Diffraction of electromagnetic waves by irregular interfaces in stratified, uniaxial anisotropic media

G. V. Rozhnov

Oplot Research Enterprise, 111402 Moscow, Russia
(Submitted 24 May 1993)
Zh. Eksp. Teor. Fiz. **104**, 3584–3602 (November 1993)

To quadratic accuracy in the amplitudes of both random and deterministic irregularities on rough surfaces, we obtain closed-form analytic expressions for the transmission and reflection coefficients, the dispersion relation, and the angular spectrum of diffracted *s*- and *p*-polarized electromagnetic waves in an arbitrary multilayer, uniaxial, stratified anisotropic medium.

1. INTRODUCTION

The scattering of electromagnetic waves from an irregular interface is one of the classic problems of physics.[1] Nevertheless, exact analytic solutions for a marginally rough surface (enabling one to calculate transmission and reflection coefficients and the dispersion relation for the eigenmodes of the medium) have only been obtained relatively recently, and then only for various special cases, such as a homogeneous[2–4] or stratified[5–7] half-space containing just a single rough boundary, and a three-layer medium (a thin film on a substrate) with two irregular interfaces.[8] For multilayer media containing an arbitrary number of rough boundaries, we presently have closed-form analytic expressions only for the angular spectrum of diffracted waves.[9,10] The calculation of transmission and reflection coefficients and the dispersion relation for such media remains an unsolved problem.

Typical approaches to this sort of problem, such as field matching at a boundary,[2] the effective boundary condition method,[3] and Green's function techniques,[4] lead either to an unwieldy set of self-consistent equations[3] (even in the simplest case, with just one irregular boundary), or they yield results inapplicable to the resonant eigenmodes of the medium.[2,4] Various methods have been used in attempting to broaden the applicability of these results. These have included, for example, artificially introducing a temporary surface impedance,[11] which however is not a logical outgrowth of the adopted solution method. Diagrammatic techniques[1,12–14] have been used to sum perturbation expansions, functional integration[15] has been used, and attempts have been made to find a self-consistent solution[16] of a simplified set of equations for the strongly-coupled eigenmodes of the medium. All of these methods, however, have either been specifically geared to strongly-reflecting metallic media, or they have been far too complex, and therefore difficult to generalize to multilayer media.

Solutions in the neighborhood of eigenmodes are of immediate practical interest as they relate to the analysis of strong electromagnetic resonance effects such as surface-enhanced Raman scattering,[17] anomalous suppression of the specular component,[18] second-harmonic generation,[19] etc., and also with regard to wave localization on a rough surface.[20] The eigenmode spectrum of a multilayer medium is much richer and more complex than that of a simple semi-infinite metallic medium, and such media are widely useful in numerous areas of physics. It would therefore be highly desirable to develop a universally applicable solution method that is suited not only to strongly reflecting metallic media, but to others as well.

In the present paper we employ Green's functions to reduce this problem to the solution of the standard equations of quantum scattering theory in the general case of an arbitrary multilayer stratified medium. To quadratic accuracy in the amplitudes of the surface irregularities, we use a simple iterative procedure—with no need to solve a highly involved set of self-consistent equations and without summing the terms of a perturbation expansion—to derive a widely applicable set of closed-form analytic expressions for the (amplitude) transmission and reflection coefficients of polarized electromagnetic waves. The poles of those coefficients yield the dispersion relation for the eigenmodes of the perturbed medium. We also present expressions for the angular spectrum of the diffracted waves.

The paper is organized as follows. In Sec. 2 we describe a multilayer medium and introduce the basic notation. In Sec. 3 we state the problem of calculating the total field of a diffracted wave in general terms, and in Sec. 4 we state the problem for the coherent component of the field. In Sec. 5 we solve the problem to second order in the amplitudes of the random irregular boundaries; section 6 summarizes the results. Section 7 discusses periodic irregular boundaries, and Sec. 8 examines the results obtained. Certain of the intermediate equations are derived in the Appendix.

2. DESCRIPTION OF THE MEDIUM. NOTATION

We work here in the context of macroscopic electrodynamics. A stratified, uniaxial anisotropic medium (Fig. 1) made up of $N=n-1$ rough interfaces with $z=h_j(\boldsymbol{\rho})$, $j=1, 2, \ldots, N$, where $\boldsymbol{\rho}=(x,y)$ is a two-dimensional vector lying in a plane at constant z, can be characterized by its dielectric constant

 1063-7761/93/110709-10$10.00

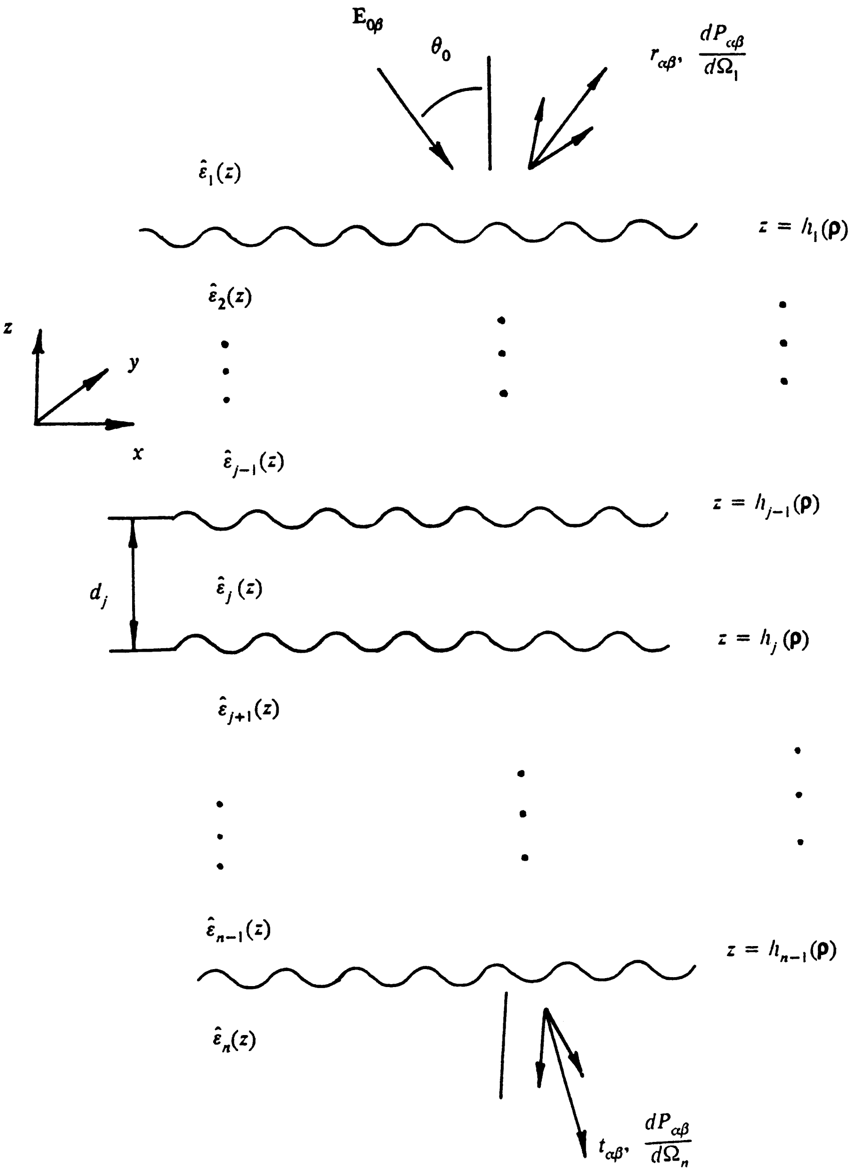

FIG. 1.

$$\hat{\varepsilon}(\mathbf{r})=\hat{\varepsilon}_1(z)+\sum_{j=1}^{N}[\hat{\varepsilon}_{j+1}(z)-\hat{\varepsilon}_j(z)]\theta[h_j(\rho)-z]$$
$$\equiv\varepsilon_{\perp}(\mathbf{r})\hat{P}_{\perp}+\varepsilon_{\parallel}(\mathbf{r})\hat{P}_{\parallel}, \qquad (1)$$

where $\theta(z)$ is the Heaviside step function, and where $\hat{P}_{\parallel}=\hat{\mathbf{z}}\hat{\mathbf{z}}$ and $\hat{P}_{\perp}=1-\hat{P}_{\parallel}$ are projection operators in the direction of the normal $\hat{\mathbf{z}}$ and the plane $z=\text{const}$, respectively. We employ dyadic notation in the present paper for second-rank tensors. We assume that the magnetic susceptibility of the medium is unity. The dielectric constant of each of the successive media,

$$\hat{\varepsilon}_j(z)=\varepsilon_{j\perp}(z)\hat{P}_{\perp}+\varepsilon_{j\parallel}(z)\hat{P}_{\parallel}$$

is arbitrary, with $\operatorname{Re}\hat{\varepsilon}_j(z)\gtrless 0$ and $\operatorname{Im}\hat{\varepsilon}_j(z)\geqslant 0$, the only constraint being that the longitudinal and transverse components of the dielectric constant of the first and last media, $\varepsilon_{j\parallel}(z)$ and $\varepsilon_{j\perp}(z)$, $j=1$, n, are asymptotically equal as $|z|\to\infty$, taking values $\varepsilon_{1\perp}(z)=\varepsilon_{1\parallel}(z)=\varepsilon_1$ as $z\to+\infty$ and $\varepsilon_{n\perp}(z)=\varepsilon_{n\parallel}(z)=\varepsilon_n$ as $z\to-\infty$. This constraint is of no fundamental importance, serving merely to simplify notation in the asymptotic expansion of the fields (see Eq. (18) below).

