by surface polaritons. This may be seen by noting that

$$\frac{1}{|k_1-\epsilon(\omega)k_z|^2}=\frac{|k_1+\epsilon(\omega)k_z|^2}{|k_1^2-\epsilon^2(\omega)k_z^2|^2}\ ,$$

or after some small rearrangements,

$$\frac{1}{|k_1-\epsilon(\omega)k_z|^2}=\frac{|k_1+\epsilon(\omega)k_z|^2}{|\epsilon^2(\omega)-1|^2}\times\left(\left|k_\parallel^2-\frac{\omega^2}{c^2}\,\frac{\epsilon(\omega)}{\epsilon(\omega)+1}\right|^2\right)^{-1}\ . \tag{4.4}$$

Thus, when the left-hand side of Eq. (4.4) is considered as a function of $k_\parallel$, when $\epsilon^{(2)}(\omega)$ is small and $\epsilon^{(1)}(\omega)$ negative, a strong resonance at the surface plasmon wave vector [Eq. (4.1)] appears. We may obtain the contribution to $f_z^{(s<)}$ from roughness-induced coupling to surface polaritons by considering only the part that arises from this resonance. We proceed to obtain this portion in the limit $\epsilon^{(2)}(\omega)\to 0$, by replacing $k_\parallel$ everywhere in slowly varying factors by the value

$$k_{sp}=\frac{\omega^2}{c^2}\,\frac{\epsilon^{(1)}(\omega)}{\epsilon^{(1)}(\omega)+1}=\frac{\omega^2}{c^2}\,\frac{|\epsilon^{(1)}(\omega)|}{|\epsilon^{(1)}(\omega)|-1}\ , \tag{4.5}$$

where, as the last step indicates, we confine our attention to frequency regions where $\epsilon^{(1)}(\omega)<0$. With such an approximation applied to Eq. (4.4), one obtains

$$\frac{1}{|k_1-\epsilon(\omega)k_z|^2}\cong\left(\frac{\omega}{c}\right)^2\frac{4|\epsilon^{(1)}(\omega)|^2}{[|\epsilon^{(1)}(\omega)|-1]^3[|\epsilon^{(1)}(\omega)|+1]^2}\times\left(\left|k_\parallel^2-\frac{\omega^2}{c^2}\,\frac{\epsilon(\omega)}{\epsilon(\omega)+1}\right|^2\right)^{-1}. \tag{4.6}$$

Note also that when $\epsilon^{(2)}(\omega)$ is small and $\epsilon^{(1)}(\omega)<0$,

$$k_1^{(1)}\cong-\frac{\omega^2}{2c^2}\,\frac{\epsilon^{(2)}(\omega)}{(k_\parallel^2+(\omega^2/c^2)|\epsilon^{(1)}(\omega)|)^{1/2}}\ , \tag{4.7}$$

i.e., the quantity $k_1^{(1)}$ is proportional to $\epsilon^{(2)}(\omega)$ in this limit.[11]

When the approximations described above are carried out for all the facors in the appropriate term of Eq. (4.8), the results may be arranged to read [for small $\epsilon^{(2)}(\omega)$]

$$f_z^{(s<)}=\frac{2\delta^2\cos\theta_0}{\pi}\left(\frac{\omega}{c}\right)^6\frac{|\epsilon^{(1)}(\omega)|^2}{[|\epsilon^{(1)}(\omega)|-1]^{9/2}}\,\epsilon^{(2)}(\omega)\times\int_0^{2\pi}d\varphi_s\sin^2\varphi_s\,g(|\hat{k}_\parallel k_{sp}-\vec{k}_\parallel^{(0)}|)\times\int_0^\infty dk_\parallel\,k_\parallel\Big/\left|k_\parallel^2-k_{sp}^2-i\left(\frac{\omega}{c}\right)^2\frac{\epsilon^{(2)}(\omega)}{[|\epsilon^{(1)}(\omega)|-1]^2}\right|^2. \tag{4.8}$$

To obtain this result, it is useful to note the identity [as $\epsilon^{(2)}(\omega)\to 0$ and with $\epsilon^{(1)}(\omega)<0$]

$$|k_z^{(i)}-k_z^{(0)}|^2=1+|\epsilon^{(1)}(\omega)|\ . \tag{4.9}$$

As $\epsilon^{(2)}(\omega)\to 0$, the integral over $k_\parallel$ is readily evaluated to give the simple result

$$f_z^{(s<)}=\left(\frac{\omega}{c}\right)^4\delta^2\cos\theta_0\,\frac{|\epsilon^{(1)}(\omega)|^2}{[|\epsilon^{(1)}(\omega)|^2-1]^{5/2}}\times\int_0^{2\pi}\frac{d\varphi_s}{\pi}\sin^2\varphi_s\,g(|\hat{k}_\parallel k_{sp}-\vec{k}_\parallel^{(0)}|)\ . \tag{4.10}$$

At normal incidence, this result becomes equivalent to the result of Crowell and Ritchie,[4] who derived it through the use of quantum-mechanical perturbation theory, and also with the recent results of Elson and Ritchie.[6] It is interesting to note that in the classical theory, this contribution comes from a small "leak" of energy out of the surface polariton into the crystalline interior, owing to the (assumed small) value of $\epsilon^{(2)}(\omega)$. This is evident from Eq. (4.7), where one sees that for each $k_\parallel$, the contribution to the time average of the Poynting vector in the direction normal to the crystal surface vanishes identically as $\epsilon^{(2)}(\omega)\to 0$. As we have seen, the integrated strength of all contributions to $f_z^{(s<)}$ remains finite as $\epsilon^{(2)}(\omega)\to 0$.

We next examine the behavior of $f_x^{(s<)}$, the fraction of the energy of the incident wave absorbed by the energy flow parallel to the surface. We shall find for $f_x^{(s<)}$ a behavior that differs qualitatively from that of $f_z^{(s<)}$, in the limit $\epsilon^{(2)}(\omega)\to 0$. As explained earlier, if the incident beam illuminates a rectangular area of the surface with length L_x for the side parallel to the x axis and L_y for the side parallel to the y axis, then

$$f_x^{(s<)}=\left(L_y\int_{-\infty}^0 dz\,\mathrm{Re}\langle S_x(z)\rangle\right)\Big/L_xL_yP_0\ ,$$

where P_0 is given in Eq. (4.2b). Thus, we have

$$f_x^{(s<)}=\frac{\delta^2\omega^3|\epsilon(\omega)-1|^2}{2\pi^2c^3L_x}\,\frac{\cos\theta_0}{|k_z^{(i)}-k_z^{(0)}|^2}\int\frac{d^2k_\parallel}{k_1^{(2)}}\,g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)k_\parallel\cos\varphi_s\times\left\{\frac{c^2}{\omega^2}\,\frac{\sin^2\varphi_s}{|k_1-\epsilon(\omega)k_z|^2}\left[(k_\parallel^2+|k_1|^2)|k_z|^2-2k_1^{(2)}k_z^{(2)}k_\parallel^2\,\theta\left(k_\parallel^2-\frac{\omega^2}{c^2}\right)\right]+\frac{\omega^2}{c^2}\,\frac{\cos^2\varphi_s}{|k_1-k_z|^2}\right\}. \tag{4.11}$$

As in the case of $f_z^{(s<)}$, the term proportional to $|k_1-\epsilon(\omega)k_z|^{-2}$ contains the contribution to the absorption that arises from the coupling of the incident wave to surface polaritons. We may proceed with the evaluation of $f_x^{(s<)}$ exactly as before. We shall simply state the result as a consequence. However, before we do this, we make two general observations.

First, note that $f_x^{(s<)}$ is proportional to L_x^{-1}. The reason for this is that the incident wave illuminates a rectangular area of the surface with area L_xL_y, while the energy absorbed from the incident wave which flows parallel to the surface is carried in a small channel of dimensions $L_y\times$(the skin depth). This is evident from the factor of $1/k_1^{(2)}$ in the integrand of Eq. (4.11). Because $f_x^{(s<)}$ is inversely proportional to L_x, it will not appear in any calculation which assumes the incident wave to illuminate the whole surface, and then takes the limit as the surface area becomes infinite. Most of the quantum field theoretic treatments discussed in Sec. I fall into this class.

It is apparent also that in the limit as $\epsilon^{(2)}(\omega)\to 0$, the quantity $f_x^{(s<)}$ will diverge as $\epsilon^{(2)}(\omega)^{-1}$. This is apparent at once because $k_\parallel \cos\varphi_s$ appears in Eq. (4.11) in place of the factor $k_1^{(1)}$ in Eq. (4.3). As we see from Eq. (4.7), as $\epsilon^{(2)}(\omega)\to 0$ [in a frequency region where $\epsilon^{(1)}(\omega)< 0$], the factor $k_1^{(1)}$ introduces a factor of $\epsilon^{(2)}(\omega)$ into $f_z^{(s<)}$, and as $\epsilon^{(2)}(\omega)\to 0$ this cancels the factor of $[\epsilon^{(2)}(\omega)]^{-1}$ that arises from integration over the surface polariton resonance. We shall discuss the physical origin of the divergence below.

