Nonlocal effective permittivity tensor of a rough interface between homogeneous and isotropic media

G. V. Rozhnov

Orion Scientific-Manufacturing Alliance
(Submitted 31 May 1990)
Zh. Eksp. Teor. Fiz. **98**, 1737–1747 (November 1990)

The relationship between the effective permittivity tensor of a layer of a rough surface and its n-dimensional height distribution functions F_n is established through a solution of Maxwell's equations. The local part of the effective permittivity tensor is determined by F_1, and the nonlocal part by F_n with $n \geqslant 2$.

The introduction of an effective permittivity operator

$$\langle \varepsilon \mathbf{E} \rangle = \hat{\varepsilon}^{eff} \langle \mathbf{E} \rangle \tag{1}$$

is a natural way, and also the most convenient way, to describe the mean field $\langle \mathbf{E} \rangle$ in composites and in randomly inhomogeneous media.[1-4] The procedure for calculating $\hat{\varepsilon}^{\text{eff}}$ is completely definite for three-dimensional composite materials and leads to various approximate expressions of the Lorenz-Lorentz type, the Maxwell-Garnett type, the Bruggemann type, and so forth.

A procedure for calculating the effective permittivity of a rough layer is also used widely in the theory of the diffraction of electromagnetic waves by rough surfaces, but there is no justification for calculating $\hat{\varepsilon}^{\text{eff}}$ of such a layer from one of the expressions named above for the theory of composite media.[5-8] Since they are strong functions of the size, shape, and density of the inclusions, none of which are considered in the original formulation [a contact of homogeneous and isotropic media along a rough interface $z = h(\rho)$; Fig. 1], the applicability of the approach taken in Refs. 5–8 is problematical and requires demonstration.

The properties of a rough surface are determined completely and unambiguously by the n-dimensional height distribution functions of this surface.[9] In the conventional approaches,[5-8] on the other hand, the relationship between the effective permittivity and the statistics of the surface is completely severed.

Our purposes in the present paper are to develop a general procedure for calculating the effective permittivity of a layer of a rough interface between homogeneous and isotropic media and to relate the effective permittivity to the statistics of the rough surface. We will impose no limitations on the statistics of the surface.

1. FORMULATION OF THE PROBLEM

In the original equation of macroscopic electrodynamics for a monochromatic electromagnetic wave,

$$(\text{rot rot} - k_0^2 \hat{\varepsilon}_z)\mathbf{E}(\mathbf{r}) = k_0^2 \Delta\hat{\varepsilon}(\mathbf{r})\mathbf{E}(\mathbf{r}) \tag{2}$$

(k_0 is the wave number in vacuum), the permittivity tensor $\hat{\varepsilon}_z$ (which we are leaving arbitrary at this point; it will be determined below) of a layered, inhomogeneous, uniaxially isotropic medium with a principal optical axis directed along the normal to the mean plane of the interface between the media, $z = \langle h(\rho) \rangle = \text{const}$, is written as follows:

$$\hat{\varepsilon}_z = \varepsilon_\perp(z)\hat{P}_\perp + \varepsilon_\parallel(z)\hat{P}_\parallel, \tag{3}$$

where $\hat{P}_\parallel = \hat{z}\hat{z}$, $\hat{P}_\perp = 1 - \hat{P}_\parallel$ are operators of projection onto the normal and onto the $z = \text{const}$ plane, respectively. The quantity $\Delta\hat{\varepsilon}(\mathbf{r})$ on the right side of (2) is the difference between the permittivity of the original medium (Fig. 1), which contains a rough interface $z = h(\boldsymbol{\rho})$,

$$\varepsilon(\mathbf{r}) = \varepsilon_1\theta[z - h(\boldsymbol{\rho})] + \varepsilon_2\theta[h(\boldsymbol{\rho}) - z] \tag{4}$$

[$\theta(z)$ is the unit step function], and the function $\hat{\varepsilon}_z$ introduced in (3):

$$\Delta\hat{\varepsilon}(\mathbf{r}) = [\varepsilon(\mathbf{r}) - \varepsilon_\perp(z)]\hat{P}_\perp + [\varepsilon(\mathbf{r}) - \varepsilon_\parallel(z)]\hat{P}_\parallel. \tag{5}$$

The only restriction on the behavior of the functions $\varepsilon_\perp(z)$ and $\varepsilon_\parallel(z)$ is that outside the rough layer, at $z \geqslant h_{\max}$ and $z \leqslant h_{\min}$, these functions take on the constant values of the permittivity of the original media:

$$\varepsilon_\perp(z) = \varepsilon_\parallel(z) = \begin{cases} \varepsilon_1 & \text{for} \quad z \geqslant h_{max}, \\ \varepsilon_2 & \text{for} \quad z \leqslant h_{min}. \end{cases} \tag{6}$$

Within this layer, the values of $\varepsilon_{\perp,\parallel}(z)$ are arbitrary. Condition (6) localizes perturbation (5) in the layer $h_{\min} \leqslant z \leqslant h_{\max}$. Outside this layer we have $\Delta\hat{\varepsilon}(\mathbf{r}) \equiv 0$.

Equation (2) can be put in integral form in the standard way:

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \int d^3\mathbf{r}' \hat{G}(\mathbf{r}, \mathbf{r}')\Delta\hat{\varepsilon}(\mathbf{r}')\mathbf{E}(\mathbf{r}'), \tag{7}$$

where $\mathbf{E}_0(\mathbf{r})$ is a general solution of the homogeneous version of Eq. (2) (with a zero right side). For this purpose we use the Green's function $\hat{G}(\mathbf{r}, \mathbf{r}')$ of Eq. (2),

$$(\text{rot rot} - k_0^2\hat{\varepsilon}_z)\hat{G}(\mathbf{r}, \mathbf{r}') = k_0^2 \hat{1}\delta(\mathbf{r} - \mathbf{r}'), \tag{8}$$

which satisfies the radiation condition at infinity. An expression for $\hat{G}(\mathbf{r}, \mathbf{r}')$ for an arbitrary function $\hat{\varepsilon}_z$ is derived in the Appendix.