In the zeroth-order (smooth boundary) approximation, the properties of each medium derive from its dielectric constant,

$$\hat{\varepsilon}_z^0=\hat{\varepsilon}_1(z)+\sum_{j=1}^{N}[\hat{\varepsilon}_{j+1}(z)-\hat{\varepsilon}_j(z)]\theta[\bar{h}_j-z]$$
$$\equiv\varepsilon_{\perp}^0(z)\hat{P}_{\perp}+\varepsilon_{\parallel}^0(z)\hat{P}_{\parallel}, \qquad (2)$$

where $\bar{h}_j=\langle h_j(\rho)\rangle$ is the mean height of the jth boundary, and angular brackets denote an ensemble average over the rough surfaces. The difference in dielectric constant between adjacent layers is

$$\Delta\varepsilon_{j\perp}(z)=\varepsilon_{j\perp}(z)-\varepsilon_{j+1,\perp}(z),$$

$$\Delta\varepsilon_{j\parallel}^{-1}(z)=\varepsilon_{j+1,\parallel}^{-1}(z)-\varepsilon_{j\parallel}^{-1}(z),$$

and the discontinuity in the dielectric and its first derivative with respect to z at the jth boundary is given by

$$(\Delta\varepsilon_\perp)_j=\Delta\varepsilon_{j\perp}(\bar h_j),\quad (\Delta\varepsilon_\parallel^{-1})_j=\Delta\varepsilon_{j\parallel}^{-1}(\bar h_j),$$

$$(\Delta\varepsilon_\perp)_j'=\frac{d}{dz}\Delta\varepsilon_{j\perp}(z)\Big|_{z=\bar h_j},$$

$$(\Delta\varepsilon_\parallel^{-1})_j'=\frac{d}{dz}\Delta\varepsilon_{j\parallel}^{-1}(z)\Big|_{z=\bar h_j}.$$

The statistical characteristics of the rough boundaries are specified by F_j and F_{ij}, the one- and two-dimensional height distribution functions:

$$F_j(z)=\langle\theta[z-h_j(\boldsymbol\rho)]\rangle,$$
$$F_{ij}(\boldsymbol\rho-\boldsymbol\rho',z,z')=\langle\theta[z-h_j(\boldsymbol\rho)]\theta[z'-h_j(\boldsymbol\rho')]\rangle. \qquad (3)$$

On average, the rough boundaries are assumed to be uniform, so $F_j(z)$ is independent of $\boldsymbol\rho$ and F_{ij} depends solely on $\boldsymbol\rho-\boldsymbol\rho'$. Below, in addition to the functions in (3), we make use of

$$\bar\lambda_j(z)=F_j(z)-\theta(z-\bar h_j),$$
$$\Phi_{ij}(\boldsymbol\rho-\boldsymbol\rho',z,z')=F_{ij}(\boldsymbol\rho-\boldsymbol\rho',z,z')-F_i(z)F_j(z'), \qquad (4)$$

whose domain is restricted to the layer given by $|z-\bar h_i|\lesssim\delta_i$, $|z'-\bar h_j|\lesssim\delta_j$, where $\delta_j=\langle(h_j(\boldsymbol\rho)-\bar h_j)^2\rangle^{1/2}$ is the rms amplitude of variations in the jth rough surface. We also have

$$\int_{-\infty}^{\infty}(z-\bar h_j)^{n-1}\bar\lambda_j(z)dz=-\frac{1}{n}\langle[h_j(\boldsymbol\rho)-\bar h_j]^n\rangle, \qquad (5)$$

$$\int_{-\infty}^{\infty}\Phi_{ij}(\boldsymbol\rho-\boldsymbol\rho',z,z')dzdz'=K_{ij}(\boldsymbol\rho-\boldsymbol\rho'), \qquad (6)$$

$$\int_{-\infty}^{\infty}\operatorname{sign}(z-z')\Phi_{jj}(\boldsymbol\rho-\boldsymbol\rho',z,z')dzdz'=0, \qquad (7)$$

where

$$K_{ij}(\boldsymbol\rho-\boldsymbol\rho')=\langle[h_i(\boldsymbol\rho)-\bar h_i][h_j(\boldsymbol\rho')-\bar h_j]\rangle$$

are correlation functions, whose Fourier transform with respect to $\boldsymbol\rho-\boldsymbol\rho'$ yields the spectral densities $S_{ij}(\mathbf q)$.

No constraints whatever are imposed on the degree to which the rough surfaces $i,j=1, 2, ..., N$ are correlated. When we derive our final results (see Sec. 6), we will assume that the roughness $\delta=\max(\delta_j)$ is small compared to the thickness $d_j=\bar h_j-\bar h_{j+1}$ of the individual layers and the reciprocal of the normal component of the wave vector in each medium j,

$$\eta_{js}(z)=[k_0^2\varepsilon_{j\perp}(z)-\mathbf b^2]^{1/2},$$

$$\eta_{jp}(z)=\left[\varepsilon_{j\perp}(z)\left(k_0^2-\frac{\mathbf b^2}{\varepsilon_{j\parallel}(z)}\right)\right]^{1/2},$$

where $k_0=\omega/c$ is the vacuum wave number and $\mathbf b$ is the projection of the wave vector in the plane $z=$const. The second of these two conditions states that surface irregularities are small compared to the characteristic scale length of field variations in the adjacent media. As $z\to\infty(-\infty)$

$$\eta_{js}=\eta_{jp}\equiv\eta_j=(k_j^2-\mathbf b^2)^{1/2},$$

in the bounding media $j=1(n)$, and we choose the sign of the square root for which $\mathrm{Re}(\mathrm{Im})\eta_j\geqslant0$; $k_j=k_0\varepsilon_j^{1/2}$ is the wave number in medium $j=1, n$.

3. GENERAL FORMULATION. BASIC RELATIONS

A monochromatic electromagnetic wave $\mathbf E(\mathbf r)\exp(-i\omega t)$ will propagate in the medium specified by (1) in accordance with the equations of macroscopic electrodynamics, such that

$$[\text{curl curl}-k_0^2\hat\varepsilon(\mathbf r)]\mathbf E(\mathbf r)=0. \qquad (8)$$

This equation normally reduces to an equation[21] for the scattering operator $\hat T$

$$\hat T=k_0^2\Delta\hat\varepsilon(1+\hat G\hat T) \qquad (9)$$

(for integral equations, we adopt a symbolic operator notation throughout), where $\Delta\hat\varepsilon(\mathbf r)=\hat\varepsilon(\mathbf r)-\hat\varepsilon_z$ is the perturbation, $\hat G$ is the Green's function, for which

$$(\text{curl curl}-k_0^2\hat\varepsilon_z)\hat G=\hat 1\delta(\mathbf r-\mathbf r'), \qquad (10)$$

and which also satisfies the radiation condition at infinity, and

$$\hat\varepsilon_z=\varepsilon_\perp(z)\hat P_\perp+\varepsilon_\parallel(z)\hat P_\parallel \qquad (11)$$

is the dielectric constant of a particular medium. The latter can be chosen arbitrarily, but the resultant perturbation $\Delta\hat\varepsilon(\mathbf r)$ must be localized within a neighborhood $|z-\bar h_j|\lesssim\delta_j$ of the rough boundary $j=1, 2, ..., N$. The dielectric constants $\varepsilon_{\perp,\parallel}(\mathbf r)$ and $\varepsilon_{\perp,\parallel}(z)$ in Eqs. (1) and (11), respectively, are different: their arguments conform to the notational convention adopted in the physics literature that distinguishes between a function and its Fourier transform, for example.