As remarked above, when $\epsilon^{(1)}(\omega)< 0$, and in the limit $\epsilon^{(2)}(\omega)\to 0$, one may evaluate the surface polariton contribution to $f_x^{(s<)}$ exactly as before. Upon carrying out the calculation, we find

$$f_x^{(s<)} = -\frac{\delta^2\omega^3|\epsilon^{(1)}(\omega)|^{5/2}\cos\theta_0}{L_x c^3[|\epsilon^{(1)}(\omega)|+1][|\epsilon^{(1)}(\omega)|-1]^2}\frac{1}{\epsilon^{(2)}(\omega)} \times\int_0^{2\pi}\frac{d\varphi_s}{\pi}\cos\varphi_s\sin^2\varphi_s\, g(|\hat{k}_\parallel k_{sp}-\vec{k}_\parallel^{(0)}|)\ . \tag{4.12}$$

At first glance, Eq. (4.12) seems curious, because of the explicit minus sign. This means that $f_x^{(s<)}$ will be negative for any surface described by a roughness structure function $g(Q_\parallel)$ which falls off monotonically as a function of its argument. (as for either a Lorentzian or a Gaussian). Thus, the energy flow described by $f_x^{(s<)}$ is in the medium, and opposed in direction to the $\hat{x}$ component of the incident wave Poynting vector. The reason for this is that the surface polariton responsible for the energy absorption occurs in a frequency region where the dielectric constant is negative, and one readily sees that in the medium, the Poynting vector is antiparallel to the wave vector $\vec{k}_\parallel$ of the surface polariton.

Actually, from the remarks of the preceding paragraph, we can appreciate that there is also an energy flow parallel to the surface which resides in the vacuum just above the surface. The electromagnetic field of the surface polariton excited by the incident wave extends into the vacuum outside the crystal, as well as into the crystal itself. To calculate the total energy flow parallel to the surface induced by the surface roughness, one needs to supplement the quantity $f_x^{(s<)}$ by the part $f_x^{(s>)}$ which resides in the vacuum outside the crystal. When we do this, we shall see that $f_x^{(s>)}$ is positive and always larger in magnitude than $f_x^{(s<)}$ in the region $\epsilon^{(1)}(\omega)< -1$, where the surface polaritons may be excited by the incident wave. Thus, when the two are combined, the total rate of energy flow $f_x^{(s<)}+f_x^{(s>)}$ is parallel to the $\hat{x}$ component of the Poynting vector of the incident wave, as one would expect intuitively.

To calculate the contribution $f_x^{(s>)}$ to the rate of energy flow parallel to the surface, in the vacuum just above the surface, we require the time average $\langle S_x(z)\rangle$ of the Poynting vector of the scattered fields outside the crystal suface, for $z>0$. In Sec. II, we display expressions for the Poynting vector associated with the scattered fields for $z>0$. However, as remarked just after Eq. (2.47), we confined our attention there to the contributions to the Poynting vector from the scattered radiation which propagates off to infinity, i.e., the integral in Eq. (2.53) is confined to the region $k_\parallel<\omega/c$, where k_z is real. For the present purposes, we require the contribution to $\langle S_x(z)\rangle$ from the region $k_\parallel>\omega/c$, since these contributions describe fields localized near the surface, with $k_z=i(k_\parallel^2-\omega^2/c^2)^{1/2}$. Given this portion of $\langle S_x(z)\rangle$, we then compute $f_x^{(s>)}$ from the relation

$$f_x^{(s>)}=\left(L_y\int_0^\infty dz\,\mathrm{Re}\langle S_x\rangle\right)\Big/ L_xL_yP_0\ . \tag{4.13}$$

It is a short exercise to obtain the general expression for $f_x^{(s>)}$, with the methods outlined in Secs. II and III. We find

$$f_x^{(s>)}=\frac{\delta^2\omega^3|\epsilon(\omega)-1|^2}{2\pi^2c^3L_x}\frac{\cos\theta_0}{|k_z^{(1)}-k_z^{(0)}|^2}\int_>\frac{d^2k_\parallel}{k_z^{(2)}}g(|\vec{k}_\parallel-\vec{k}_\parallel^{(0)}|)\,k_\parallel\cos\varphi_s \times\left(\frac{c^2}{\omega^2}\frac{\sin^2\varphi_s}{|k_1-\epsilon(\omega)k_z|^2}[(k_\parallel^2+|k_z|^2)|k_1|^2-2k_1^{(2)}k_z^{(2)}k_\parallel^2]+\frac{\omega^2}{c^2}\frac{\cos^2\varphi_s}{|k_1-k_z|^2}\right)\ . \tag{4.14}$$

The symbol > appended to the integral sign reminds the reader that the integral covers the region $k_\parallel>\omega/c$, where the scattered fields are localized near the surface. (The contribution from the region $k_\parallel<\omega/c$ has been included in the cross sections defined in Sec. III.)

In the limit of small $\epsilon^{(2)}(\omega)$, we may extract from Eq. (4.14) the contribution from the surface polaritons. The method for doing this is precisely the same as that outlined earlier in this section. After carrying out this calculation we find

$$f_x^{(s>)}=-|\epsilon^{(1)}(\omega)|^2 f_x^{(s<)}\ , \tag{4.15}$$

so that the total rate of energy flow parallel to the surface generated by the driving field is

$$f_x^{(s)}=f_x^{(s>)}+f_x^{(s<)}$$

or

$$f_x^{(s)} = \frac{\delta^2}{L_x}\frac{\omega^3}{\pi c^3}\frac{\cos\theta_0 |\epsilon^{(1)}(\omega)|^{5/2}}{|\epsilon^{(1)}(\omega)|-1}\frac{1}{\epsilon^{(2)}(\omega)} \times \int_0^{2\pi} d\varphi_s \cos\varphi_s \sin^2\varphi_s g(|\hat{k}_\parallel k_{sp} - \vec{k}_\parallel^{(0)}|) . \quad (4.16)$$

The physical meaning of this result becomes more apparent if we introduce the mean free path $l_{sp}(\omega)$ of the surface polariton. The mean free path is defined by

$$\frac{1}{l_{sp}(\omega)} = \mathrm{Im}(k_\parallel) , \quad (4.17)$$

where $\mathrm{Im}(k_\parallel)$ is the imaginary part of $k_\parallel$, calculated by inserting the complex dielectric constant in the right-hand side of Eq. (4.1). As $\epsilon^{(2)}(\omega) \to 0$, and with $\epsilon^{(1)}(\omega)$ negative one has

$$\frac{1}{l_{sp}(\omega)} = \frac{\omega}{2c}\frac{\epsilon^{(2)}(\omega)}{|\epsilon^{(1)}(\omega)|^{1/2}[|\epsilon^{(1)}(\omega)|-1]^{3/2}} , \quad (4.18)$$

so that we have

$$|f_x^{(s)}| = \frac{\delta^2\omega^4}{2c^4}\frac{|\epsilon^{(1)}(\omega)|^2\cos\theta_0}{[|\epsilon^{(1)}(\omega)|-1]^{5/2}}\frac{l_{sp}(\omega)}{L_x} \times \int_0^{2\pi}\frac{d\varphi_s}{\pi}\cos\varphi_s \sin^2\varphi_s g(|\hat{k}_\parallel k_{sp} - \vec{k}_\parallel^{(0)}|) . \quad (4.19)$$

At normal incidence, $\vec{k}_\parallel^{(0)} = 0$, and the angular integral on the right-hand side of Eq. (4.19) vanishes, as symmetry dictates.

The physical interpretation of the result in Eq. (4.18) is the following. The incident wave has frequency ω that matches that of a surface polariton [when $\epsilon^{(1)}(\omega) < 0$ as assumed here], but its wave-vector component $k_\parallel^{(0)}$ in the plane of the surface does not, since necessarily $ck_\parallel^{(0)} < \omega$, while for surface polaritons $ck_\parallel^{(0)} > \omega$, as remarked above. The effect of the surface roughness is to mix into the incident wave a broad spectrum of spatial Fourier components $k_\parallel$, and the electric field at each $k_\parallel$ oscillates with frequency ω. There is thus in the scattered field a component which matches both the frequency of the surface polariton and its wave vector, the latter computed from Eq. (4.1), with $\epsilon(\omega)$ replaced by $\epsilon^{(1)}(\omega)$. Thus, in the language of nonlinear optics, the surface-roughness-induced interaction between the incident wave and the surface polariton is phase matched. For the incident wave, $k_\parallel$ is purely real, while the surface polariton has the finite mean free path $l_{sp}(\omega)$ parallel to the surface. Thus, the surface polariton mean free path $l_{sp}(\omega)$ plays the role of the coherence length of the phase-matched interaction, and the energy stored in the driven surface polariton is proportional to the coherence length.

We can see from the discussion of the preceding paragraph that the result displayed in Eq. (4.18) is valid only in one limit (which in many circumstances is the one relevant to experimental situations). If $\epsilon^{(2)}(\omega)$ is so small, or the incident beam so well focused, that $l_{sp}(\omega) > L_x$, then quite clearly the coherence length of the phase-matched interaction becomes L_x rather than $l_{sp}(\omega)$. In our discussions, we have implicitly assumed L_x and L_y are both very large, and integrations over spatial coordinates parallel to the surface have been freely extended to $\pm\infty$. Had they been kept finite, then we would have found Eq. (4.15) valid only when $l_{sp}(\omega) < L_x$, and when $l_{sp}(\omega) > L_x$, the factor $l_{sp}(\omega)/L_x$ would have been replaced by unity. Throughout the visible range of frequencies and into the ultraviolet, $\epsilon^{(2)}(\omega)$ is large enough that the condition $l_{sp}(\omega) < L_x$ should be satisfied, unless the beam is focused very sharply. However, in the infrared, it has been demonstrated that $l_{sp}(\omega)$ can become very large[12] and the limit $l_{sp}(\omega) > L_x$ may be appropriate most commonly here.