The solution of Eq. (7) is expressed in terms of the scattering operator[10] $\hat{T}$ (we will be using symbolic operator notation below):

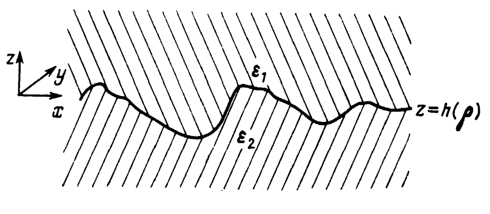

FIG. 1. Rough interface between homogeneous and isotropic media.

 0038-5646/90/110975-06$03.00

$$\mathbf{E}=(1+\hat{G}\hat{T})\mathbf{E}_0. \tag{9}$$

The scattering operator is determined by the solution of the equation

$$\hat{T}=\Delta\hat{\varepsilon}(1+\hat{G}\hat{T}). \tag{10}$$

Substituting (9) into (1), and noting that the choice of $\mathbf{E}_0$ is arbitrary, we find the following expression for the effective permittivity of the rough layer, using (10):

$$\hat{\varepsilon}^{eff}(\mathbf{r},\mathbf{r}')=\hat{\varepsilon}_z\delta(\mathbf{r}-\mathbf{r}')+\hat{\Sigma}(\mathbf{r},\mathbf{r}'). \tag{11}$$

The nonlocal part of the permittivity, $\hat{\Sigma}(\mathbf{r},\mathbf{r}')$, is expressed in terms of the mean value of the scattering operator $\hat{T}$ over the ensemble:

$$\hat{\Sigma}=\langle\hat{T}\rangle(1+\hat{G}\langle\hat{T}\rangle)^{-1}. \tag{12}$$

The calculation of the effective permittivity (11), (12) of the rough layer thus reduces to solving Eq. (10) for the matrix $\hat{T}$ and then taking its average. However, the general method for calculating the effective permittivity outlined above is incomplete. It requires refinement, since expansion (11) is ambiguous and can be carried out by an infinite number of methods because of the arbitrariness in the choice of the local part $\hat{\varepsilon}_z$ of the effective permittivity.

2. LOCAL PART OF THE EFFECTIVE PERMITTIVITY TENSOR $\hat{\varepsilon}_z$

To make expansion (11) for the effective permittivity unambiguous, we require that in the approximation of independent scatterers, in which the relation

$$\left\langle\prod_{i=1}^{n}\Delta\hat{\varepsilon}(\mathbf{r}_i)\right\rangle=\prod_{i=1}^{n}\langle\Delta\hat{\varepsilon}(\mathbf{r}_i)\rangle \quad \text{for} \quad \mathbf{r}_1\neq\mathbf{r}_2\neq\ldots\neq\mathbf{r}_n \tag{13}$$

holds, the mean value of the scattering vanish:

$$\langle\hat{T}\rangle=0. \tag{14}$$

Since $\hat{T}$ is a function of $\hat{\varepsilon}_z$, Eq. (14) is an equation for $\hat{\varepsilon}_z$, whose solution gives us the local part of the effective permittivity (11). Under conditions (13) and (14), the nonlocal part of the effective permittivity, (12), also vanishes. By virtue of our conditions (13) and (14), the nonlocal part of the effective permittivity is nonzero only because of the statistical dependence of the scatterers. Expansion (11) thus acquires a clear physical meaning: The local part, $\hat{\varepsilon}_z$, stems from single scattering (one-particle scattering) of waves, while the nonlocal part, $\hat{\Sigma}$, stems from multiple-scattering effects (effects of multiparticle or collective scattering). In Sec. 4 this assertion is verified by direct calculations. It is shown there that $\hat{\varepsilon}_z$ is determined exclusively by the one-dimensional height distribution $F_1(h)$, while $\hat{\Sigma}$ is determined exclusively by multidimensional distribution functions $F_n(h_1,\ldots,h_n)$ with $n\geqslant 2$.

To solve Eq. (14), we replace the scattering operator $\hat{T}$ by an iterative series expansion in powers of $\Delta\hat{\varepsilon}$,

$$\hat{T}=\Delta\hat{\varepsilon}+\Delta\hat{\varepsilon}\hat{G}\Delta\hat{\varepsilon}+\Delta\hat{\varepsilon}\hat{G}\Delta\hat{\varepsilon}\hat{G}\Delta\hat{\varepsilon}+\ldots, \tag{15}$$

and we use condition (13). If the Green's function (A4) (see the Appendix) had no singular part, the solution of Eq. (14) under condition (13) would be

$$\langle\Delta\hat{\varepsilon}(\mathbf{r})\rangle=0. \tag{16}$$

From this equation and (5) we find $\varepsilon_\perp(z)=\varepsilon_\parallel(z)=\langle\varepsilon(\mathbf{r})\rangle$. However, the presence of a local part $\alpha\delta(z-z')$ in Green's function (A4) makes Eqs. (14) and (16) nonequivalent, since terms of the type $\langle\Delta\varepsilon^n(\mathbf{r})\rangle$ with $n\geqslant 2$ are present when $\hat{T}$ is averaged, because of the local term in $\hat{G}$ in expansion (15). The contribution of these terms to $\langle\hat{T}\rangle$ is nonzero even under conditions (13) and (16). To solve (14), we must therefore either sum all the terms of this type or put our original equation, (10), in a form such that the Green's function in it contains no singular increment. Below we first find the transformation which we need, and we then show that it is equivalent to the summation method.