For arbitrary $\hat\varepsilon_z$, the Green's function $\hat G$ is built up from basis functions $\mathbf E_{m\alpha}^{+}$ that are the solutions of the equation

$$(\text{curl curl}-k_0^2\hat\varepsilon_z^0)\mathbf E_{m\alpha}^{+}=k_0^2(\hat\varepsilon_z-\hat\varepsilon_z^0)\mathbf E_{m\alpha}^{+}, \qquad (12)$$

the subscript $m=1, n$ identifies here the medium at which the incident wave is specified, and $\alpha=s, p$ gives its polarization state.[10]

The solution of Eq. (8) can be expressed in terms of the general solution $\mathbf E_0$ of Eq. (12):

$$\mathbf E=(1+\hat G\hat T)\mathbf E_0. \qquad (13)$$

The Green's function $\hat G(\mathbf r,\mathbf r')$ contains a singular term $\sim\delta(\mathbf r-\mathbf r')$, while the basis functions $\mathbf E_{m\alpha}^{+}$ that make it up are discontinuous at the interfaces between media. These two circumstances are interrelated, and can be disposed of by transforming[22] to basis functions that are continuous at the boundaries,

$$X^{+}_{m\alpha}=\hat{\mathscr{P}}\mathbf{E}^{+}_{m\alpha},$$

$$\hat{\mathscr{P}}=\hat{P}_{\perp}+\varepsilon_{\parallel}(z)\hat{P}_{\parallel}.$$

We then obtain in place of (9) an equivalent equation for the scattering operator $\hat{t}=\hat{\mathscr{P}}^{-1}\hat{T}\hat{\mathscr{P}}^{-1}$,

$$\hat{t}=k_0^2\hat{v}(1+\hat{G}_0\hat{t}), \tag{14}$$

in which the Green's function $\hat{G}_0=\hat{\mathscr{P}}\hat{G}'\hat{\mathscr{P}}$ contains no singular terms and whose basis is continuous at the function boundaries; $\hat{G}'$ is the regular part of the Green's function $\hat{G}$,

$$\hat{G}_0(\mathbf{b},z,z')=\frac{i}{2\eta_1}\sum_{\alpha=s,p}t_\alpha(\delta)[\mathbf{X}^{+}_{n\alpha}(\mathbf{b},z)\mathbf{X}^{-}_{1\alpha}(\mathbf{b},z')\theta(z-z')+\mathbf{X}^{+}_{1\alpha}(\mathbf{b},z)\mathbf{X}^{-}_{n\alpha}(\mathbf{b},z')\theta(z'-z)], \tag{15}$$

where

$$\mathbf{X}^{-}_{ms}=\mathbf{X}^{+}_{ms},\quad \mathbf{X}^{\pm}_{mp}=\mathbf{D}_{mz}\pm\mathbf{E}_{mb},\quad \mathbf{D}_{mz}=\varepsilon_{\parallel}(z)\mathbf{E}_{mz},$$

$t_\alpha(\delta)$ is the (amplitude) transmission coefficient of the medium $\hat{\varepsilon}_z$ for a wave incident from above ($z\to\infty$) [see Eq. (27)]. Since in general $\hat{\varepsilon}_z$ depends on the parameters of a rough surface, as do the solution of Eq. (12), the basis functions $\mathbf{X}^{\pm}_{m\alpha}$, and the transmission coefficients $t_\alpha(\delta)$. This is made explicit by the argument δ in the coefficients $t_\alpha(\delta)$. Similarly, $\mathbf{E}^{\pm}_{m\alpha}$ and $\mathbf{X}^{\pm}_{m\alpha}$ also depend on δ, but to keep the notation simple we will not show that dependence explicitly.

The new perturbation $\hat{v}(\mathbf{r})$ is then given by

$$\hat{v}(\mathbf{r})=\Delta\varepsilon_{\perp}(\mathbf{r})\hat{P}_{\perp}+\Delta\varepsilon_{\parallel}^{-1}(\mathbf{r})\hat{P}_{\parallel},$$

$$\Delta\varepsilon_{\perp}(\mathbf{r})=\varepsilon_{\perp}(\mathbf{r})-\varepsilon_{\perp}(z), \tag{16}$$

$$\Delta\varepsilon_{\parallel}^{-1}(\mathbf{r})=\varepsilon_{\parallel}^{-1}(z)-\varepsilon_{\parallel}^{-1}(\mathbf{r}).$$

The matrix elements $\mathbf{E}^{lm}_{\alpha\beta}$ of the operator $\hat{t}$,

$$E^{lm}_{\alpha\beta}(\mathbf{b},\mathbf{b}_0)=\frac{it_\alpha(\delta)t_{\beta_0}(\delta)}{2\eta_1}\times\int dzdz'\mathbf{X}^{-}_{l\alpha}(\mathbf{b},z)\hat{t}(\mathbf{b},\mathbf{b}_0,z,z')\mathbf{X}^{+}_{m\beta}(\mathbf{b}_0,z'), \tag{17}$$

determine the coefficients of the asymptotic expansion of the total diffracted field (13) as $|z|\to\infty$ in the bounding media:

$$\mathbf{E}(\mathbf{r})=\exp(i\mathbf{b}_0\boldsymbol{\rho})[\exp(-i\eta_{10}z)\hat{\mathbf{e}}^{+}_{1\beta0}+r_{\beta0}(\delta)\exp(i\eta_{10}z)\hat{\mathbf{e}}^{-}_{1\beta0}]+\sum_{\alpha=s,p}\int d^2\mathbf{b}\exp[i(\mathbf{b}\boldsymbol{\rho}+\eta_1z)]\hat{\mathbf{e}}^{-}_{1\alpha}E^{11}_{\alpha\beta}(\mathbf{b},\mathbf{b}_0),$$

$$z\to+\infty,$$

$$\mathbf{E}(\mathbf{r})=\exp[i(\mathbf{b}_0\boldsymbol{\rho}-\eta_{n0}z)]\hat{\mathbf{e}}^{+}_{n\beta0}t_{\beta0}(\delta)+\sum_{\alpha=s,p}\int d^2\mathbf{b}\exp[i(\mathbf{b}\boldsymbol{\rho}-\eta_nz)]\hat{\mathbf{e}}^{+}_{n\alpha}E^{n1}_{\alpha\beta}(\mathbf{b},\mathbf{b}_0),$$

$$z\to-\infty. \tag{18}$$

With no loss of generality, we have assumed here that the incident polarized electromagnetic wave, with $\beta=s, p$, has been specified in the upper medium. The $r_\beta(\delta)$ are reflection coefficients in the medium given by (11) [see Eq. (27)], and the $\hat{\mathbf{e}}^{\pm}_{m\alpha}$ are polarization unit vectors,

$$\hat{\mathbf{e}}^{\pm}_{ms}=\hat{s}=[\hat{\mathbf{b}}\hat{\mathbf{z}}],\quad \hat{\mathbf{e}}^{\pm}_{mp}=(b\hat{\mathbf{z}}\pm\eta_m\hat{\mathbf{b}})/k_m.$$

Only $E^{11}_{\alpha\beta}$ and $E^{n1}_{\alpha\beta}$ appear in Eq. (18). The coefficients $E^{1n}_{\alpha\beta}$ and $E^{nn}_{\alpha\beta}$ govern the asymptotic expansion of the diffracted field for a wave incident from below. In (18) and throughout the rest of this paper, the additional subscript 0 denotes quantities that depend on the variables $\mathbf{b}$ or $\mathbf{b}_0$: for example, $\eta_1=\eta_1(\mathbf{b})$, $\eta_{10}=\eta_1(\mathbf{b}_0)$, etc.

Averaging (18) over an ensemble of rough surfaces yields an expression for the transmission and reflection coefficients $r_{\alpha\beta}$ and $t_{\alpha\beta}$ of a perturbed medium:

$$r_{\alpha\beta}=r_\alpha(\delta)\delta_{\alpha\beta}+\bar{E}^{11}_{\alpha\beta}(\mathbf{b}),$$

$$t_{\alpha\beta}=t_\alpha(\delta)\delta_{\alpha\beta}+\bar{E}^{n1}_{\alpha\beta}(\mathbf{b}), \tag{19}$$

where $\delta_{\alpha\beta}$ is the Kronecker delta and $\langle E^{lm}_{\alpha\beta}(\mathbf{b},\mathbf{b}_0)\rangle=\bar{E}^{lm}_{\alpha\beta}(\mathbf{b})\delta(\mathbf{b}-\mathbf{b}_0)$.

Thus, in the general case of an arbitrary stratified medium, the problem of electromagnetic wave diffraction by rough interfaces reduces to the solution of the standard equation (14) of quantum scattering theory. If the solution is known, the matrix elements of $\hat{t}$ in (17) will determine the total diffracted field (18), as well as the transmission and reflection coefficients (19). This general approach, however, which has been employed under the assumption of slightly rough surfaces in the special cases of a homogeneous medium,[4,11,23] a stratified half-space,[7] and a three-layer medium,[8] yields results of limited utility, since the neighborhood of eigenmodes of the medium is not taken into consideration. In the next section we develop an alternative approach that yields analytically correct results at all frequencies, including those in the neighborhood of eigenmodes.

4. STATEMENT OF THE PROBLEM FOR A COHERENT COMPONENT OF THE FIELD

To calculate the transmission and reflection coefficients (19) and the eigenmode dispersion relation for a perturbed medium, if suffices to find only the coherent component $\langle E(\mathbf{r})\rangle$ of the diffracted field. We average Eq. (8) over an ensemble of rough surfaces, introducing the operator $\hat{\varepsilon}_{\text{eff}}$ for the effective dielectric constant of the medium:

$$\langle\hat{\varepsilon}(\mathbf{r})\mathbf{E}(\mathbf{r})\rangle=\int\hat{\varepsilon}_{\text{eff}}(\mathbf{r},\mathbf{r}')\langle\mathbf{E}(\mathbf{r}')\rangle d^3\mathbf{r}',$$

$$\hat{\varepsilon}_{\text{eff}}(\mathbf{r},\mathbf{r}')=\hat{\varepsilon}_z\delta(\mathbf{r}-\mathbf{r}')+\hat{\Sigma}(\mathbf{r},\mathbf{r}'),$$

where $\hat{\varepsilon}_z$ is the local and $\hat{\Sigma}(\mathbf{r},\mathbf{r}')$ the nonlocal part of $\hat{\varepsilon}_{\text{eff}}$. We then obtain a closed-form equation for the coherent component $\langle \mathbf{E}(\mathbf{r})\rangle = \mathbf{E}(\mathbf{b},z)\exp(i\mathbf{b}\boldsymbol{\rho})$,

$$(\text{curl curl} - k_0^2\hat{\varepsilon}_z)\mathbf{E}(\mathbf{b},z) = k_0^2 \int \hat{\Sigma}(\mathbf{b},z,z')\mathbf{E}(b,z')dz', \tag{20}$$

with $\text{curl} = (i\mathbf{b} + \hat{z}d/dz)$, where it has been assumed that $\hat{\Sigma}(\mathbf{r},\mathbf{r}')$ for uniformly rough surfaces depends solely on the coordinate difference $\boldsymbol{\rho}-\boldsymbol{\rho}'$ (the Fourier transform variable). The nonlocal part $\hat{\Sigma}$ is guaranteed to be unique by the solution of Eq. (9) for the scattering operator $\hat{T}$,[24]

$$k_0^2\hat{\Sigma} = \langle \hat{T}\rangle(1+\hat{G}\langle\hat{T}\rangle)^{-1}. \tag{21}$$