Note that when $l_{sp}(\omega) > L_x$, $|f_x^{(s)}|$ and $f_z^{(s)}$ become comparable in magnitude, so both components of the Poynting vector must be considered when the total surface-roughness-induced absorption is calculated. When $l_{sp}(\omega) \ll L_x$, then $|f_x^{(s)}|$ is small in magnitude. However, the energy density stored in the surface polariton can be very large when $\epsilon^{(2)}(\omega)$ is small and this may lead to a number of physical effects, such as the diffuse scattering of the incident radiation through the surface polariton as an intermediate state, a phenomenon observed in a number of experiments.[13] This question, along with related problems, is currently under investigation.

The discussion presented above is confined entirely to the case of s-polarized incident radiation. We conclude this section by stating the expression for the contribution from surface polaritons to $f_z^{(p)}$, the fraction of the energy absorbed from the incident wave due to surface roughness that comes about because of the presence of $\langle S_z \rangle$. When $l_{sp}(\omega) \ll L_x$, this is the dominant contribution to the roughness-induced absorption, as in the case of s polarization.

We find, after a series of manipulations very similar to those above, that the surface polariton contribution to $f_z^{(p)}$ is

$$f_z^{(p)} = \delta^2\left(\frac{\omega}{c}\right)^4 \frac{|\epsilon^{(1)}(\omega)|\cos\theta_0}{[|\epsilon^{(1)}(\omega)|\cos^2\theta_0 + \sin^2\theta_0]}\frac{1}{[|\epsilon^{(1)}(\omega)|-1]^{5/2}}$$

$$\times \int_0^{2\pi} \frac{d\varphi_s}{\pi} g(|\hat{k}_{\parallel} k_{sp} - \vec{k}_{\parallel}^{(0)}|) \{\cos\varphi_s[|\epsilon^{(1)}(\omega)|^2 + |\epsilon^{(1)}(\omega)|\sin^2\theta_0]^{1/2} - \tfrac{1}{2}[1+|\epsilon^{(1)}(\omega)|^2]\sin\theta_0\}^2 . \quad (4.20)$$

Of course, there is also an energy flow $f_x^{(p)}$ parallel to the surface for p-polarized incident radiation as well as for s-polarized incident radiation. We do not display $f_x^{(p)}$ explicitly here, since [for finite $\epsilon^{(2)}(\omega)$] it is proportional to $l_{sp}(\omega)/L_x$, and is negligible for our purposes.

V. NUMERICAL STUDIES OF ROUGHNESS-INDUCED SCATTERING AND ABSORPTION

In this section, we explore the predictions of the results derived in Secs. II–IV. The purpose of the calculations is to explore the dependence of the roughness-induced scattering on the polarization of the incident wave, on polarization at normal incidence, and to test the accuracy of the simple results given by Eqs. (4.10) and (4.16) against the predictions for aluminum, both because it is the material which most closely approximates the nearly-free-electron metal for which one would expect Eqs. (4.10) and (4.16) to be valid, and because one can prepare films of this material with well characterized surface roughness. We refer the reader to the very complete study of aluminum films carried out by Endriz and Spicer as an example of such studies.[14]

In the numerical calculations reported below, we have presumed a Gaussian distribution function for the surface-roughness correlation function. More specifically, the correlation function $\langle\zeta(\vec{x}_{\parallel}) \times\zeta(\vec{0})\rangle$ is related to the quantity $g(\vec{Q}_{\parallel})$ introduced in Sec. IV in the following manner:

$$\langle\zeta(\vec{x}_{\parallel})\zeta(\vec{0})\rangle = \delta^2 \int \frac{d^2Q_{\parallel}}{(2\pi)^2} g(\vec{Q}_{\parallel}) e^{i\vec{Q}_{\parallel}\cdot\vec{x}_{\parallel}} , \quad (5.1)$$

where if $g(\vec{Q}_{\parallel})$ is normalized so that

$$\int \frac{d^2Q_{\parallel}}{(2\pi)^2} g(\vec{Q}_{\parallel}) = 1 , \quad (5.2)$$

then $\langle\zeta^2(\vec{0})\rangle = \langle\zeta^2\rangle = \delta^2$, so the parameter δ is then the rms height of the surface roughness. In the calculations reported below, we have used a Gaussian for $g(\vec{Q}_{\parallel})$:

$$g(\vec{Q}_{\parallel}) = \pi a^2 e^{(-a^2/4)Q_{\parallel}^2} , \quad (5.3)$$

where a is a transverse correlation length. With this form of $g(\vec{Q}_{\parallel})$, one finds

$$\langle\zeta(\vec{x}_{\parallel})\zeta(\vec{0})\rangle = \delta^2 e^{-x_{\parallel}^2/a^2} . \quad (5.4)$$

The Gaussian form for $g(\vec{Q}_{\parallel})$ has the virtue that all the integrations over φ_s may be performed analytically, and expressed in terms of the modified Bessel functions $I_n(x)$. Thus, the numerical calculations involve only a single integration over θ_s in the case of the scattering calculation, or $k_{\parallel}$ for the case of the absorption calculations. In our numerical calculations, we have chosen 500 Å as the value of the transverse correlation length a which enters $g(\vec{Q}_{\parallel})$. The real and imaginary parts of $\epsilon(\omega)$ have been extracted from the analysis of the optical properties of aluminum by Ehrenreich, Phillipp, and Segall.[15]

We first consider the behavior of the roughness-induced scattering of light from aluminum. If we let $f(s)$ and $f(p)$ denote the fraction of the energy scattered away from an incident wave of s and p polarization, respectively, then we write

$$f(s) = f(s\to s) + f(s\to p) \quad (5.5a)$$

and

$$f(p) = f(p\to s) + f(p\to p) , \quad (5.5b)$$

where $f(i\to j)$ denotes the fraction of the energy of the incident wave of polarization i scattered into the final state of polarization j. Of course,

$$f(i\to j) = \int d\Omega_s \frac{df(i\to j)}{d\Omega_s} , \quad (5.6a)$$

where the integration is over solid angle with $0\le\theta_s\le\frac{1}{2}\pi$, and the $df(i\to j)/d\Omega_s$ are the differential scattering cross sections presented in Eqs. (2.69)–(2.72).

To present the results, it is useful to introduce dimensionless quantities $R(i\to j)$ related to the $f(i\to j)$ of Eq. (5.5) as follows:

$$f(i\to j) = \delta^2 a^2(\omega/c)^4 R(i\to j) . \quad (5.6b)$$

In Fig. 2, we show the variation with angle of incidence of the two functions $R(s\to s)$ and $R(s\to p)$, for a photon of energy 7 eV incident on aluminum. The two functions are comparable in magnitude, and they both fall off smoothly and monotonically with angle of incidence.

In Fig. 3, we show the behavior of $R(p\to s)$ and $R(p\to p)$ again for $\hbar\omega = 7$ eV on aluminum. The behavior of $R(p\to p)$ is quite striking, since it exhibits the pronounced broad maximum centered about $\theta_0 \approx 50°$.

In Fig. 4, we illustrate the variation with angle of incidence of the total reduced scattering efficiences $R(s)$ and $R(p)$, defined by

$$R(s) = R(s\to s) + R(s\to p)$$

and

$$R(p) = R(p\to s) + R(p\to p) .$$

The broad shoulder in $R(p)$ reflects the off-center maximum in $R(p\to p)$ illustrated in Fig. 3.

In Fig. 5, we show the variation of $R(s)$ with fre-

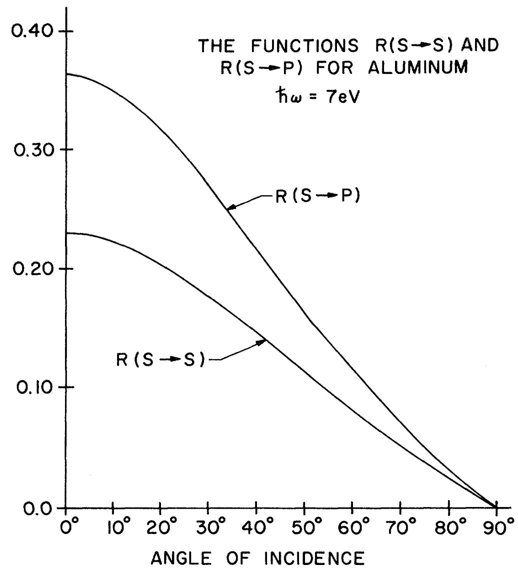

FIG. 2. Variation of the scattering functions $R(s\to s)$ and $R(s\to p)$ with angle of incidence, for a 7-eV photon incident on aluminum. The transverse correlation length a has been chosen equal to 500 Å.