Substituting expansion (A4) for the Green's function $\hat{G}$ in Eq. (10) for the scattering operator $\hat{T}$, and moving the local part $-\Delta\hat{\varepsilon}\varepsilon_\parallel^{-1}\hat{P}_\parallel\hat{T}$ to the left side of Eq. (10), we find an equation equivalent to (10) for the scattering operator $\hat{T}$:

$$\hat{T}=\hat{\mathscr{P}}_\varepsilon\Delta\hat{\varepsilon}(1+\hat{G}'\hat{T}). \tag{17}$$

In this equation $\hat{G}'$, defined by (A5), no longer has a singular increment; the operator $\hat{\mathscr{P}}_\varepsilon$ depends on the permittivity (4) of the original medium, perturbed by the rough surface:

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

The perturbed permittivity $\varepsilon(\mathbf{r})$ in Eq. (17) appears in both $\mathscr{P}_\varepsilon$ and $\Delta\hat{\varepsilon}(\mathbf{r})$, so it poses several inconveniences in the calculation of mean values. We separate $\varepsilon(\mathbf{r})$ into a single factor, making use of the following identity for this purpose:

$$\hat{\mathscr{P}}_\varepsilon\Delta\hat{\varepsilon}=(\varepsilon-\varepsilon_\perp)\hat{P}_\perp+\varepsilon_\parallel^2(\varepsilon_\parallel^{-1}-\varepsilon^{-1})\hat{P}_\parallel=\hat{\mathscr{P}}\hat{v}\hat{\mathscr{P}}, \tag{18}$$

where $\hat{v}$ is the new perturbation of the problem, which also vanishes outside the rough layer:

$$\hat{v}(\mathbf{r})=[\varepsilon(\mathbf{r})-\varepsilon_\perp(z)]\hat{P}_\perp+\varepsilon_1\varepsilon_2[\varepsilon_\parallel^{-1}(z)-\varepsilon^{-1}(\mathbf{r})]\hat{P}_\parallel. \tag{19}$$

The operator $\hat{\mathscr{P}}$ does not depend on $\varepsilon(\mathbf{r})$; it renormalizes the z components of the fields:

$$\hat{\mathscr{P}}=\hat{P}_\perp+\frac{\varepsilon_\parallel}{(\varepsilon_1\varepsilon_2)^{1/2}}\hat{P}_\parallel. \tag{20}$$

The reason for singling out the factor $\varepsilon_1\varepsilon_2$ in (19) and (20) will be seen later [see (28) below].

From (17) and (18) we find the following representation of the operator $\hat{T}$:

$$\hat{T}=\hat{\mathscr{P}}\hat{t}\hat{\mathscr{P}}, \tag{21}$$

where $\hat{t}$ is a new scattering operator which satisfies an equation like (10),

$$\hat{t}=\hat{v}(1+\hat{G}_0\hat{t}). \tag{22}$$

This representation, however, differs from (10) in that it contains only a regular Green's function:

$$\hat{G}_0=\hat{\mathscr{P}}\hat{G}'\hat{\mathscr{P}}. \tag{23}$$

Introducing the new basis system of functions $\mathbf{X}_{j\gamma}^{\pm}=\mathscr{P}\mathbf{E}_{j\gamma}^{\pm}$, where $\mathbf{E}_{j\gamma}^{\pm}$ are given in (A2),

$$\mathbf{X}_{js}^{\pm}(\mathbf{b},z)=\hat{\mathbf{s}}E_j(\mathbf{b},z),$$

$$\mathbf{X}_{jp}^{\pm}(\mathbf{b},z)=\frac{1}{k_0}\left(\frac{b\hat{z}}{(\varepsilon_1\varepsilon_2)^{1/2}}\pm i\frac{\hat{\mathbf{b}}}{\varepsilon_\perp(z)}\frac{d}{dz}\right)H_j(\mathbf{b},z), \quad (24)$$

we find the following expression for $\hat{G}_0(\mathbf{b},z,z')$ from (23) and (A5):

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

$$+\mathbf{X}_{1\alpha}^{+}(\mathbf{b},z)\mathbf{X}_{2\alpha}^{-}(\mathbf{b},z')\theta(z'-z)]. \quad (25)$$

The equation which the Green's function $\hat{G}_0$ satisfies is given below [see (33)].

To prove that transformations (21) and (23) are equivalent to the summation in the expansion in (15) of the entire set of local terms of the type $\Delta\hat{\varepsilon}^n$, we replace $\hat{G}$ in (15) by its singular part from (A4). With respect to the longitudinal part of the permittivity, $\Delta\varepsilon_\parallel=\varepsilon-\varepsilon_\parallel$, we then find a geometric progression, which can be summed:

$$\Delta\varepsilon_\parallel-\Delta\varepsilon_\parallel\varepsilon_\parallel^{-1}\Delta\varepsilon_\parallel+\Delta\varepsilon_\parallel\varepsilon_\parallel^{-1}\Delta\varepsilon_\parallel\varepsilon_\parallel^{-1}\Delta\varepsilon_\parallel-\ldots$$

$$=\frac{\Delta\varepsilon_\parallel}{1+\Delta\varepsilon_\parallel/\varepsilon_\parallel}=\frac{\varepsilon_\parallel}{\varepsilon}\Delta\varepsilon_\parallel=\frac{\varepsilon_\parallel^2}{\varepsilon_1\varepsilon_2}(\hat{z}\hat{v}\hat{z})=\hat{\mathscr{P}}\hat{P}_\parallel\hat{v}\hat{\mathscr{P}}.$$

The result gives us the longitudinal part of this term of the expansion of $\hat{t}$ in powers of $\hat{v}$ in Eq. (22).