Equation (20) is completely equivalent to the original Eq. (8), but it governs only the coherent component of the total diffracted field. The variable $\mathbf{b}$, whose value is determined either by the incident wave vector or a solution of the dispersion relation, is merely a parameter, and can be omitted. The integrodifferential equation (20) describes a narrower class of solution than (8). In a previous paper,[22] the author developed the general theory of analytic correct solutions of equations like (20) for arbitrary functions $\hat{\varepsilon}_z$ and $\hat{\Sigma}(\mathbf{b},z,z')$. The equation can be solved by reducing it to an equivalent equation for the retarded scattering operator $\hat{T}^+$:

$$\hat{T}^+ = k_0^2\hat{\Sigma}(1+\hat{G}^+\hat{T}^+), \tag{22}$$

where the retarded Green's function $\hat{G}^+$ is a solution of the same Eq. (10) as the radiation Green's function $\hat{G}$; however, it satisfies the condition $\hat{G}^+=0$ as $z\to-\infty$. Solving Eq. (22) yields a solution for the field $\mathbf{E}(\mathbf{b},z)$:

$$\mathbf{E}(\mathbf{b},z) = (1+\hat{G}^+\hat{T}^+)\mathbf{E}_{1\alpha}^+.$$

Just like Eq. (9), Eq. (22) can be transformed to a set of basis functions $t^+ = \hat{\mathscr{P}}^{-1}T^+\hat{\mathscr{P}}^{-1}$ that are continuous at a boundary, and the singular term can likewise be eliminated from the Green's function $\hat{G}^+$. In place of (22), we thereby obtain the equivalent equation

$$\hat{t}^+ = k_0^2\hat{\sigma}(1+\hat{G}_0^+\hat{t}^+) \tag{23}$$

$$\hat{G}_0^+(\mathbf{b},z,z') = \frac{i}{2\eta_1}\sum_{\alpha=s,p} t_\alpha(\delta)[\mathbf{X}_{n\alpha}^+(\mathbf{b},z)\mathbf{X}_{1\alpha}^-(\mathbf{b},z') - \mathbf{X}_{1\alpha}^+(\mathbf{b},z)\mathbf{X}_{n\alpha}^-(\mathbf{b},z')]\theta(z-z'), \tag{24}$$

in which the perturbation $\hat{\sigma}$ can be defined in terms of the mean value of the operator (14),

$$k_0^2\hat{\sigma} = \langle\hat{t}\rangle(1+\hat{G}_0\langle\hat{t}\rangle)^{-1}. \tag{25}$$

Assuming the solution of (23) to be known, the matrix elements of the operator $\hat{t}^+$ then determine the coefficient functions $A_{\alpha\beta}^{\pm} = A_{\alpha\beta}^-(\mp\eta_1)$,[22] with

$$A_{\alpha\beta}^-(\eta_1) = a_{1\alpha}^-(\delta)\delta_{\alpha\beta} - \frac{i}{2\eta_1} \times \int dzdz'\mathbf{X}_{n\alpha}^-(\mathbf{b},z)\hat{t}^+(\mathbf{b},z,z')\mathbf{X}_{1\beta}^+(\mathbf{b},z'), \tag{26}$$

in terms of which one can express the transmission and reflection coefficients $r_{\alpha\beta}$ and $t_{\alpha\beta}$ of the perturbed medium (1). The final equations linking $r_{\alpha\beta}$, $t_{\alpha\beta}$, and $A_{\alpha\beta}^{\pm}$ can be found in Ref. 22 (in the next section, we solve this problem in the quadratic approximation; the equations appear below as (42) to that order). The coefficients $a_{1\alpha}^{\pm}(\delta)$ have the same meaning as the $A_{\alpha\beta}^{\pm}$, and we can express the transmission and reflection coefficients of a medium with the dielectric constant (11) in terms of those coefficients:

$$r_\alpha(\delta) = \frac{a_{1\alpha}^+(\delta)}{a_{1\alpha}^-(\delta)}, \quad t_\alpha(\delta) = \frac{1}{a_{1\alpha}^-(\delta)}. \tag{27}$$

These coefficients also appear in Eqs. (15), (17)–(19), and (24).

One typical peculiarity of Eq. (23), as compared with Eq. (14), is that the Green's function $\hat{G}_0^+$ has no poles.[22] A simple iterative solution of (23) will converge uniformly over the whole frequency domain, including any neighborhood of the medium's eigenmodes.

The scattering operators $\langle\hat{t}\rangle$ and $\hat{t}^+$, whose matrix elements determine the transmission and reflection coefficients given by (17) and (19), as well as the coefficient functions (26), are related to one another. Eliminating the perturbation $\hat{\sigma}$ from (23) and (25), we have

$$\langle\hat{t}\rangle - \hat{t}^+ = \langle\hat{t}\rangle(\hat{G}_0 - \hat{G}_0^+)\hat{t}^+. \tag{28}$$

The kernel of this equation is degenerate,

$$\hat{G}_0(z,z') - \hat{G}_0^+(z,z') = \frac{i}{2\eta_1}\sum_{\alpha=s,p}\frac{\mathbf{X}_{1\alpha}^+(\mathbf{b},z)\mathbf{X}_{n\alpha}^-(\mathbf{b},z')}{a_{1\alpha}^-(\delta)},$$

so Eq. (28) can be solved exactly. Solving for the matrix elements (17) of the operator $\langle\hat{t}\rangle$, we obtain the general expressions relating $r_{\alpha\beta}$, $t_{\alpha\beta}$, and $A_{\alpha\beta}^{\pm}$.[22] If instead of (28) we solve for the matrix elements (26) of the operator $\hat{t}^+$, we obtain the inverse relations. The latter can be used to reduce the previously obtained results for $r_{\alpha\beta}$ and $t_{\alpha\beta}$ to analytic form and to derive the dispersion relation.

Thus far, we have treated the value of the dielectric constant (11) as being arbitrary. Analyzing Eq. (14), we see that it is desirable to choose $\hat{\varepsilon}_z$ such that $\langle\hat{v}\rangle=0$. The first nonvanishing approximation to the solution of Eqs. (14) and (28) will then be quadratic in the perturbation $\hat{v}$,

$$\hat{t}^+ = \langle\hat{t}\rangle = k_0^4\langle\hat{v}\hat{G}_0\hat{v}\rangle + \dots. \tag{29}$$

The condition $\langle\hat{v}\rangle=0$ is ensured by the fact that $\varepsilon_\perp(z) = \langle\varepsilon_\perp(\mathbf{r})\rangle$ and $\varepsilon_\parallel(z) = \langle\varepsilon_\parallel^{-1}(\mathbf{r})\rangle^{-1}$, whereupon we obtain for the multilayer stratified medium (1)

$$\varepsilon_\perp(z) = \varepsilon_{n\perp}(z) + \sum_{j=1}^{n-1}\Delta\varepsilon_{j\perp}(z)F_j(z),$$
$$\varepsilon_\parallel^{-1}(z) = \varepsilon_{n\parallel}^{-1}(z) + \sum_{j=1}^{n-1}\Delta\varepsilon_{j\parallel}^{-1}(z)F_j(z). \tag{30}$$

When (30) is substituted into (16), the dependence of the perturbation $\hat{v}(\mathbf{r})$ on the surface profile of the various boundaries and the dielectric constants of the adjacent media factors:

$$\hat{v}(\mathbf{r})=\sum_{j=1}^{n-1}\hat{v}_j(z)\lambda_j(\mathbf{r}),$$

$$\hat{v}_j(z)=\Delta\varepsilon_{j\perp}(z)\hat{P}_\perp+\Delta\varepsilon_{j\parallel}^{-1}(z)\hat{P}_\parallel, \tag{31}$$

$$\lambda_j(\mathbf{r})=\theta[z-h_j(\boldsymbol{\rho})]-F_j(z).$$

Furthermore, $\hat{v}(\mathbf{r})$ is an additive function of the number of rough boundaries. With the same choice of $\hat{\varepsilon}_z$, the original perturbation $\Delta\varepsilon(\mathbf{r})$ lacks this property. Equations (30) and (31) generalize our previous results[24] for a uniform, isotropic, semi-infinite medium, to arbitrary, stratified, uniaxial anisotropic media containing N rough interfaces.