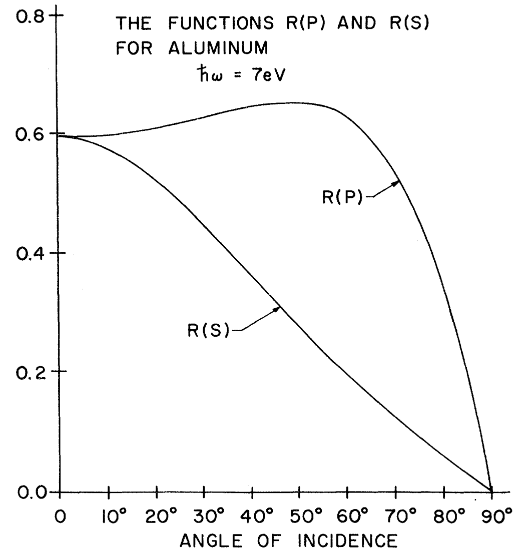

FIG. 4. Variation of the scattering functions $R(s)$ and $R(p)$ with angle of incidence, for a 7-eV photon incident on aluminum. The transverse correlation length a has been chosen equal to 500 Å.

quency, for three angles of incidence. The fact that $R(s)$ decreases substantially as ω increases means that the total scattering efficiency varies with frequency considerably more slowly than ω^4. Of course, this comes about because $\epsilon(\omega)$ is strongly dependent on frequency in this region. Note that at normal incidence, $R(s)$ displays a feature at the bulk plasma frequency ω_p where $\epsilon^{(1)}(\omega)=0$. This feature becomes small by the time $\theta_0=40°$.

We next turn our attention to the roughness-induced-absorption cross section. We introduce

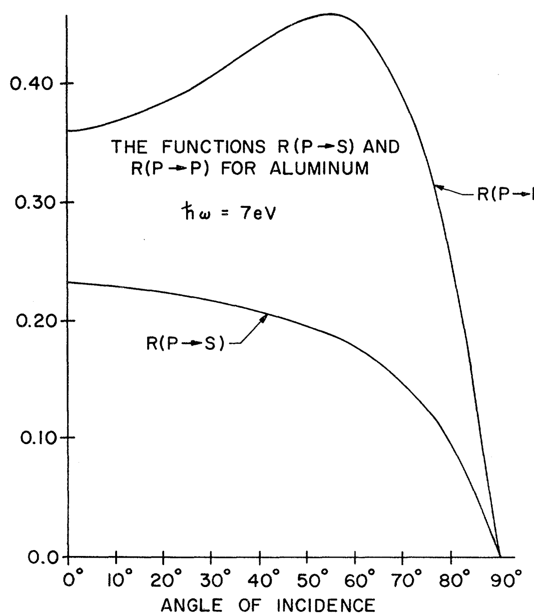

FIG. 3. Variation of the scattering functions $R(p\to s)$ and $R(p\to p)$ with angle of incidence, for a 7-eV photon incident on aluminum. The transverse correlation length a has been chosen equal to 500 Å.

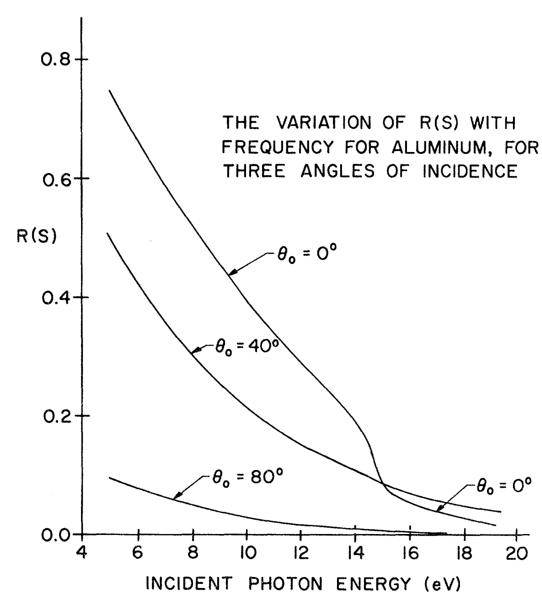

FIG. 5. Variation of $R(s)$ with frequency for several angles of incidence, at 7 eV for aluminum. The transverse correlation length a has been chosen equal to 500 Å.

dimensionless measures of the absorption rate A_{ij} similar to those employed in the scattering calculations through the relations

$$f_z^{(s)} = \delta^2 a^2 (\omega/c)^4 (A_{sp} + A_{ss}) \tag{5.7a}$$

and

$$f_z^{(p)} = \delta^2 a^2 (\omega/c)^4 (A_{ps} + A_{pp}) . \tag{5.7b}$$

The function A_{ij} is a dimensionless measure of the contribution to the rate of absorption of radiation of polarization i through roughness-induced coupling to final states of polarization j. In the general expression for $f_z^{(s)}$, A_{sp} comes from the contributions proportional to $\sin^2\varphi_s$ while A_{ss} comes from those proportional to $\cos^2\varphi_s$. In $f_z^{(p)}$, A_{ps} arises from the portion proportional to $\sin^2\varphi_s$ and A_{pp} from the remainder.

In Fig. 6, we show the angular variation of A_{sp} and A_{pp}, for the case where $\hbar\omega = 7$ eV. Note the similarity in the dependence on angle of incidence to the variation with θ_0 of the reduced scattering cross sections R_{sp} and R_{pp}. The solid lines in the figure are obtained by fully evaluating the integrals

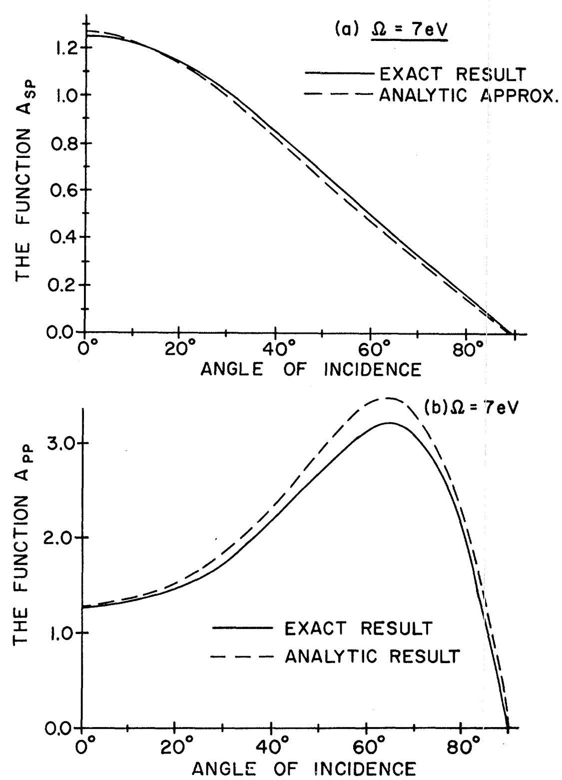

FIG. 6. Functions A_{sp} and A_{pp} as functions of the angle of incidence, for a photon of $\hbar\omega = 7$ eV incident on aluminum. The solid line is a result of a numerical integration over the exact formulas, and the dashed lines are obtained from Eqs. (4.10) and (4.15). The transverse correlation length a has been chosen equal to 500 Å.

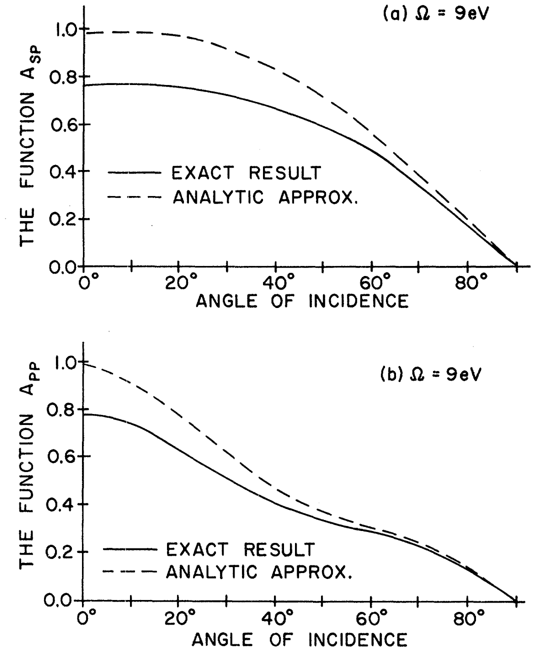

FIG. 7. Functions A_{sp} and A_{pp} as functions of the angle of incidence, for a photon of energy $\hbar\omega = 9$ eV incident on aluminum. The solid line is a result of a numerical integration over the exact formula, and the dashed lines are obtained from Eq. (4.10) and (4.15). The transverse correlation length a has been chosen equal to 500 Å.

numerically, and the dashed lines have been calculated from the approximate expressions presented in Eqs. (4.10) and (4.16). The agreement between the analytical approximation and the full calculation is remarkably good at 7 eV although for reasons discussed below, we will see it is less good at both lower and higher photon energies. At 7 eV, we find both A_{ss} and A_{ps} are quite small, of the order of 2 or 3% of A_{sp} and A_{pp} at all angles of incidence.