Similarly, we convolve all the remaining series in all the subsequent terms of expansion (15):

$$\Delta\hat{\varepsilon}\hat{G}\Delta\hat{\varepsilon}+\ldots\rightarrow\hat{v}\hat{G}_0\hat{v}\text{ etc.}$$

Transformations (21), (23) have thus reduced Eq. (10) for the scattering operator $\hat{T}$, which contains a singular Green's function $\hat{G}$, to Eq. (22) for the modified scattering operator $\hat{t}$, in which the Green's function $\hat{G}_0$ is regular. When we then repeat the arguments following (15), we can assert that the condition

$$\langle\hat{v}(\mathbf{r})\rangle=0 \quad (26)$$

gives us the solution of the equation $\langle\hat{t}\rangle=0$ under condition (13). By virtue of the linear dependence in (21) of the operators $\hat{T}$ and $\hat{t}$, this solution is equivalent to the solution of our original equation, (14).

Substituting (19) into Eq. (26), and solving the latter, we find the following expressions for the components of the tensor local part of the effective permittivity, $\hat{\varepsilon}_z$ [using (4)]:

$$\varepsilon_\perp(z)=\langle\varepsilon(\mathbf{r})\rangle=\varepsilon_2+(\varepsilon_1-\varepsilon_2)F_1(z),$$

$$\varepsilon_\parallel^{-1}(z)=\langle\varepsilon^{-1}(\mathbf{r})\rangle=\varepsilon_2^{-1}+(\varepsilon_1^{-1}-\varepsilon_2^{-1})F_1(z), \quad (27)$$

where $F_1(z)=\langle\theta[z-h(\rho)]\rangle$ is a one-dimensional height distribution $[0\leqslant F_1(z)\leqslant 1]$, given by

$$F_1(z)=\int_{-\infty}^{z}p_1(h)\,dh,$$

and $p_1(h)$ is a one-dimensional distribution density.

The quantity $\beta(z)=[\varepsilon_\perp(z)-\varepsilon_\parallel(z)]/\varepsilon_\parallel(z)$, the relative anisotropy of a medium with the permittivity in (27),

$$\beta(z)=\frac{(\varepsilon_1-\varepsilon_2)^2}{\varepsilon_1\varepsilon_2}F_1(z)[1-F_1(z)],$$

vanishes outside the rough layer and reaches a maximum

$$\beta_{max}=(\varepsilon_1-\varepsilon_2)^2/4\varepsilon_1\varepsilon_2$$

on the plane on which $F_1(z)=0.5$. The typical width of the anisotropy region is on the order of H, which is the mean square amplitude of the roughness.

Substituting (27) into (19), we can transform perturbation tensor $\hat{v}(\mathbf{r})$ into a unit tensor $\hat{1}v(\mathbf{r})$, and we can factorize the functional dependence of $v(\mathbf{r})$ on the irregularity profile $h(\rho)$ and the permittivities of the media in contact:

$$v(\mathbf{r})=(\varepsilon_1-\varepsilon_2)\lambda(\mathbf{r}),$$

$$\lambda(\mathbf{r})=\theta[z-h(\rho)]-\langle\theta[z-h(\rho)]\rangle=\theta[z-h(\rho)]-F_1(z). \quad (28)$$

This property, which is not shared by the original perturbation, (5), explains the introduction of the additional factor $\varepsilon_1\varepsilon_2$ in (19) and (20). The function $\lambda(\mathbf{r})$ is zero except in the layer $h_{\min}\leqslant z\leqslant h_{\max}$, where its values are $|\lambda(\mathbf{r})|\leqslant 1$.

3. NONLOCAL PART $\hat{\Sigma}(\mathbf{r},\mathbf{r}')$ OF THE EFFECTIVE PERMITTIVITY TENSOR

The nonlocal part $\hat{\Sigma}(\mathbf{r},\mathbf{r}')$ of the effective permittivity tensor can be expressed in terms of the mean value of the scattering operator $\hat{t}$ according to (12) and (21):

$$\hat{\Sigma}=\hat{\mathscr{P}}\langle\hat{t}\rangle(1+\hat{\mathscr{P}}\hat{G}\hat{\mathscr{P}}\langle\hat{t}\rangle)^{-1}\hat{\mathscr{P}}. \quad (29)$$

In contrast with Eq. (22) for the operator $\hat{t}$, which contains a regular Green's function G_0, expression (29) retains the complete Green's function, with the singular increment

$$\hat{\mathscr{P}}(z)\hat{G}(\mathbf{b},z,z')\hat{\mathscr{P}}(z')=\hat{G}_0(\mathbf{b},z,z')-\frac{\varepsilon_\parallel(z)}{\varepsilon_1\varepsilon_2}\hat{P}_\parallel\delta(z-z'). \quad (30)$$

This increment leads to a partial summation and to a change in the structure of the series, as was shown in the preceding section of this paper. [In the case at hand, it is the structure of series (29) which is changed, in the expansion of $\hat{\Sigma}$ in powers of $\langle\hat{t}\rangle$.] Below we will see the meaning of this circumstance, and we will find an expression for $\hat{\Sigma}$ which does not contain singular terms.