The dielectric constant $\hat{\varepsilon}_z$ introduced by (30) depends on the one-dimensional height distribution function $F_j(z)$ of the various rough surfaces; accordingly, so do the basis functions $\mathbf{E}_{m\alpha}^{+}$ of Eq. (12), the Green's functions $\hat{G}$, $\hat{G}_0$, $\hat{G}^{+}$, and $\hat{G}_0^{+}$, and the transmission and reflection coefficients (27). The latter can be distinguished by the argument δ in the functions $r_\alpha(\delta)$, $t_\alpha(\delta)$, and $a_{1\alpha}^{-}(\delta)$.

In general, Eq. (12) cannot be solved in terms of analytic functions, and some approximation scheme is required. Equation (12) is a special case of Eq. (20), so that (23), (24), and (26) still hold. In what follows, we denote functions that refer to the unperturbed medium (2), which has smooth boundaries, by a bar (e.g., $\bar{\mathbf{E}}_{m\alpha}^{+}$, $\bar{G}$, etc.). By analogy with (23), Eq. (12) can then be replaced by its equivalent,

$$\hat{\hat{t}}^{+}=k_0^2\hat{v}(1+\hat{\hat{G}}_0^{+}\hat{\hat{t}}^{+}), \tag{32}$$

in which the perturbation $\hat{v}(z)$ is given in terms of the differences $\hat{\varepsilon}_z-\hat{\varepsilon}_z^0$; from (30),

$$\hat{v}(z)=\sum_{j=1}^{n-1}\hat{v}_j(z)\bar{\lambda}_j(z), \tag{33}$$

where the $\bar{\lambda}_j(z)$ are given by (4), and the $\hat{v}_j(z)$ by (31). As with (23) and (26), the matrix elements of Eq. (32) yield the coefficients $a_{1\alpha}^{-}(\delta)$,

$$a_{1\alpha}^{-}(\delta)=a_{1\alpha}^{-}-\frac{i}{2\eta_1}\times\int dzdz'\bar{\mathbf{X}}_{n\alpha}^{-}(\mathbf{b},z)\hat{\hat{t}}^{+}(\mathbf{b},z,z')\bar{\mathbf{X}}_{1\alpha}^{+}(\mathbf{b},z'). \tag{34}$$

The coefficients $a_{1\alpha}^{\pm}=a_{1\alpha}^{-}(\mp\eta_1)$ yield the transmission and reflection coefficients r_α and t_α of the unperturbed, smooth-boundary medium (2) for an $\alpha=s$- or p-polarized electromagnetic wave incident from above:

$$r_\alpha=\frac{a_{1\alpha}^{+}}{a_{1\alpha}^{-}},\quad t_\alpha=\frac{1}{a_{1\alpha}^{-}}. \tag{35}$$

The argument δ does not appear here, in contrast to Eq. (27).

Imposing no constraints at all on the nature, amplitude, or number of rough boundaries, we have thus reduced the calculation of the dispersion relation and the transmission and reflection coefficients to the solution of the standard equations (14), (23), and (32) of quantum scattering theory for the scattering matrices $\hat{t}$, $\hat{t}^{+}$, and $\hat{\hat{t}}^{+}$. The desired quantities can be expressed in terms of the matrix elements (26) and (34) of the corresponding operators. In the next section, we apply this general approach to the quadratic approximation in the amplitudes of the irregular boundaries.

5. CALCULATION OF THE COEFFICIENTS $A_{\alpha\beta}^{-}$ AND $a_{1\alpha}^{-}(\delta)$ IN THE QUADRATIC APPROXIMATION

To calculate the $a_{1\alpha}^{-}(\delta)$ in the quadratic approximation, it suffices to stop after the first iteration when we solve Eq. (32). Using (33), we then have

$$a_{1\alpha}^{-}(\delta)=a_{1\alpha}^{-}-\frac{ik_0^2}{2\eta_1}\sum_{j=1}^{n-1}\int\bar{\mathbf{X}}_{n\alpha}^{-}(z)\hat{v}_j(z)\bar{\mathbf{X}}_{1\alpha}^{+}(z)\bar{\lambda}_j(z)dz. \tag{36}$$

The functions $\bar{\lambda}_j(z)$ are localized within the layer $|z-\bar{h}_j|\lesssim\delta_j$. For slightly rough surfaces, the fields in the integrand of (36) will be smooth functions of z, and they can therefore be expanded in powers of $z-\bar{h}_j$ in the neighborhood of each boundary $z=\bar{h}_j$:

$$\bar{\mathbf{X}}_{ms}^{\pm}(\mathbf{b},z)=[E_{ms}^{j}+E_{ms}'^{j}(z-\bar{h}_j)+\dots]\hat{s},$$

$$\bar{\mathbf{X}}_{mp}^{\pm}(\mathbf{b},z)=(D_m^j\hat{\mathbf{z}}\pm E_{mb}^j\hat{\mathbf{b}})-i\left[bE_{mb}^j\varepsilon_\perp^0(z)\hat{\mathbf{z}}\pm\frac{D_m^j}{b}\times\left(k_0^2-\frac{b^2}{\varepsilon_\parallel^0(z)}\right)\hat{\mathbf{b}}\right](z-\bar{h}_j)+\dots, \tag{37}$$

where E_{ms}^j, $E_{ms}'^j$, E_{mb}^j, and D_m^j are the values of the corresponding functions $E_{ms}(z)$, $dE_{ms}(z)/dz$, $E_{mb}(z)$, and $D_m(z)$ at the boundary $z=\bar{h}_j$. These values are known, since we assume that we know the analytic solution of the unperturbed equation (12) when the right-hand side vanishes. Specifically, if one of the two bounding media is homogeneous and isotropic all the way through to the first rough boundary, if there are no other rough boundaries, and if (as before) the remainder of the medium is arbitrarily stratified and uniaxially anisotropic, then these fields can be expressed in terms of the external parameters of the unperturbed problem—the transmission and reflection coefficients (35). For example, if $\hat{\varepsilon}_1(z)=\varepsilon_1\hat{1}=\text{const}$ for $z\geqslant\bar{h}_1$ (but $\varepsilon_{\perp,\parallel}(z)$ are arbitrary for $z\leqslant\bar{h}_1$), then at the boundary $z=\bar{h}_1$ we have

$$E_{1s}=a_{1s}^{+}+a_{1s}^{-},\quad E_{ns}=1,$$

$$E_{1s}'=i\eta_1(a_{1s}^{+}-a_{1s}^{-}),\quad E_{ns}'=i\eta_1,$$

$$E_{1b}=(a_{1p}^{-}-a_{1p}^{+})\eta_1/k_1,\quad E_{nb}=-\eta_1/k_1, \tag{38}$$

$$D_1=(a_{1p}^{-}+a_{1p}^{+})b\varepsilon_1/k_1,\quad D_n=b\varepsilon_1/k_1.$$

The unperturbed fields at the boundaries $z=\bar{h}_j$ of a plane-parallel multilayer medium can be found in Ref. 10. The functions (37) have been normalized to an incident wave of unit amplitude. In writing (37), we have used the fact that the fields $\bar{\mathbf{X}}_{m\alpha}^{\pm}(z)$ are continuous at the boundaries, but that their z-derivatives are discontinuous. The latter results in the dielectric constants $\varepsilon^0_{\perp,\parallel}(z)$ showing up in the linear terms of the field expansion for p-polarized waves. Integrals over z in (36) can be calculated explicitly using (5). For the discontinuous part of the $\bar{\mathbf{X}}^{\pm}_{jp}$, we also have

$$\int_{-\infty}^{\infty}(z-\bar{h}_j)\left[b^2\Delta\varepsilon^{-1}_{j\parallel}(z)\varepsilon^0_{\perp}(z)-\Delta\varepsilon_{j\perp}(z)\times\left(k_0^2-\frac{b^2}{\varepsilon^0_{\parallel}(z)}\right)\right]\bar{\lambda}_j(z)dz=\frac{\delta_j^2}{2}\left(\frac{\varepsilon_{j\perp}}{\varepsilon_{j+1,\perp}}\eta^2_{j+1,p}-\frac{\varepsilon_{j+1,\perp}}{\varepsilon_{j\perp}}\eta^2_{jp}\right)_{z=\bar{h}_j}.$$

Finally, we have

$$a^-_{1\alpha}(\delta)=a^-_{1\alpha}+\frac{k_0^2}{2}\sum_{j=1}^{n-1}V_{\alpha j}(\mathbf{b})\delta_j^2, \qquad (39)$$

the functions $V_{\alpha j}$ are given in the Appendix.