In Fig. 7, we present calculations similar to those in Fig. 6 for $\hbar\omega = 9$ eV. The agreement between the analytic approximation and the full calculations is now less good than that at 7 eV. We believe that the reason why this is so is apparent from the form of the integral over $k_\parallel$ in Eq. (4.8). One sees that the width of the resonance in the integral scales as $\epsilon^{(2)}(\omega)/[|\epsilon^{(1)}(\omega)| - 1]^2$. As ω increases, $|\epsilon^{(1)}(\omega)|$ decreases until at ≈ 10.6 eV, the surface plasmon energy in aluminum, $|\epsilon^{(1)}(\omega)|$ approaches unity. Thus, even though $\epsilon^{(2)}(\omega)$ may be small, as ω increases, the simple Lorentzian approximation to the structure of the integrand in the full expression for A_{ip} becomes less good. At 9 eV, both A_{ss} and A_{ps} remain a very small fraction of the total absorption rate.

In Fig. 8, we present the frequency dependence of the various contributions to the roughness-in-

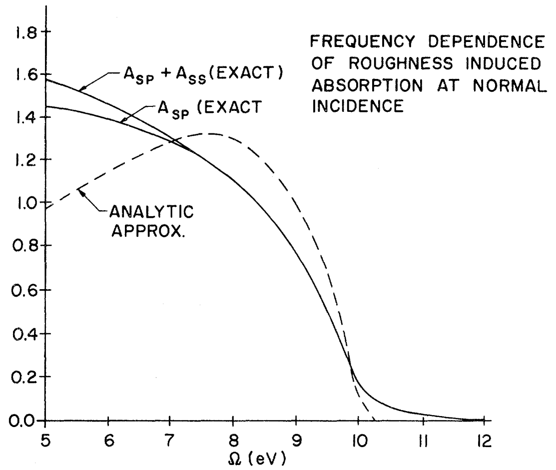

FIG. 8. Variation with frequency at normal incidence of A_{sp}, A_{ss}, and the analytic approximation to the roughness-induced-absorption cross section. The calculations have been performed for an aluminum substrate with the transverse correlation length a equal to 500 Å.

duced-absorption rate, for the case of normal incidence. The results of the numerical calculations are shown as full lines, and the analytic approximation as a dashed line. The roughness-induced-absorption rate falls off dramatically as one passes through the surface plasmon frequency at 10.6 eV, and one can see that while the analytic approximation represents the trend well, the agreement with the full calculations is semiquantitative, with discrepancies of up to 50% in the range of energies displayed in Fig. 7. Note particularly that the analytic approximation falls below the full curves below 7 eV. We ascribe this to the fact that at these lower energies, roughness-induced absorption by free-particle–hole pairs becomes a significant fraction of the total, so the picture which assigns all the absorption to roughness-induced coupling to surface polaritons underestimates the total roughness-induced absorption. In the figure, the importance of roughness-induced coupling to single-particle excitations is illustrated by the fact that A_{ss} now contributes to the absorption rate significantly, while above 7 eV it represents a very small fraction of the total.

These calculations suggest that while the simple analytic expressions in Eqs. (4.10) and (4.16) provide reasonable semiquantitative estimates of the roughness-induced-absorption rates, attempts to provide quantitative contact between theory and experiment should proceed with the use of the full expressions. In this regard, the calculations presented here should place the analytic approximations in a most favorable light, since aluminum is the metal most accurately approximated by the free-electron model.

APPENDIX

In this Appendix we outline the derivation of the elements of the Green's-function tensor $D_{\mu\nu}(\vec{x}, \vec{x}'; \omega)$, which is the solution of the equation

$$\sum_{\mu}\left(\epsilon_0(z;\omega)\frac{\omega^2}{c^2}\delta_{\lambda\mu}-\frac{\partial^2}{\partial x_\lambda\,\partial x_\mu}+\delta_{\lambda\mu}\nabla^2\right)D_{\mu\nu}(\vec{x},\vec{x}';\omega)=4\pi\delta_{\lambda\nu}\,\delta(\vec{x}-\vec{x}')\ , \tag{A1}$$

where

$$\begin{aligned}\epsilon_0(z;\omega)&=1, & z>0\\ &=\epsilon(\omega)\ , & z<0\ ,\end{aligned} \tag{A2}$$

together with boundary conditions which will be specified below.

We begin by Fourier analyzing $D_{\mu\nu}(\vec{x}, \vec{x}'; \omega)$ and $\delta(\vec{x}-\vec{x}')$ according to

$$D_{\mu\nu}(\vec{x},\vec{x}';\omega)=\int\frac{d^2k_\parallel}{(2\pi)^2}\,e^{i\vec{k}_\parallel\cdot(\vec{x}_\parallel-\vec{x}_\parallel')}\,d_{\mu\nu}(\vec{k}_\parallel\,\omega\,|\,zz')\ , \tag{A3}$$

$$\delta(\vec{x}-\vec{x}')=\delta(z-z')\int\frac{d^2k_\parallel}{(2\pi)^2}\,e^{i\vec{k}_\parallel\cdot(\vec{x}_\parallel-\vec{x}_\parallel')}\ , \tag{A4}$$

where $\vec{k}_\parallel$ and $\vec{x}_\parallel$ are two-dimensional vectors given by $(k_x, k_y, 0)$ and $(x, y, 0)$, respectively. The decomposition (A3) reflects the fact that the system for which the Green's function $D_{\mu\nu}(\vec{x}, \vec{x}'; \omega)$ is being sought retains infinitesimal translational invariance in the x and y directions, even if it has lost it in the z direction. Substitution of Eqs. (A3) and (A4) into Eq. (A1) yields the following set of differential equations for the Fourier coefficients $d_{\mu\nu}(\vec{k}_\parallel\,\omega\,|\,zz')$:

$$\begin{pmatrix}\epsilon_0\dfrac{\omega^2}{c^2}-k_y^2+\dfrac{d^2}{dz^2} & k_xk_y & -ik_x\dfrac{d}{dz}\\ k_xk_y & \epsilon_0\dfrac{\omega^2}{c^2}-k_x^2+\dfrac{d^2}{dz^2} & -ik_y\dfrac{d}{dz}\\ -ik_x\dfrac{d}{dz} & -ik_y\dfrac{d}{dz} & \epsilon_0\dfrac{\omega^2}{c^2}-k_\parallel^2\end{pmatrix}\begin{pmatrix}d_{xx} & d_{xy} & d_{xz}\\ d_{yx} & d_{yy} & d_{yz}\\ d_{zx} & d_{zy} & d_{zz}\end{pmatrix}=4\pi\delta(z-z')\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\ . \tag{A5}$$

At this point it is convenient to exploit the isotropy of our system in the xy plane by premultiplying and postmultiplying Eq. (A5) by the matrices $\vec{S}(\vec{k}_\parallel)$ and $\vec{S}^{-1}(\vec{k}_\parallel)$, respectively, where

$$\underline{S}(\vec{k}_\parallel)=\frac{1}{k_\parallel}\begin{pmatrix}k_x & k_y & 0\\ -k_y & k_x & 0\\ 0 & 0 & k_\parallel\end{pmatrix},\quad \underline{S}^{-1}(\vec{k}_\parallel)=\frac{1}{k_\parallel}\begin{pmatrix}k_x & -k_y & 0\\ k_y & k_x & 0\\ 0 & 0 & k_\parallel\end{pmatrix}\ . \tag{A6}$$

[The matrix $\underline{S}(\vec{k}_\parallel)$ is recognized as the matrix which rotates the vector $(k_x, k_y, 0)$ into the vector $(k_\parallel, 0, 0)$.] The result of this transformation is the simpler equation

$$\begin{pmatrix}\epsilon_0\frac{\omega^2}{c^2}+\frac{d^2}{dz^2} & 0 & -ik_\parallel\frac{d}{dz}\\ 0 & \epsilon_0\frac{\omega^2}{c^2}-k_\parallel^2+\frac{d^2}{dz^2} & 0\\ -ik_\parallel\frac{d}{dz} & 0 & \epsilon_0\frac{\omega^2}{c^2}-k_\parallel^2\end{pmatrix}\begin{pmatrix}g_{xx} & g_{xy} & g_{xz}\\ g_{yx} & g_{yy} & g_{yz}\\ g_{zx} & g_{zy} & g_{zz}\end{pmatrix}=4\pi\delta(z-z')\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix} \tag{A7}$$

for Fourier coefficients $g_{\mu\nu}(k_\parallel\omega\,|\,zz')$ which are related to the coefficients $d_{\mu\nu}(\vec{k}_\parallel\omega\,|\,zz')$ by

$$d_{\mu\nu}(\vec{k}_\parallel\omega\,|\,zz')=\sum_{\mu'\nu'} g_{\mu'\nu'}(k_\parallel\omega\,|\,zz')\times S_{\mu'\mu}(\vec{k}_\parallel)\,S_{\nu'\nu}(\vec{k}_\parallel)\ . \tag{A8}$$

In what follows we will obtain only the coefficients $g_{\mu\nu}(k_\parallel\omega\,|\,zz')$.