For this purpose we rewrite our original equation (2) in field components:

$$\mathbf{X}(\mathbf{r})=\begin{pmatrix}E_x\\E_y\\(\varepsilon_1\varepsilon_2)^{-1/2}D_z\end{pmatrix}, \quad (31)$$

where $D_z(\mathbf{r})=\varepsilon(\mathbf{r})E_z(\mathbf{r})$ is the z component of the displacement vector, and $\varepsilon(\mathbf{r})$ is given by expression (4). The choice of specifying these field components for rewriting Eqs. (2) stems from the circumstance that transformation (21), (23) by the operator $\hat{\mathscr{P}}$ in (20) is in a sense the best transformation, since it reduces the perturbation tensor $\hat{v}(\mathbf{r})$ in (19) to a scalar function (28) with a factorized dependence on the profile $h(\boldsymbol{\rho})$ and on the permittivity ε_j. In place of (2) we then find the equivalent system

$$\hat{l}\mathbf{X}(\mathbf{r})=\hat{m}\hat{v}(\mathbf{r})\mathbf{X}(\mathbf{r}), \quad (32)$$

where $\hat{l}$ and $\hat{m}$ are 3×3 matrix differential operators of the type

$$
\hat{l}=\begin{pmatrix} -(\partial_y^2+\partial_z^2+k_0^2\varepsilon_\perp(z)) & \partial_x\partial_y & (\varepsilon_1\varepsilon_2)^{1/2}\partial_x\partial_z\varepsilon_\parallel^{-1}(z) \\ \partial_y\partial_x & -(\partial_z^2+\partial_x^2+k_0^2\varepsilon_\perp(z)) & (\varepsilon_1\varepsilon_2)^{1/2}\partial_y\partial_z\varepsilon_\parallel^{-1}(z) \\ \partial_z\partial_x & \partial_z\partial_y & -(\varepsilon_1\varepsilon_2)^{1/2}[(\partial_x^2+\partial_y^2)\times \\ & & \times\,\varepsilon_\parallel^{-1}(z)+k_0^2] \end{pmatrix},
$$

$$
\hat{m}=k_0^2\begin{pmatrix} 1 & 0 & (k_1k_2)^{-1}\partial_x\partial_z \\ 0 & 1 & (k_1k_2)^{-1}\partial_y\partial_z \\ 0 & 0 & -(k_1k_2)^{-1}(\partial_x^2+\partial_y^2) \end{pmatrix}
$$

and $\hat{v}(\mathbf{r})$ is given by (19). The differential operators $\partial_x=\partial/\partial x$, etc., act on all the functions which follow them.

The complete set of solutions of the homogeneous version of Eq. (32) (with a zero right side), $\mathbf{X}_{j\gamma}(\mathbf{r})=\mathbf{X}_{j\gamma}^{+}(\mathbf{b},z)\exp(i\,\mathbf{b}\boldsymbol{\rho})$, $(j=1,2;\ r=s,p)$, is given by functions (24). Its Green's function, which satisfies the equation

$$
\hat{l}\hat{G}_0(\mathbf{r},\mathbf{r}')=\hat{m}\delta(\mathbf{r}-\mathbf{r}') \tag{33}
$$

and the radiation condition at infinity, is given by (25) in the mixed $(\mathbf{b},z)$ representation.

Using (33), we can put Eq. (32) in integral form, $\mathbf{X}=\mathbf{X}_0+\hat{G}_0\hat{v}\mathbf{X}$. Its solution

$$
\mathbf{X}=(1+\hat{G}_0\hat{t})\mathbf{X}_0 \tag{34}
$$

is expressed in terms of the scattering operator $\hat{t}$ given by Eq. (22). We define the eigenenergy operator $\hat{\sigma}$ of Eq. (32) by

$$
\langle\hat{v}\mathbf{X}\rangle=\hat{\sigma}\langle\mathbf{X}\rangle. \tag{35}
$$

We then find the following equation for the mean field $\langle\mathbf{X}\rangle$:

$$
(\hat{l}-\hat{m}\hat{\sigma})\langle\mathbf{X}\rangle=0. \tag{36}
$$

Substituting (34) into (35), and making use of the arbitrariness in the choice of $\mathbf{X}_0$, we find the following expression for the operator $\hat{\sigma}$:

$$
\hat{\sigma}=\langle\hat{t}\rangle(1+\hat{G}_0\langle\hat{t}\rangle)^{-1}. \tag{37}
$$

This expression is an analog of the corresponding expression (12) for $\hat{\Sigma}$, and contains only the regular part of the Green's function, $\hat{G}_0$, in contrast with (29).

To relate the components of the tensor nonlocal part of the effective permittivity $\hat{\Sigma}$ to the components of the eigenenergy operator $\hat{\sigma}$, we take an average of Eq. (2),

$$
(\mathrm{rot\,rot}-k_0^2\hat{\varepsilon}^{eff})\langle\mathbf{E}\rangle=0 \tag{38}
$$

and we transform it to the same field components [see (31)] with respect to which Eq. (36) is written. Comparing these equations, we find the relationship which we are seeking between the operators $\hat{\varepsilon}_{ij}^{\mathrm{eff}}=\hat{\varepsilon}_{ij}$ and $\hat{\sigma}_{ij}$:

$$
\begin{gathered}
\hat{\varepsilon}_{\alpha\beta}-\hat{\varepsilon}_{\alpha z}\hat{\varepsilon}_{zz}^{-1}\hat{\varepsilon}_{z\beta}=\varepsilon_\perp(z)\delta(\mathbf{r}-\mathbf{r}')\delta_{\alpha\beta}+\hat{\sigma}_{\alpha\beta},\\
\hat{\varepsilon}_{zz}^{-1}=\varepsilon_\parallel^{-1}(z)\delta(\mathbf{r}-\mathbf{r}')-(\varepsilon_1\varepsilon_2)^{-1}\hat{\sigma}_{zz},\\
\hat{\varepsilon}_{\alpha z}\hat{\varepsilon}_{zz}^{-1}=(\varepsilon_1\varepsilon_2)^{-1/2}\hat{\sigma}_{\alpha z},\\
\hat{\varepsilon}_{zz}^{-1}\hat{\varepsilon}_{z\alpha}=(\varepsilon_1\varepsilon_2)^{-1/2}\hat{\sigma}_{z\alpha},
\end{gathered} \tag{39}
$$

where $\delta_{\alpha\beta}$ is the Kronecker delta, and $\alpha,\beta=x,y$. The eigenenergy operator $\hat{\sigma}$ thus does not determine the actual components of the effective-permittivity tensor but only a certain combination of them.