To calculate the coefficients of the functions $A^-_{\alpha\beta}$ in the quadratic approximation, we need merely keep the first nonvanishing approximation to $\langle\hat{t}\rangle$ in (29). Making use of (31) and defining $\Phi_{ij}(\mathbf{r},\mathbf{r}')=\langle\lambda_i(\mathbf{r})\lambda_j(\mathbf{r}')\rangle$ (see (4)), we have then for the expansion of $\hat{t}^+$ in the coordinate representation

$$\hat{t}^+(\mathbf{r},\mathbf{r}')=k_0^4\sum_{i,j=1}^{n-1}\hat{v}_i(z)\hat{G}_0(\mathbf{r},\mathbf{r}')\hat{v}_j(z')\Phi_{ij}(\mathbf{r},\mathbf{r}').$$

All of the functions in this expression depend solely on the coordinate difference $\boldsymbol{\rho}-\boldsymbol{\rho}'$, so the matrix elements (26) contain spectral-type integrals of the functions $G_0(\mathbf{b},z,z')$ and $\Phi_{ij}(\mathbf{b},z,z')$ over b. The remaining integrals over z and z' can be calculated explicitly if we take account of the smooth variation of the fields $\mathbf{X}^{\pm}_{m\alpha}(\mathbf{b},z)$ in the neighborhood of the rough boundaries, and expand them as power series in $z-\bar{h}_j$, bearing in mind (6) and (7). In the quadratic approximation, it is sufficient to retain the zeroth-order terms in the power-series expansion in $z-\bar{h}_j$, replace $\mathbf{X}^{\pm}_{m\alpha}$ with the unperturbed $\bar{\mathbf{X}}^{\pm}_{m\alpha}$ given by (37), and keep only the symmetric part $\hat{G}^s_0$ of the radiation Green's function $\hat{G}_0$

$$G^s_0(\mathbf{b},z,z')=\frac{i}{2\eta_1}\sum_{\gamma=s,p}t_\gamma\begin{cases}\frac{1}{2}[\mathbf{X}^+_{n\gamma}(\mathbf{b},z)\mathbf{X}^-_{1\gamma}(\mathbf{b},z')+\mathbf{X}^+_{1\gamma}(\mathbf{b},z)\mathbf{X}^-_{n\gamma}(\mathbf{b},z')], & \text{for } z=z',\\ \mathbf{X}^+_{n\gamma}(\mathbf{b},z)\mathbf{X}^-_{1\gamma}(\mathbf{b},z'), & \text{for } z>z',\\ \mathbf{X}^+_{1\gamma}(\mathbf{b},z)\mathbf{X}^-_{n\gamma}(\mathbf{b},z'), & \text{for } z<z'.\end{cases}$$

For the coefficient functions (26), we obtain the resulting expansion

$$A^-_{\alpha\beta}(\eta_{10})=a^-_{1\alpha 0}(\delta)\delta_{\alpha\beta}+\frac{k_0^2}{2\eta_{10}}\sum_{i,j=1}^{n-1}\int\frac{d^2\mathbf{b}}{2\eta_1}U^{ij}_{\alpha\beta}(\mathbf{b},\mathbf{b}_0)S_{ij}(\mathbf{b}_0-\mathbf{b}). \qquad (40)$$

The explicit form of the functions

$$U^{ij}_{\alpha\beta}(\mathbf{b},\mathbf{b}_0)=-2i\eta_1\bar{\mathbf{X}}^-_{n\alpha}(\mathbf{b}_0,\bar{h}_i)\hat{v}_i(\bar{h}_i)\hat{G}^s_0\times(\mathbf{b},h_i,h_j)\hat{v}_j(h_j)\bar{\mathbf{X}}^+_{1\beta}(\mathbf{b}_0,\bar{h}_j)$$

is given in the Appendix. It follows from (40) that the off-diagonal coefficients $A^-_{\alpha\beta}$ with $\alpha\neq\beta$ are of order δ^2. We can therefore neglect products of these coefficients in the general equations[22] relating $r_{\alpha\beta}$, $t_{\alpha\beta}$, and $A^{\pm}_{\alpha\beta}$. We detail the relationship between $r_{\alpha\beta}$, $t_{\alpha\beta}$, and $A^{\pm}_{\alpha\beta}$ in the next section.

For the sake of completeness, we also give the equation for the angular spectrum of diffracted waves in the medium (1). In the quadratic approximation, it is sufficient to stop after the first iteration in solving (14), obtaining

$$\hat{t}(\mathbf{r},\mathbf{r}')=k_0^2\hat{v}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')+\dots .$$

Substituting this result into (17) and (18), calculating the electromagnetic flux density, and averaging the latter over an ensemble of rough surfaces (we make use of (6) for the angular spectrum), we obtain the angular spectrum given below by Eq. (45), in which the expansion coefficients are given by

$$Q^{lm}_{j\alpha\beta}(\mathbf{b},\mathbf{b}_0)=\frac{k_0^2t_\alpha t_{\beta 0}}{4\eta_1\eta_{10}}\bar{\mathbf{X}}^-_{l\alpha}(\mathbf{b},\bar{h}_j)\hat{v}_j(\bar{h}_j)\bar{\mathbf{X}}^+_{m\beta}(\mathbf{b}_0,\bar{h}_j). \qquad (41)$$

These are written out explicitly in the Appendix.

6. RESULTS

In the quadratic approximation to the amplitudes of the irregularities in the stratified, uniaxial, anisotropic medium (1), the transmission and reflection coefficients $r_{\alpha\beta}$ and $t_{\alpha\beta}$ for an incident $\beta=s$- or p-polarized electromagnetic wave are given by

$$r_{\alpha\alpha}=\frac{A^+_{\alpha\alpha}}{A^-_{\alpha\alpha}},\quad r_{sp}=\frac{A^+_{sp}a^-_{1s}-A^-_{sp}a^+_{1s}}{A^-_{ss}A^-_{pp}},$$
$$r_{ps}=\frac{A^+_{ps}a^-_{1p}-A^-_{ps}a^+_{1p}}{A^-_{ss}A^-_{pp}}, \qquad (42)$$
$$t_{\alpha\alpha}=\frac{1}{A^-_{\alpha\alpha}},\quad t_{sp}=-\frac{A^-_{sp}}{A^-_{ss}A^-_{pp}},\quad t_{ps}=-\frac{A^-_{ps}}{A^-_{ss}A^-_{pp}},$$

with $\alpha=s$, p. The coefficients of the functions $A^{\pm}_{\alpha\beta}=A^-_{\alpha\beta}(\mp\eta_1)$ follow directly from (39) and (40):

$$A^-_{\alpha\beta}(\eta_{10}) = \left[a^-_{1\alpha 0} + \frac{k_0^2}{2} \sum_{j=1}^{n-1} V_{\alpha j}(\mathbf{b}_0)\delta_j^2 \right] \delta_{\alpha\beta} + \frac{k_0^4}{2\eta_{10}} \sum_{i,j=1}^{n-1} \int \frac{d^2\mathbf{b}}{2\eta_1} U^{ij}_{\alpha\beta}(\mathbf{b},\mathbf{b}_0) S_{ij}(\mathbf{b}_0 - \mathbf{b}). \tag{43}$$

The expansion coefficients $V_{\alpha j}(\mathbf{b}_0)$ and $U^{ij}_{\alpha\beta}(\mathbf{b},\mathbf{b}_0)$ are written out in full in the Appendix.

The dispersion relation for the eigenmodes of the perturbed medium depends on the poles of the coefficients (42), and to the same approximation, it separates into two independent equations for $\alpha = s$- and p-polarized modes,

$$A^-_{\alpha\alpha}(\eta_1) = 0. \tag{44}$$

This statement holds only if the dispersion curves of the eigenmodes do not intersect, i.e., if the equation $a^-_{1\alpha} = 0$ has different solutions for $\alpha = s$ and $\alpha = p$. Polarization mixing effects will then be of order δ^4. If the eigenmodes do intersect, so that $a^-_{1s} = a^-_{1p} = 0$ simultaneously, then polarization mixing effects will be of order δ^2, and it will be necessary to solve the exact dispersion relation $A^-_{ss}A^-_{pp} = A^-_{sp}A^-_{ps}$ in the vicinity of the intersection point.[22]

The location of Brewster's angle, at which an initially unpolarized incident beam emerges completely polarized upon reflection,[25] is also given by two independent equations in the present quadratic approximation,

$$A^+_{\alpha\alpha}(\eta_1) = 0.$$

The angular spectrum $dP_{\alpha\beta}/d\Omega_m$ of the $\alpha = s$- or p-polarized electromagnetic wave scattered into medium $m = 1, n$ with dielectric constant ε_m for some incident $\beta = s$- or p-polarized wave from the upper medium is

$$\frac{dP_{\alpha\beta}}{P_{0z} d\Omega_m} = 4\eta_{10}\eta_m k_m^2 \sum_{i,j=1}^{n-1} Q^{m1}_{i\alpha\beta}(\mathbf{b},\mathbf{b}_0) \bar{Q}^{m1}_{j\alpha\beta}(\mathbf{b},\mathbf{b}_0) S_{ij}(\mathbf{b}_0 - \mathbf{b}); \tag{45}$$

a bar denotes here complex conjugation; P_{0z} is the normal component of the incoming wave, with angle of incidence θ_0; $d\Omega_m = \sin\theta_m d\theta_m d\varphi$ is the scattering solid angle in medium $m = 1, n$; θ_m is the scattering angle in medium m; $b = k_m \sin\theta_m$, $b_0 = k_1 \sin\theta_0$; and φ is the angle between the unit vectors $\hat{\mathbf{b}}$ and $\hat{\mathbf{b}}_0$. Equation (45) makes sense only if the final medium ($m = n$) is nondissipative and transparent, i.e., if $k_n^2 = 0$. The expansion coefficients $Q^{lm}_{j\alpha\beta}(\mathbf{b},\mathbf{b}_0)$ are given in full in the Appendix.