We note first from Eq. (A7) that the functions g_{yx} and g_{yz} satisfy homogeneous equations

$$\left(\epsilon_0\frac{\omega^2}{c^2}-k_\parallel^2+\frac{d^2}{dz^2}\right)g_{yx}=0\ , \tag{A9a}$$

$$\left(\epsilon_0\frac{\omega^2}{c^2}-k_\parallel^2+\frac{d^2}{dz^2}\right)g_{yz}=0\ . \tag{A9b}$$

The functions g_{xy} and g_{zy} satisfy a pair of coupled homogeneous equations

$$\left(\epsilon_0\frac{\omega^2}{c^2}+\frac{d^2}{dz^2}\right)g_{xy}-ik_\parallel\frac{d}{dz}\,g_{zy}=0\ , \tag{A10a}$$

$$-ik_\parallel\frac{d}{dz}\,g_{xy}+\left(\epsilon_0\frac{\omega^2}{c^2}-k_\parallel^2\right)g_{zy}=0\ . \tag{A10b}$$

These four functions therefore vanish. We are thus left with the following sets of equations to solve:

$$\left(\epsilon_0\frac{\omega^2}{c^2}-k_\parallel^2+\frac{d^2}{dz^2}\right)g_{yy}=4\pi\delta(z-z')\ , \tag{A11}$$

$$\left(\epsilon_0\frac{\omega^2}{c^2}+\frac{d^2}{dz^2}\right)g_{xx}-ik_\parallel\frac{d}{dz}\,g_{zx}=4\pi\delta(z-z')\ , \tag{A12a}$$

$$-ik_\parallel\frac{d}{dz}\,g_{xx}+\left(\epsilon_0\frac{\omega^2}{c^2}-k_\parallel^2\right)g_{zx}=0\ , \tag{A12b}$$

$$\left(\epsilon_0\frac{\omega^2}{c^2}+\frac{d^2}{dz^2}\right)g_{xz}-ik_\parallel\frac{d}{dz}\,g_{zz}=0\ , \tag{A13a}$$

$$-ik_\parallel\frac{d}{dz}\,g_{xz}+\left(\epsilon_0\frac{\omega^2}{c^2}-k_\parallel^2\right)g_{zz}=4\pi\delta(z-z')\ . \tag{A13b}$$

From Eqs. (A11)–(A13) we see that we can regard the Green's functions g_{xx}, g_{yy}, and g_{xz} as the primary functions to be solved for, since the remaining functions g_{zx} and g_{zz} can be obtained from g_{xx} and g_{xz}, respectively.

We must now consider the boundary conditions which supplement the differential equations (A11)–(A13). They are of two types: (i) boundary conditions at $z=\pm\infty$, and (ii) boundary conditions at the interface $z=0$. For the former we assume either outgoing waves at infinity or exponentially decaying waves at infinity, depending on the values of $k_\parallel$ and ω. To obtain the boundary conditions at the interface $z=0$ we proceed as follows.

It is straightforward to obtain from the Maxwell equations in the presence of an external current $\vec{j}^{\,\mathrm{ext}}(\vec{x},t)$, in a gauge in which the scalar potential $\varphi(\vec{x},t)$ vanishes,

$$\nabla\times\vec{H}=\frac{4\pi}{c}\,\vec{j}^{\,\mathrm{ext}}+\frac{1}{c}\,\dot{\vec{D}}\ ,$$

$$\nabla\times\vec{E}=-\frac{1}{c}\,\dot{\vec{H}}\ , \tag{A14a}$$

$$\vec{H}=\nabla\times\vec{A}\ ,\quad \vec{E}=-\frac{1}{c}\,\dot{\vec{A}}\ ,\quad \varphi=0 \tag{A14b}$$

$$\vec{B}=\vec{H}\ ,\quad \vec{D}=\epsilon_0\vec{E}\ , \tag{A14c}$$

that the vector potential $A_\alpha(\vec{x},\omega)$ is related to the external current $j_\beta^{\mathrm{ext}}(\vec{x},\omega)$ by

$$A_\alpha(\vec{x},\omega)=-\frac{1}{c}\sum_\beta\int d^3x'\,D_{\alpha\beta}(\vec{x},\vec{x}';\omega)\,j_\beta^{\mathrm{ext}}(\vec{x}',\omega)\ , \tag{A15}$$

where $D_{\alpha\beta}(\vec{x},\vec{x}';\omega)$ is the same Green's function as appears in Eq. (A1). It follows from Eqs. (A14) that the electric and magnetic fields induced by the external current are given by

$$E_\alpha(\vec{x},\omega)=-\frac{i\omega}{c^2}\sum_\beta\int d^3x'\,D_{\alpha\beta}(\vec{x},\vec{x}';\omega)\,j_\beta^{\mathrm{ext}}(\vec{x}',\omega) \tag{A16}$$

$$H_\alpha(\vec{x}, \omega) = -\frac{1}{c} \sum_{\beta\gamma\delta} \epsilon_{\alpha\beta\gamma} \frac{\partial}{\partial x_\beta} \int d^3x'\, D_{\gamma\delta}(\vec{x}, \vec{x}'; \omega) \times j_\delta^{\text{ext}}(\vec{x}', \omega) . \tag{A17}$$

The boundary conditions on $D_{\alpha\beta}(\vec{x}, \vec{x}'; \omega)$ follow from the continuity of the tangential components of $\vec{E}$ and $\vec{H}$, and the normal components of $\vec{D}$ and $\vec{H}$ across the plane $z=0$. Since $\vec{j}^{\text{ext}}(\vec{x}, \omega)$ is arbitrary, we see that the following quantities must be continuous across the plane $z=0$, for $\beta = x, y, z$:

$$D_{x\beta}(\vec{x}, \vec{x}'; \omega) , \quad D_{y\beta}(\vec{x}, \vec{x}'; \omega) ,$$
$$\sum_\gamma \epsilon_{z\gamma}(\vec{x}; \omega) D_{\gamma\beta}(\vec{x}, \vec{x}'; \omega) , \tag{A18}$$

$$\frac{\partial}{\partial y} D_{z\beta}(\vec{x}, \vec{x}'; \omega) - \frac{\partial}{\partial z} D_{y\beta}(\vec{x}, \vec{x}'; \omega) , \tag{A19a}$$

$$\frac{\partial}{\partial z} D_{x\beta}(\vec{x}, \vec{x}'; \omega) - \frac{\partial}{\partial x} D_{z\beta}(\vec{x}, \vec{x}'; \omega) , \tag{A19b}$$

$$\frac{\partial}{\partial x} D_{y\beta}(\vec{x}, \vec{x}'; \omega) - \frac{\partial}{\partial y} D_{x\beta}(\vec{x}, \vec{x}'; \omega) . \tag{A19c}$$

In writing the third of the quantities in (A18) we have assumed, for greater generality, an arbitrary position-dependent dielectric tensor $\epsilon_{\alpha\beta}(\vec{x}; \omega)$ which, however, still possesses a discontinuity across the plane $z=0$. The boundary conditions which follow from the continuity of the six quantities given by (A18) and (A19) are not all independent, however.

With the aid of Eq. (A3) we find that these boundary conditions translate into the following conditions on the Fourier coefficient $d_{\mu\nu}(\vec{k}_\parallel \omega | zz')$. The quantities

$$d_{x\beta}(\vec{k}_\parallel \omega | zz') , \quad d_{y\beta}(\vec{k}_\parallel \omega | zz') ,$$
$$\epsilon_0(z; \omega) d_{z\beta}(\vec{k}_\parallel \omega | zz') , \tag{A20a}$$

$$ik_y d_{z\beta}(\vec{k}_\parallel \omega | zz') - \frac{d}{dz} d_{y\beta}(\vec{k}_\parallel \omega | zz') , \tag{A20b}$$

$$\frac{d}{dz} d_{x\beta}(\vec{k}_\parallel \omega | zz') - ik_x d_{z\beta}(\vec{k}_\parallel \omega | zz') , \tag{A20c}$$

$$ik_x d_{y\beta}(\vec{k}_\parallel \omega | zz') - ik_y d_{x\beta}(\vec{k}_\parallel \omega | zz') \tag{A20d}$$

must be continuous across the plane $z=0$. Note that the first two conditions imply the last, which will therefore be discarded in what follows. We have also assumed a z-dependent scalar dielectric constant in writing these conditions, the situation appropriate to the problem at hand.