Relations (39) are linear in $\hat{\sigma}_{ij}$. Substituting them into the expression $\hat{\mathscr{P}}\hat{\sigma}\hat{\mathscr{P}}$, and writing $\hat{\varepsilon}$ as a sum of local and nonlocal parts [see (11)], we find the relationship between the operators $\hat{\sigma}$ and $\hat{\Sigma}$:

$$
\hat{\mathscr{P}}\hat{\sigma}\hat{\mathscr{P}}=\left(1+\hat{\Sigma}\frac{\hat{P}_\parallel}{\varepsilon_\parallel}\right)^{-1}\hat{\Sigma}. \tag{40}
$$

Alternatively, solving for $\hat{\Sigma}$, we find the nonlocal part of the effective permittivity $\hat{\Sigma}$ as a function of the eigenenergy operator $\hat{\sigma}$:

$$
\hat{\Sigma}=\hat{\mathscr{P}}\hat{\sigma}\hat{\mathscr{P}}\left(1-\frac{\hat{P}_\parallel}{\varepsilon_\parallel}\hat{\mathscr{P}}\hat{\sigma}\hat{\mathscr{P}}\right)^{-1}=\hat{\mathscr{P}}\hat{\sigma}\left(1-\frac{\varepsilon_\parallel}{\varepsilon_1\varepsilon_2}\hat{P}_\parallel\hat{\sigma}\right)^{-1}\hat{\mathscr{P}}. \tag{41}
$$

Relation (41) can also be found from (29) by expressing $\langle\hat{t}\rangle$ in terms of $\hat{\sigma}$ in the latter and replacing $\hat{\mathscr{P}}\hat{G}\hat{\mathscr{P}}$ in accordance with (30).

Relations (40) and (41) thus establish a mutually one-to-one correspondence between the nonlocal part of the effective-permittivity tensor $\hat{\Sigma}$ and the eigenenergy operator $\hat{\sigma}$ of Eq. (36). Calculating the latter operator [see (37)] reduces to solving the standard equation [see (22)] for $\hat{t}$: a scattering operator with a regular Green's function $\hat{G}_0$.

4. ITERATIVE EXPANSION OF $\hat{t}$ AND $\hat{\Sigma}$

Let us examine the structure of the nonlocal part of the effective permittivity, solving Eq. (22) by an iterative method. Taking the average of an expansion of $\hat{t}$ in powers of v, we find the series

$$
\begin{aligned}
\langle\hat{t}(1,2)\rangle=\hat{G}_0(1,2)\langle v(1)v(2)\rangle+\hat{G}_0(1,3)\hat{G}_0(3,2)\langle v(1)v(2)\\
\times v(3)\rangle+\dots,
\end{aligned} \tag{42}
$$

We introduce the n-dimensional distribution functions of the heights of the random process $z=h(\rho)$:

$$
\begin{aligned}
F_n(1,\dots,n)=\left\langle\prod_{j=1}^{n}\theta[z_j-h(\boldsymbol{\rho}_j)]\right\rangle=\int_{-\infty}^{z_1}dh_1\dots\\
\dots\int_{-\infty}^{z_n}dh_n p_n(h_1,\dots,h_n;\ \boldsymbol{\rho}_1,\dots\boldsymbol{\rho}_n),
\end{aligned} \tag{43}
$$

$0\leqslant F_n\leqslant 1$; here $p_n(h_1,\dots,h_n;\boldsymbol{\rho}_1,\dots,\boldsymbol{\rho}_n)$ are n-dimensional height distributions. Using (28), we then find the following expression for the mean values of the product $v(\mathbf{r}_i)$:

$$
\left\langle\prod_{j=1}^{n}v(j)\right\rangle=(\varepsilon_1-\varepsilon_2)^n\Phi_n(1,\dots,n).
$$

Here Φ_n are determined by the central moments of the random process $\lambda(\mathbf{r})$:

$$
\Phi_n(1,\dots,n)=\left\langle\prod_{j=1}^{n}\lambda(j)\right\rangle.
$$

They can be expressed directly in terms of distributions functions (43). In particular, for $n=2, 3$ we find

$$\Phi_2(1,2)=F_2(1,2)-F_1(1)F_1(2)$$

$$=\int_{-\infty}^{z_1} dh_1\int_{-\infty}^{z_2} dh_2[p_2(h_1,h_2)-p_1(h_1)p_1(h_2)],$$

$$\Phi_3(1,2,3)=F_3(1,2,3)-\Phi_2(1,2)F_1(3)$$
$$-\Phi_2(2,3)F_1(1)-\Phi_2(3,1)F_1(2)-F_1(1)F_1(2)F_1(3). \quad (44)$$