7. MULTILAYER MEDIUM WITH PERIODIC BOUNDARY IRREGULARITIES

It was assumed in the foregoing that the boundary irregularities are random functions of the profiles $z = h_j(\boldsymbol{\rho})$, but our results also hold for deterministic, periodic boundaries such as those of a diffraction grating, with

$$h_j(\boldsymbol{\rho}) \equiv h_j(x,y) = h_j(x + a_j, y + b_j),$$

where a_j and b_j are the periods of the jth boundary in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions. The Fourier components of the profile are

$$[\tilde{h}_j]_{lm} = \int \frac{d^2\rho}{S_j} \tilde{h}_j(\boldsymbol{\rho}) \exp(-i\mathbf{q}^j_{lm}\boldsymbol{\rho}),$$

$$\mathbf{q}^j_{lm} = 2\pi\left(\frac{l}{a_j}\hat{x} + \frac{m}{b_j}\hat{y}\right),$$

where $\tilde{h}_j(\boldsymbol{\rho}) = h_j(\boldsymbol{\rho}) - \bar{h}_j$, $l,m = 0, \pm 1, \pm 2, \ldots$, and S_j is the area of an integration cell.

For a deterministic boundary, the averaging scheme employed to go from Eq. (8) to Eq. (20) is no longer appropriate, and we must turn instead to a reanalysis of the original equation (14). The random profile of boundary irregularities enters into the final equations (42), (43), and (45) via the spectral densities $S_{ij}(\mathbf{q})$. To establish the relationship between the densities S_{ij} and the Fourier components of the periodic boundaries, we choose the dielectric constant $\hat{\varepsilon}_z$ of the unperturbed medium [Eq. (14)] to be that of a medium with smooth boundaries (2). The perturbation (16) takes then the form (31), where

$$\lambda_j(\mathbf{r}) = \theta[z - h_j(\boldsymbol{\rho})] - \theta(z - \bar{h}_j).$$

For slightly rough surfaces, this function can be expanded in powers of $\tilde{h}_j(\boldsymbol{\rho})$:

$$\lambda_j(\mathbf{r}) = -\tilde{h}_j(\boldsymbol{\rho})\delta(z - \bar{h}_j) + \frac{\tilde{h}_j^2(\boldsymbol{\rho})}{2}\delta'(z - \bar{h}_j) + \ldots,$$

and the iterative solution of Eq. (14) will contain linear ($\sim [\tilde{h}_j]_{\mathbf{b}-\mathbf{b}_0}$) and quadratic ($\sim \int d^2\mathbf{b}[\tilde{h}_i]_{\mathbf{b}-\mathbf{b}'}[\tilde{h}_j]_{\mathbf{b}'-\mathbf{b}_0}$) terms in the Fourier components of the arbitrary deterministic profile $\tilde{h}_j(\boldsymbol{\rho})$. For periodic irregularities,

$$[\tilde{h}_j]_{\mathbf{q}} = \sum_{l,m} [\tilde{h}_j]_{l,m}\delta(\mathbf{q} - \mathbf{q}^j_{lm}).$$

These same terms enter into the matrix elements (17) and the full diffracted field (18). The zeroth diffraction order yields the transmission and reflection coefficients (19). But those equations should also turn into the final results (42) if we expand them in powers of the boundary irregularities. A comparison yields

$$\delta_j^2 = [\tilde{h}_j^2]_{00} = \sum_{l,m} |[\tilde{h}_j]_{lm}|^2,$$
$$S_{jj}(\mathbf{q}) = \sum_{l,m} |[\tilde{h}_j]_{lm}|^2 \delta(\mathbf{q} - \mathbf{q}^j_{lm}). \tag{46}$$

The situation is more complicated when we look at the cross-spectral densities $S_{ij}(\mathbf{q})$ with $i \neq j$. In the zeroth diffraction order, profiles $\tilde{h}_i(\boldsymbol{\rho})$ and $\tilde{h}_j(\boldsymbol{\rho})$, with $i \neq j$, contribute only when their periods are commensurate, i.e., when there is some set of l, m, l', m' for which

$$\mathbf{q}^i_{lm} + \mathbf{q}^j_{l'm'} = 0. \tag{47}$$

This will be the case when the period ratio $a_i/a_j = b_i/b_j$ of profiles $\tilde{h}_i$ and $\tilde{h}_j$ is a rational number. We then have

$$S_{ij}(\mathbf{q}) = \sum_{l,m} [\tilde{h}_i]_{lm}[\tilde{h}_j]_{l'm'}\delta(\mathbf{q} - \mathbf{q}^j_{l'm'}), \tag{48}$$

where l', m' can be obtained from (47). When $i = j$, (48) is the same as (46).

If in fact the profiles $\tilde{h}_i$ and $\tilde{h}_j$ are incommensurate, i.e., their periods are related by an irrational factor, then (47) cannot be satisfied for any choice of l, m, l', m'. In that event, the cross-spectral densities S_{ij} with $i \neq j$ (and accordingly, bilinear combinations of the profiles (48)) will contribute neither to the zeroth diffraction order, nor to the transmission and reflection coefficients (42).

Substituting (46) and (48) into the final equations (43) and (45) changes the integrals over $d^2\mathbf{b}$ in the transmission and reflection coefficients and in the angular spectrum into a corresponding sum over diffraction orders; note that in (45), $d^2\mathbf{b} = \eta_m k_m d\Omega_m$. The resulting equations provide a basis for dealing analytically with the numerical calculations of Ref. 26 for the special case of a three-layer medium.

8. DISCUSSION

In the present paper, we have reduced the problem of electromagnetic wave diffraction from rough interfaces (either random or deterministic) between stratified, uniaxial, isotropic media in the general case—imposing no prior constraints upon the amplitude of boundary irregularities—to a solution of the standard equations of quantum scattering theory, Eqs. (14), (23), (25), and (32). A simple iterative solution yields closed-form analytic expressions for the transmission and reflection coefficients of the perturbed medium [Eqs. (42) and (43)]. These apply to a wider domain than previously, including the neighborhood of resonant eigenmodes. The dispersion relation (44) for the eigenmodes of the perturbed medium depends on the poles of the coefficients (42).

Equations (42) and (43) subsume all previous results as special cases. Equation (45) for the angular spectrum of the diffracted waves extends the results obtained in Refs. 9 and 10 for the special case of plane-stratified isotropic media to the present case of arbitrary stratified, uniaxial, anisotropic media.

The technique of averaging the original equation (8) and reducing it to Eq. (20) in order to derive the final expressions (42) and (43) shows that, with regard to the coherent component of the diffracted field, surface roughness is always manifested as a sort of surface layer with effective dielectric constant $\hat{\varepsilon}_{\text{eff}} - \hat{\varepsilon}_z^0 = (\hat{\varepsilon}_z - \hat{\varepsilon}_z^0) + \hat{\Sigma}$. Equations (9) and (21) yield a regular procedure for calculating $\hat{\varepsilon}_{\text{eff}}$. No further modeling assumptions are required to calculate $\hat{\varepsilon}_{\text{eff}}$, in constrast to those of numerous other approaches to this problem (see, e.g., Refs. 27–30). As before, the present approach constitutes a rigorous solution.

Equations (42) and (43) are exact, in the sense that they include all terms of order δ^2. In particular, in the neighborhood of Brewster's angle and of the eigenmodes of the unperturbed medium, the zeroth-order terms $a^{+}_{1\alpha 0}$ and $a^{-}_{1\alpha 0}$ vanish, and corrections $\sim \delta^2$ are no longer small, making a substantial contribution.

The parameters of the unperturbed medium enter into the final expressions (see Appendix) through discontinuities in the dielectric constant and its z-derivative at a boundary, through the transmission coefficients t_s and t_p of the unperturbed medium, and through the values of the unperturbed fields E^j_{ms}, E'^j_{ms}, E^j_{mb}, and D^j_m at the jth rough boundary. Those fields are known, since we have assumed that we have an analytic solution for the unperturbed equation (12) of a medium with smooth boundaries. The way in which the result depends on the fields at the jth boundary is physically reasonable—to a first approximation, neglecting retardation, the final equations can only depend on the field values in those regions where the perturbation $\Delta\hat{\varepsilon}$ is located. Previous conclusions[6,7] that the final expressions depend only on the external characteristics of the unperturbed problem hold only in the special case that one of the outermost media is homogeneous all the way through to the boundary, and that there is but a single rough surface, located at the boundary of the homogeneous outermost medium [see Eq. (38)]. Equations (42) and (45) make it possible to reinforce or suppress the contribution of the jth rough boundary to the observed effects by altering the boundary field distributions.