To obtain the boundary conditions on the functions $g_{\mu\nu}(k_\parallel \omega | zz')$ for which we are solving, we must combine the conditions (A20) with the inverse of Eq. (A8),

$$g_{\mu\nu}(k_\parallel \omega | zz') = \sum_{\mu'\nu'} S_{\mu\mu'}(\vec{k}_\parallel) S_{\nu\nu'}(\vec{k}_\parallel) d_{\mu'\nu'}(\vec{k}_\parallel \omega | zz') , \tag{A21}$$

and the differential equations (A5). For example, we have that

$$g_{xx} = \frac{1}{k_\parallel^2} (k_x^2 d_{xx} + k_x k_y d_{xy} + k_x k_y d_{yx} + k_y^2 d_{yy}) .$$

Since each term on the right-hand side is continuous across the plane $z=0$, we obtain the boundary condition

$$g_{xx}|_{0-} = g_{xx}|_{0+} . \tag{A22a}$$

In addition, we have that

$$\begin{aligned}\frac{d}{dz} g_{xx} &= \frac{k_x}{k_\parallel^2}\left(k_x \frac{d}{dz} d_{xx} + k_y \frac{d}{dz} d_{yx}\right) + \frac{k_y}{k_\parallel^2}\left(k_x \frac{d}{dz} d_{xy} + k_y \frac{d}{dz} d_{yy}\right) \\ &= \frac{ik_x}{k_\parallel^2}\left(-ik_x \frac{d}{dz} d_{xx} - ik_y \frac{d}{dz} d_{yx}\right) + i\frac{k_y}{k_\parallel^2}\left(-ik_x \frac{d}{dz} d_{xy} - ik_y \frac{d}{dz} d_{yy}\right) \\ &= \frac{i}{k_\parallel^2}\left(k_\parallel^2 - \epsilon_0(z; \omega)\frac{\omega^2}{c^2}\right)(k_x d_{zx} + k_y d_{zy}) ,\end{aligned}$$

where we have used Eq. (A5) in going from the second equation to the third. Multiplying both sides of this equation by $\epsilon_0(z; \omega)[k_\parallel^2 - \epsilon_0(z; \omega)(\omega^2/c^2)]^{-1}$ we obtain

$$\frac{\epsilon_0(z; \omega)}{k_\parallel^2 - \epsilon_0(z; \omega)(\omega^2/c^2)} \frac{d}{dz} g_{xx} = \frac{i}{k_\parallel^2}[k_x \epsilon_0(z; \omega) d_{zx} + k_y \epsilon_0(z; \omega) d_{zy}] .$$

According to (A20a), the right-hand side of this equation is continuous across the plane $z=0$. Thus we obtain the second boundary condition

$$\frac{\epsilon_0}{k_\parallel^2 - \epsilon_0 \omega^2/c^2} \frac{d}{dz} g_{xx}\Big|_{0-} = \frac{\epsilon_0}{k_\parallel^2 - \epsilon_0 \omega^2/c^2} \frac{d}{dz} g_{xx}\Big|_{0+} . \tag{A22b}$$

In the same way we obtain the remaining boundary conditions

$$g_{yy}|_{0-} = g_{yy}|_{0+} , \tag{A22c}$$

$$\frac{d}{dz} g_{yy}\Big|_{0-} = \frac{d}{dz} g_{yy}\Big|_{0+} , \tag{A22d}$$

$$g_{xz}|_{0-} = g_{xz}|_{0+} , \tag{A22e}$$

$$\frac{\epsilon_0}{k_\parallel^2 - \epsilon_0 \omega^2/c^2} \frac{d}{dz} g_{xz}\Big|_{0-} = \frac{\epsilon_0}{k_\parallel^2 - \epsilon_0 \omega^2/c^2} \frac{d}{dz} g_{xz}\Big|_{0+} . \tag{A22f}$$

Equations (A22) constitute the boundary conditions at the plane $z=0$ on the primary Green's functions g_{xx}, g_{yy}, and g_{xz}.

In solving the differential equations (A11)–(A13) the following two results are useful for obtaining the particular integrals:

$$\left(\frac{d^2}{dz^2} + \alpha^2\right)\frac{e^{i\alpha|z-z'|}}{2i\alpha} = \delta(z - z') , \tag{A23a}$$

$$\left(\frac{d^2}{dz^2}+\alpha^2\right)\tfrac{1}{2}e^{i\alpha|z-z'|}\operatorname{sgn}(z-z')=\frac{d}{dz}\,\delta(z-z')\ . \tag{A23b}$$

We illustrate the determination of the $g_{\mu\nu}(k_\parallel\,\omega\,|\,zz')$ by working out $g_{xz}(k_\parallel\,\omega\,|\,zz')$. We assume first that $z'<0$. On combining Eqs. (A13a) and (A13b), and recalling Eq. (A2), we find that the equations satisfied by this function are

$$\left(\frac{d^2}{dz^2}+k^2\right)g_{xz}=0\ ,\quad z>0 \tag{A24a}$$

$$\left(\frac{d^2}{dz^2}+k_1^2\right)g_{xz}=ik_\parallel\,\frac{4\pi c^2}{\epsilon(\omega)\,\omega^2}\,\frac{d}{dz}\,\delta(z-z')\ ,\quad z<0 \tag{A24b}$$

where we have introduced the functions

$$k=\begin{cases}\left(\dfrac{\omega^2}{c^2}-k_\parallel^2\right)^{1/2}, & \dfrac{\omega^2}{c^2}>k_\parallel^2\\[2ex] i\left(k_\parallel^2-\dfrac{\omega^2}{c^2}\right)^{1/2}, & \dfrac{\omega^2}{c^2}<k_\parallel^2\end{cases} \tag{A25}$$

$$k_1^2=-\left(\epsilon(\omega)\,\frac{\omega^2}{c^2}-k_\parallel^2\right)^{1/2}. \tag{A26}$$

The choice of the sign in Eq. (A26), together with the fact that $\operatorname{Im}\epsilon(\omega)>0$, ensures that $\operatorname{Im}k_1<0$.

The solutions of Eqs. (A24) can be written in the forms

$$g_{xz}=\begin{cases}Ae^{ikz}\ , & z>0\\[1ex] ik_\parallel\,\dfrac{2\pi c^2}{\epsilon(\omega)\omega^2}\,e^{-ik_1|z-z'|}\operatorname{sgn}(z-z')+Be^{ik_1z}\ , & z<0\ ,\end{cases}$$

which, in view of Eqs. (A25) and (A26), satisfy the boundary conditions at infinity. We now apply the boundary conditions (A22e) and (A22f) to obtain the following equations for the coefficients A and B,

$$A=B+2\pi i\,\frac{k_\parallel c^2}{\epsilon(\omega)\omega^2}\,e^{ik_1z'}\ ,$$

$$\frac{k_1A}{k\epsilon(\omega)}=B-2\pi i\,\frac{k_\parallel c^2}{\epsilon(\omega)\omega^2}\,e^{ik_1z'}\ .$$

In obtaining the second equation we have assumed that $z'\neq 0$. We thus find that

$$A=-\frac{4\pi ik_\parallel c^2}{\omega^2}\,\frac{k}{k_1-\epsilon(\omega)k}\,e^{ik_1z'}\ ,$$

$$B=-\frac{2\pi ik_\parallel c^2}{\epsilon(\omega)\omega^2}\,\frac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik_1z'}\ ,$$

from whence it follows that

$$g_{xz}(k_\parallel\,\omega\,|\,zz')=\begin{cases}-\dfrac{4\pi ik_\parallel c^2}{\omega^2}\,\dfrac{k}{k_1-\epsilon(\omega)k}\,e^{ikz+ik_1z'}\ , & z>0\ ,\quad z'<0\\[2ex] -\dfrac{2\pi ik_\parallel c^2}{\epsilon(\omega)\,\omega^2}\left(\dfrac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik_1(z+z')}-e^{-ik_1|z-z'|}\operatorname{sgn}(z-z')\right)\ , & z<0\ ,\quad z'<0\ .\end{cases}$$

When $z'>0$, the equations obeyed by $g_{xz}(k_\parallel\,\omega\,|\,zz')$ become

$$\left(\frac{d^2}{dz^2}+k^2\right)g_{xz}=\frac{4\pi ik_\parallel c^2}{\omega^2}\,\frac{d}{dz}\,\delta(z-z'),\quad z>0$$

$$\left(\frac{d^2}{dz^2}+k_1^2\right)g_{xz}=0\ ,\quad z<0\ .$$

The solutions satisfying the boundary conditions are

$$g_{xz}(k_\parallel\,\omega\,|\,zz')=\begin{cases}-\dfrac{2\pi ik_\parallel c^2}{\omega^2}\left(\dfrac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik(z+z')}-e^{ik|z-z'|}\operatorname{sgn}(z-z')\right)\ , & z>0\ ,\quad z'>0\\[2ex] -\dfrac{4\pi ik_\parallel c^2}{\omega^2}\,\dfrac{k_1}{k_1-\epsilon(\omega)k}\,e^{ik_1z+ikz'}\ , & z<0\ ,\quad z'>0\ .\end{cases}$$

All of the remaining Green's functions can be obtained in the same way. The results of these calculations are summarized below.