In general we have $\Phi_n = F_n - \Phi_{n-1}F_1 - ...$, i.e., incorporating the nth term of the expansion in (42) requires the use of an n-dimensional height distribution function. An expansion of $\langle \hat{t}\rangle$ in powers of v is therefore a power series in the multiplicity of the collective effects taken into account. In this sense the local part of the effective permittivity [(3), (27)], incorporates all single-scattering effects, while the first nonvanishing approximation for $\langle \hat{t}\rangle$,

$$\langle \hat{t}(\mathbf{r},\mathbf{r}')\rangle=(\varepsilon_1-\varepsilon_2)^2\Phi_2(\mathbf{r},\mathbf{r}')\hat{G}_0(\mathbf{r},\mathbf{r}'), \quad \text{(h)}$$

incorporates all effects of double wave scattering. In the same approximation, $\sim v^2$, we have $\hat{\sigma}=\langle \hat{t}\rangle$, $\hat{\Sigma}=\hat{\mathscr{P}}\hat{\sigma}\hat{\mathscr{P}}$ according to (37) and (41). For a uniform rough surface the dependence of $\Phi_2(\mathbf{r},\mathbf{r}')$ on the coordinates $\boldsymbol{\rho}$ and $\boldsymbol{\rho}'$ appears only as the difference $\boldsymbol{\rho}-\boldsymbol{\rho}'$, in terms of which Fourier transforms are taken. In the mixed $(\mathbf{b}, z)$ representation, where $\mathbf{b}$ is the vector conjugate to $\boldsymbol{\rho}-\boldsymbol{\rho}'$ in the Fourier transformation, we find the following expression for the nonlocal part of the effective permittivity tensor $\hat{\Sigma}$ in the approximation $\sim v^2$:

$$\hat{\Sigma}(\mathbf{b},z,z')=\hat{\mathscr{P}}(z)\hat{\sigma}(\mathbf{b},z,z')\hat{\mathscr{P}}(z'),$$

$$\hat{\sigma}(\mathbf{b},z,z')=(\varepsilon_1-\varepsilon_2)^2\int d^2\mathbf{b}'\Phi_2(\mathbf{b}-\mathbf{b}',z,z')\hat{G}_0(\mathbf{b}',z,z'). \quad (45)$$

The scale size of the nonlocal part of the effective permittivity along the variables z and z' is on the order of the mean square roughness amplitude H, while that along the variable $\boldsymbol{\rho}-\boldsymbol{\rho}'$ is of the order of the correlation length l, since outside the regions $h_{\min}\leqslant z(z')\leqslant h_{\max}$, $|\boldsymbol{\rho}-\boldsymbol{\rho}'|\lesssim l$ the function $\Phi_2(\boldsymbol{\rho}-\boldsymbol{\rho}',z,z')$ vanishes according to (44).

Writing (45) in the coordinate system defined by the unit vectors $\hat{s}$, $\hat{\mathbf{b}}$, $\hat{z}$ (see the Appendix), we find the following complete expression:

$$\sigma_{\alpha\beta}(\mathbf{b},z,z')=(\varepsilon_1-\varepsilon_2)^2\int d^2\mathbf{b}'\Phi_2(\mathbf{b}-\mathbf{b}',z,z')\begin{pmatrix} [(\hat{\mathbf{b}}\hat{\mathbf{b}}')^2G_{ss}+(\hat{\mathbf{s}}\hat{\mathbf{b}}')^2G_{bb}] & (\hat{\mathbf{b}}\hat{\mathbf{b}}')(\hat{\mathbf{b}}'\hat{\mathbf{s}})[-G_{ss}+G_{bb}] & (\hat{\mathbf{b}}'\hat{\mathbf{s}})G_{bz} \\ (\hat{\mathbf{b}}\hat{\mathbf{b}}')(\hat{\mathbf{b}}'\hat{\mathbf{s}})[-G_{ss}+G_{bb}] & [(\hat{\mathbf{s}}\hat{\mathbf{b}}')^2G_{ss}+(\hat{\mathbf{b}}\hat{\mathbf{b}}')^2G_{bb}] & (\hat{\mathbf{b}}'\hat{\mathbf{b}})G_{bz} \\ (\hat{\mathbf{b}}'\hat{\mathbf{s}})G_{zb} & (\hat{\mathbf{b}}'\hat{\mathbf{b}})G_{zb} & G_{zz} \end{pmatrix}, \quad (46)$$

where $\alpha,\beta=s,b,z$ and the components $G_{\alpha\beta}$ are determined by the Green's function $\hat{G}_0(\mathbf{b}',z,z')$, which is itself given by (25) in the proper frame of reference $\hat{\mathbf{s}}$, $\hat{\mathbf{b}}'$, $\hat{\mathbf{z}}$.

In the general case of anisotropic rough surfaces, all the components of the tensor $\sigma_{\alpha\beta}$ are nonzero. In the case of isotropic surfaces, in contrast, in which $\Phi_2(\mathbf{b}-\mathbf{b}',z,z')$ depends on only the absolute value $|\mathbf{b}-\mathbf{b}'|$, matrix (46) becomes cellular, since in this case we have $\sigma_{sb}=\sigma_{sz}=\sigma_{bs}=\sigma_{bz}=0$.

CONCLUSION

We have derived a regular procedure for calculating the effective permittivity of a layer of a rough interface between homogeneous and isotropic media. This procedure is not based on a model. Instead, it is based on a systematic solution of the original Maxwell's equation, (2). In general, the effective permittivity of such a layer, (11), is a tensor and breaks up into the sum of a local term $\hat{\varepsilon}_z$ and a nonlocal term $\hat{\Sigma}(\mathbf{r},\mathbf{r}')$. The local part, (3), (27), which describes a uniaxial anisotropic medium with a stratification nonuniformity, is characterized unambiguously by single wave scattering and is determined entirely by a one-dimensional height distribution function. The components of the tensor $\hat{\varepsilon}_z$ [see (27)] are not independent; they are related by

$$\varepsilon_\perp(z)+\frac{\varepsilon_1\varepsilon_2}{\varepsilon_\parallel(z)}=\varepsilon_1+\varepsilon_2,$$

since they are expressed in terms of the same height distribution. This circumstance has several consequences in the reflection spectrum of such a medium for electromagnetic waves.