APPENDIX

The dependence on $\mathbf{b}$ or $\mathbf{b}_0$ of each quantity in the following equations is signified by an additional subscript 0 (for example, in η_1, η_{10}, D^j_n, D^j_{n0}).

$$V_{sj}(\mathbf{b}_0) = \frac{i}{2\eta_{10}} \frac{d}{dz} [E_{ns0}(z) \Delta\varepsilon_{j\perp}(z) E_{1s0}(z)] \big|_{z=\bar{h}_j},$$

$$V_{pj}(\mathbf{b}_0) = \frac{i}{2\eta_{10}} \Big[D^j_{n0} D^j_{10} (\Delta\varepsilon^{-1}_{\parallel})'_j - E^j_{nb0} E^j_{1b0} (\Delta\varepsilon_{\perp})'_j + \frac{i}{b_0} (D^j_{n0} E^j_{1b0} + D^j_{10} E^j_{nb0}) \Big(\frac{\varepsilon_{j\perp}}{\varepsilon_{j+1,\perp}} \eta^2_{j+1,p0} - \frac{\varepsilon_{j+1,\perp}}{\varepsilon_{j\perp}} \eta^2_{jp0} \Big) \Big]_{z=\bar{h}_j},$$

$$U^{ij}_{ss} = (\Delta\varepsilon_{\perp})_i (\Delta\varepsilon_{\perp})_j E^i_{ns0} E^j_{1s0} [t_s E^{in}_{ns} E^{jx}_{1s} - L^{ij}_{\perp} (\hat{b}\hat{s}_0)^2],$$

$$U^{ij}_{pp} = (\Delta\varepsilon_{\perp})_i (\Delta\varepsilon_{\perp})_j E^i_{nb0} E^j_{1b0} [t_p E^{in}_{nb} E^{jx}_{1b} - L^{ij}_{\perp} (\hat{b}\hat{s}_0)^2] + (\Delta\varepsilon^{-1}_{\parallel})_i (\Delta\varepsilon^{-1}_{\parallel})_j D^i_{n0} D^j_{10} t_p D^{in}_n D^{jx}_1 - t_p (\hat{b}\hat{b}_0) \times [(\Delta\varepsilon_{\perp})_i (\Delta\varepsilon^{-1}_{\parallel})_j E^i_{nb0} D^j_{10} L^{ij}_{\parallel} + (\Delta\varepsilon^{-1}_{\parallel})_i (\Delta\varepsilon_{\perp})_j D^i_{n0} E^j_{1b0} L^{ji}_{\parallel}],$$

$$U^{ij}_{sp} = -(\Delta\varepsilon_{\perp})_i E^i_{ns0} (\hat{b}\hat{s}_0) [(\Delta\varepsilon_{\perp})_j E^j_{1b0} (\hat{b}\hat{b}_0) L^{ij}_{\perp} - (\Delta\varepsilon^{-1}_{\parallel})_j D^j_{10} t_p L^{ij}_{\parallel}],$$

$$U^{ij}_{ps} = (\Delta\varepsilon_{\perp})_j E^j_{1s0} (\hat{b}\hat{s}_0) [(\Delta\varepsilon_{\perp})_i E^i_{nb0} (\hat{b}\hat{b}_0) L^{ij}_{\perp} - (\Delta\varepsilon^{-1}_{\parallel})_i D^i_{n0} t_p L^{ji}_{\parallel}],$$

where

$$in = \min(i,j), \quad jx = \max(i,j),$$

$$L^{ij}_{\perp} = t_s E^{in}_{ns} E^{jx}_{1s} + t_p E^{in}_{nb} E^{jx}_{1b},$$

$$L_{\parallel}^{ij}=\begin{cases} E_{nb}^{i}D_{1}^{j}, & i<j,\\ \frac{1}{2}(E_{nb}^{i}D_{1}^{j}+E_{1b}^{i}D_{n}^{j}), & i=j,\\ E_{1b}^{i}D_{n}^{j}, & i>j. \end{cases}$$

The expansion coefficients $Q_{j\alpha\beta}^{lm}(\mathbf{b},\mathbf{b}_0)$, which define the angular spmectrum (45), follow directly from Eqs. (37) and (41).

$$Q_{jss}^{lm}(\mathbf{b},\mathbf{b}_0)=\frac{k_0^2(\Delta\varepsilon_{\perp})_j t_s t_{s0}}{4\eta_1\eta_{10}}E_{ls}^{j}E_{ms0}^{j}(\hat{\mathbf{b}}\hat{\mathbf{b}}_0),$$

$$Q_{jpp}^{lm}(\mathbf{b},\mathbf{b}_0)=\frac{k_0^2 t_p t_{p0}}{4\eta_1\eta_{10}}[(\Delta\varepsilon_{\parallel}^{-1})_j D_l^j D_{m0}^j - (\Delta\varepsilon_{\perp})_j E_{lb}^{j}E_{mb0}^{j}(\hat{\mathbf{b}}\hat{\mathbf{b}}_0)],$$

$$Q_{jsp}^{lm}(\mathbf{b},\mathbf{b}_0)=-\frac{k_0^2(\Delta\varepsilon_{\perp})_j t_s t_{p0}}{4\eta_1\eta_{10}}E_{ls}^{j}E_{mb0}^{j}(\hat{\mathbf{b}}\hat{\mathbf{s}}_0),$$

$$Q_{jps}^{lm}(\mathbf{b},\mathbf{b}_0)=-\frac{k_0^2(\Delta\varepsilon_{\perp})_j t_p t_{s0}}{4\eta_1\eta_{10}}E_{lb}^{j}E_{ms0}^{j}(\hat{\mathbf{b}}\hat{\mathbf{s}}_0).$$

[1] F. G. Bass and I. M. Fuks, *Wave Scattering from Statistically Rough Surfaces*, Nauka, Moscow (1972) [Pergamon Press, Oxford (1977)].
[2] V. A. Antonov and V. I. Pshenitsyn, Opt. Spektrosk. **56**, 146 (1984) [Opt. Spectrosc. (USSR) **56**, 89 (1984)].
[3] N. P. Zhuk, Opt. Spektrosk. **61**, 560 (1986) [Opt. Spectrosc. (USSR) **61**, 351 (1986)].
[4] G. V. Rozhnov, *Ellipsometry: Theory, Methods, and Applications* [in Russian], Nauka (Siberian Division), Novosibirsk (1987).
[5] N. P. Zhuk, Izv. Vyssh. Uchebn. Zaved., Radiofiz. **30**, 592 (1987).
[6] N. P. Zhuk, Zh. Tekhn. Fiz. **59**, 12 (1989) [Sov. Phys. Tech. Phys. **34**, 6 (1989)].
[7] G. V. Rozhnov, *Ellipsometry in Science and Engineering, No. 2* [in Russian], Institute of Semiconductor Physics (Siberian Branch), USSR Academy of Sciences.
[8] G. V. Rozhnov, N. V. Bukhtiyarova, V. A. Kemarskii *et al.*, *Ellipsometry: Theory, Methods, and Applications* [in Russian], Nauka (Siberian Division), Novosibirsk (1991).
[9] P. Bousquet, F. Flory, P. Roche, J. Opt. Soc. Amer. **71**, 1115 (1984).
[10] G. V. Rozhnov, Zh. Eksp. Teor. Fiz. **96**, 1137 (1989) [Sov. Phys. JETP **69**, 646 (1989)].
[11] G. V. Rozhnov, Zh. Eksp. Teor. Fiz. **94**, No. 2, 50 (1988) [Sov. Phys. JETP **67**, 240 (1988)].
[12] A. A. Maradudin and W. Zierau, Phys. Rev. **B14**, 484 (1976).
[13] A. M. Brodsky and M. I. Urbakh, Surf. Sci. **115**, 417 (1982).
[14] G. A. Farias and A. A. Maradudin, Phys. Rev. **B28**, 5675 (1983).
[15] A. M. Brodsky and M. I. Urbakh, Surf. Sci. **167**, 231 (1986).
[16] S. A. Akhmanov, V. N. Seminogov, and V. I. Sokolov, Zh. Eksp. Teor. Fiz. **93**, 1654 (1987).
[17] R. K. Chang and T. E. Furtak (eds.), *Surface Enhanced Raman Scattering*, Plenum Press, New York (1982).
[18] M. Hatley and D. Maystre, Opt. Commun. **19**, 431 (1976).
[19] C. K. Chen, A. R. B. de Castro, and Y. R. Shen, Phys. Rev. Lett. **46**, 145 (1981).
[20] A. M. Brodsky and M. I. Urbakh, Progr. Surf. Sci. **33**, 91 (1990).
[21] R. G. Newton, *Scattering Theory of Waves and Particles*, McGraw-Hill, New York (1969).
[22] G. V. Rozhnov, Zh. Eksp. Teor. Fiz. **103**, 740 (1993) [Sov. Phys. JETP **76**, 364 (1993)].
[23] G. V. Rozhnov, Izv. Vyssh. Uchebn. Zaved., Radiofiz. **32**, 451 (1989).
[24] G. V. Rozhnov, Zh. Eksp. Teor. Fiz. **98**, 1737 (1990) [Sov. Phys. JETP **71**, 975 (1990)].
[25] L. A. Apresyan and Yu. A. Kravtsov, *Theory of Radiative Transfer* [in Russian], Nauka, Moscow (1983).
[26] Yu. M. Dikaev, Opt. Spektrosk. **73**, 566 (1992) [Opt. Spectrosc. (USSR) **73**, 332 (1992)].
[27] D. E. Aspnes and J. B. Theetin, Phys. Rev. **B20**, 3292 (1979).
[28] A. V. Rzhanov, K. K. Svitashev, A. I. Semenenko *et al.*, *Fundamentals of Ellipsometry* [in Russian], Nauka, Novosibirsk (1979).
[29] R. Azzam and N. Bashara, *Ellipsometry and Polarized Light*, Elsevier Publ. Co., New York (1977).
[30] A. V. Rzhanov, S. N. Svitasheva, and K. K. Svitashev, Dokl. Akad. Nauk SSSR **273**, 1123 (1983) [Sov. Phys. Doklady **28**, 1059 (1983)].

Translated by Marc Damashek