$$\begin{aligned}g_{yy}(k_\parallel\,\omega\,|\,zz')&=\frac{4\pi i}{k_1-k}\,e^{ikz+ik_1z'}\ , && z>0\ ,\quad z'<0\\ &=\frac{2\pi i}{k_1}\left(\frac{k_1+k}{k_1-k}\,e^{ik_1(z+z')}+e^{-ik_1|z-z'|}\right), && z<0\ ,\quad z'<0\\ &=\frac{2\pi i}{k}\left(\frac{k_1+k}{k_1-k}\,e^{ik(z+z')}-e^{ik|z-z'|}\right), && z>0\ ,\quad z'>0\\ &=\frac{4\pi i}{k_1-k}\,e^{ik_1z+ikz'}\ , && z<0\ ,\quad z'>0\end{aligned}$$

$$g_{xz}(k_\parallel\,\omega|\,zz') = -\frac{4\pi i k_\parallel c^2}{\omega^2}\,\frac{k}{k_1-\epsilon(\omega)k}\,e^{ikz+ik_1z'}\,, \qquad z>0\,,\quad z'<0$$

$$= -\frac{2\pi i k_\parallel c^2}{\epsilon(\omega)\omega^2}\left(\frac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik_1(z+z')} - e^{-ik_1|z-z'|}\,\mathrm{sgn}(z-z')\right), \qquad z<0\,,\quad z'<0$$

$$= -\frac{2\pi i k_\parallel c^2}{\omega^2}\left(\frac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik(z+z')} - e^{ik|z-z'|}\,\mathrm{sgn}(z-z')\right), \qquad z>0\,,\quad z'>0$$

$$= -\frac{4\pi i k_\parallel c^2}{\omega^2}\,\frac{k_1}{k_1-\epsilon(\omega)k}\,e^{ik_1z+ikz'}\,, \qquad z<0\,,\quad z'>0$$

$$g_{zz}(k_\parallel\,\omega|\,zz') = \frac{4\pi i k_\parallel^2 c^2}{\omega^2}\,\frac{1}{k_1-\epsilon(\omega)k}\,e^{ikz+ik_1z'}\,, \qquad z>0\,,\quad z'<0$$

$$= \frac{2\pi i k_\parallel^2 c^2}{k_1\epsilon(\omega)\omega^2}\left(\frac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik_1(z+z')} + e^{-ik_1|z-z'|}\right) + \frac{4\pi c^2}{\epsilon(\omega)\omega^2}\,\delta(z-z')\,, \qquad z<0\,,\quad z'<0$$

$$= \frac{2\pi i k_\parallel^2 c^2}{k\omega^2}\left(\frac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik(z+z')} - e^{ik|z-z'|}\right) + \frac{4\pi c^2}{\omega^2}\,\delta(z-z')\,, \qquad z>0\,,\quad z'>0$$

$$= \frac{4\pi i k_\parallel^2 c^2}{\omega^2}\,\frac{1}{k_1-\epsilon(\omega)k}\,e^{ik_1z+ikz'}\,, \qquad z<0\,,\quad z'>0$$

$$g_{xx}(k_\parallel\,\omega|\,zz') = -\frac{4\pi i c^2}{\omega^2}\,\frac{kk_1}{k_1-\epsilon(\omega)k}\,e^{ikz+ik_1z'}\,, \qquad z>0\,,\quad z'<0$$

$$= -\frac{2\pi i k_1 c^2}{\epsilon(\omega)\omega^2}\left(\frac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik_1(z+z')} - e^{-ik_1|z-z'|}\right), \qquad z<0\,,\quad z'<0$$

$$= -\frac{2\pi i k c^2}{\omega^2}\left(\frac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik(z+z')} + e^{ik|z-z'|}\right), \qquad z>0\,,\quad z'>0$$

$$= -\frac{4\pi i k c^2}{\omega^2}\,\frac{k_1}{k_1-\epsilon(\omega)k}\,e^{ik_1z+ikz'}\,, \qquad z<0\,,\quad z'>0$$

$$g_{zx}(k_\parallel\,\omega|\,zz') = \frac{4\pi i k_\parallel c^2}{\omega^2}\,\frac{k_1}{k_1-\epsilon(\omega)k}\,e^{ikz+ik_1z'}\,, \qquad z>0,\quad z'<0$$

$$= \frac{2\pi i k_\parallel c^2}{\epsilon(\omega)\omega^2}\left(\frac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik_1(z+z')} + e^{-ik_1|z-z'|}\,\mathrm{sgn}(z-z')\right), \qquad z<0\,,\quad z'<0$$

$$= \frac{2\pi i k_\parallel c^2}{\omega^2}\left(\frac{k_1+\epsilon(\omega)k}{k_1-\epsilon(\omega)k}\,e^{ik(z+z')} + e^{ik|z-z'|}\,\mathrm{sgn}(z-z')\right), \qquad z>0\,,\quad z'>0$$

$$= \frac{4\pi i k_\parallel c^2}{\omega^2}\,\frac{k}{k_1-\epsilon(\omega)k}\,e^{ik_1z+ikz'}\,, \qquad z<0\,,\quad z'>0\,.$$

We conclude the Appendix by pointing out that in addition to the uses to which they are put in the present paper, the Green's functions $D_{\mu\nu}(\vec{x},\vec{x}';\omega)$, whose Fourier coefficients $g_{\mu\nu}(k_\parallel\,\omega\,|zz')$ have been presented here, also arise in the evaluation of thermodynamic and double-time Green's functions, and correlation functions of the electromagnetic fields in the layered medium for which the present calculations have been carried out.[16]

For example, we consider the retarded Green's function

$$D^R_{\alpha\beta}(\vec{x}_1,\vec{x}_2;t_1-t_2) = -i\Theta(t_1-t_2) \times\langle[A_\alpha(\vec{x}_1 t_1),\ A_\beta(\vec{x}_2 t_2)]\rangle\,, \tag{A27}$$

where $\vec{A}(\vec{x},t)$ is now the operator of the vector potential in the Heisenberg representation, and the angular brackets denote an average with respect to the canonical ensemble described by the Hamiltonian of the electromagnetic field. The Fourier transform of this Green's function can be written in the form

$$D^R_{\alpha\beta}(\vec{x}_1,\vec{x}_2;\omega) = \int_{-\infty}^{\infty} d(t_1-t_2)\,e^{i\omega(t_1-t_2)} \times D^R_{\alpha\beta}(\vec{x}_1,\vec{x}_2;t_1-t_2) = -\int_{-\infty}^{\infty} dx\,(1-e^{-\beta\hbar x})\,\frac{\rho_{\alpha\beta}(\vec{x}_1,\vec{x}_2;x)}{x-\omega-i\delta}\,, \tag{A28}$$

where the spectral density $\rho_{\alpha\beta}(\vec{x}_1,\vec{x}_2;x)$ is given by

$$\rho_{\alpha\beta}(\vec{x}_1, \vec{x}_2; x) = \sum_{mn} \frac{e^{-\beta E_m}}{Z} \langle m|A_\alpha(\vec{x}_1)|n\rangle \times \langle n|A_\beta(\vec{x}_2)|m\rangle\, \delta\left(x - \frac{1}{\hbar}(E_n - E_m)\right) \quad (A29)$$

in terms of the eigenfunctions $|n\rangle$ and eigenvalues E_n of the system Hamiltonian; Z is the partition function. We can express the Fourier transforms of several useful correlation functions in terms of $\rho_{\alpha\beta}(\vec{x}_1, \vec{x}_2; x)$. For example, we have that

$$\int_{-\infty}^{\infty} d(t_1 - t_2)\, e^{i\omega(t_1 - t_2)} \langle A_\alpha(\vec{x}_1 t_1) A_\beta(\vec{x}_2 t_2)\rangle = 2\pi\rho_{\alpha\beta}(\vec{x}_1, \vec{x}_2; \omega), \quad (A30)$$

$$\int_{-\infty}^{\infty} d(t_1 - t_2)\, e^{i\omega(t_1 - t_2)} \langle E_\alpha(\vec{x}_1 t_1) E_\beta(\vec{x}_2 t_2)\rangle = 2\pi(\omega^2/c^2)\rho_{\alpha\beta}(\vec{x}_1, \vec{x}_2; \omega). \quad (A31)$$

The spectral density $\rho_{\alpha\beta}(\vec{x}_1, \vec{x}_2; \omega)$ can be obtained in a standard fashion.[17] We introduce a function of the complex variable z by

$$\hat{D}_{\alpha\beta}(\vec{x}_1, \vec{x}_2; z) = -\int_{-\infty}^{\infty} dx\,(1 - e^{-\beta\hbar x}) \frac{\rho_{\alpha\beta}(\vec{x}_1, \vec{x}_2; x)}{x - z}, \quad (A32)$$

which coincides with $D^R_{\alpha\beta}(\vec{x}_1, \vec{x}_2; \omega)$ for $\mathrm{Im}\, z > 0$. [For $\mathrm{Im}\, z < 0$ $\hat{D}_{\alpha\beta}(\vec{x}_1, \vec{x}_2; z)$ coincides with the Fourier transform of the advanced Green's function.] Then we have that

$$\rho_{\alpha\beta}(\vec{x}_1; \vec{x}_2; \omega) = \frac{i}{2\pi} \frac{1}{1 - e^{-\beta\hbar\omega}} \times [\hat{D}_{\alpha\beta}(\vec{x}_1, \vec{x}_2; \omega + i0) - \hat{D}_{\alpha\beta}(\vec{x}_1, \vec{x}_2; \omega - i0)]. \quad (A33)$$

The importance of the Green's functions $D_{\alpha\beta}(\vec{x}_1, \vec{x}_2; \omega)$ studied in this Appendix for such calculations lies in the fact that Dzyaloshinski and Pitayevski[18] have established the relation

$$D^R_{\alpha\beta}(\vec{x}, \vec{x}'; \omega) = \hbar D_{\alpha\beta}(\vec{x}, \vec{x}'; \omega), \quad (A34)$$

from which $\hat{D}_{\alpha\beta}(\vec{x}, \vec{x}'; z)$ can be obtained, and hence the spectral density $\rho_{\alpha\beta}(\vec{x}, \vec{x}'; \omega)$ and other useful correlation functions.

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