The nonlocal part of the effective permittivity [see (41)] is determined by solving the standard equation [see (22)] for the scattering matrix $\hat{t}$ and then calculating the eigenenergy operator (37). An iterative solution of (22) gives us an expansion of $\hat{\Sigma}(\mathbf{r},\mathbf{r}')$ in n-dimensional height distribution functions (43), i.e., in powers of the multiplicity of the collective effects which are taken into consideration. In terms of the variables z, z', it is localized in the slab $|z|$, $|z'|\lesssim H$, while in terms of the variables along the surface, $\boldsymbol{\rho}$ and $\boldsymbol{\rho}'$, it is localized in the region $|\boldsymbol{\rho}-\boldsymbol{\rho}'|\lesssim l$. Consequently, its contribution to the effective permittivity is small under the conditions $k_0H\ll 1$, $k_0 l\ll 1$. However, a small change in the permittivity can lead to important changes in observable physical quantities.[11]

APPENDIX

As in Ref. 12, we seek a solution of Eq. (8) for the Green's function $\hat{G}(\mathbf{b},z,z')$ [Fourier transforms are taken in the difference argument $\hat{G}(\boldsymbol{\rho}-\boldsymbol{\rho}',z,z')$] in the form of a bilinear combination of independent solutions $\mathbf{E}_{j\alpha}^{\pm}(\mathbf{b},z)$ $(j=1,2;\ \alpha=s,p)$, of the corresponding homogeneous version of Eq. (2) (with a zero right side). The functions $\mathbf{E}_{j\alpha}^{\pm}(\mathbf{b},z)$ are expressed in terms of the independent solutions $E_j(\mathbf{b},z)$ and $H_j(\mathbf{b},z)$ of the scalar equations

$$\left[\frac{d^2}{dz^2}+k_0^2\varepsilon_\perp(z)-b^2\right]E_j(\mathbf{b},z)=0,$$

$$\left[\frac{d}{dz}\varepsilon_\perp^{-1}(z)\frac{d}{dz}+k_0^2-b^2\varepsilon_\parallel^{-1}(z)\right]H_j(\mathbf{b},z)=0, \qquad \text{(A1)}$$

into which system (2) decomposes with $\Delta\hat{\varepsilon}=0$ for the s- and p-components of the polarized electromagnetic waves:

$$\mathbf{E}_{js}^{\pm}(\mathbf{b},z)=\hat{\mathbf{s}}E_j(\mathbf{b},z), \qquad \mathbf{E}_{jp}^{\pm}(\mathbf{b},z)$$

$$=\frac{1}{k_0}\left(\frac{b\hat{\mathbf{z}}}{\varepsilon_\parallel(z)}\pm i\frac{\hat{\mathbf{b}}}{\varepsilon_\perp(z)}\frac{d}{dz}\right)H_j(\mathbf{b},z). \qquad \text{(A2)}$$

Here $\hat{s}=[\hat{\mathbf{b}},\hat{\mathbf{z}}]$ and $\hat{\mathbf{b}}=\mathbf{b}/b$, $\hat{z}$ are the unit vectors of a right-handed coordinate system. By virtue of restriction (6), imposed above on the behavior of the functions $\varepsilon_{\perp,\parallel}(z)$ at $z\geqslant h_{\max}$ and $z\lesssim h_{\min}$, solutions of (A1) can always be normalized by the conditions

$$E_1(\mathbf{b},z)=k_0\exp(-i\eta_2 z), \qquad H_1(\mathbf{b},z)$$
$$=k_2\exp(-i\eta_2 z) \quad \text{for} \quad z\leqslant h_{min},$$
$$E_2(\mathbf{b},z)=k_0\exp(i\eta_1 z),\ H_2(\mathbf{b},z)=k_1\exp(i\eta_1 z) \quad \text{for} \quad z\geqslant h_{max}, \qquad \text{(A3)}$$

where $k_j - k_0\varepsilon_j^{1/2}$ is the wave number in medium $j=1, 2$; and $\eta_j=(k_j^2-b^2)^{1/2}$ is the component of the wave vector in medium j along the normal to the $z=\text{const}$ plane. We choose that branch of the root for which the relation $\text{Re(Im)}\ \eta_j\geqslant 0$ holds with $\text{Im}\varepsilon_j\geqslant 0$. We then find the following representation for the Green's function $\hat{G}(\mathbf{b},z,z')$, which satisfies the radiation condition at infinity:

$$\hat{G}(\mathbf{b},z,z')=-\frac{\hat{\mathbf{z}}\hat{\mathbf{z}}}{\varepsilon_\parallel(z)}\delta(z-z')+\hat{G}'(\mathbf{b},z,z'), \qquad \text{(A4)}$$

$$\hat{G}'(\mathbf{b},z,z')=\frac{i}{2\eta_1}\sum_{\alpha=s,p}t_\alpha[\mathbf{E}_{2\alpha}^{+}(\mathbf{b},z)\mathbf{E}_{1\alpha}^{-}(\mathbf{b},z')\theta(z-z')$$
$$+\mathbf{E}_{1\alpha}^{+}(b,z)\mathbf{E}_{2\alpha}^{-}(\mathbf{b},z')\theta(z'-z)]. \qquad \text{(A5)}$$

Here t_α are the amplitude transmission coefficients for the case in which an electromagnetic wave is incident from the upper medium with the permittivity ε_1. Expressions (A4) and (A5) are written in dyad notation. The normalization of the solutions in (A3) and the notation used in (A5) are consistent with each other. Expressions (A4) and (A5) are a generalization of the corresponding equations[12–15] found for the case of plane-layer media to the case of media with a stratification inhomogeneity.

[1] V. M. Finkel'berg, Zh. Eksp. Teor. Fiz. **46**, 725 (1964) [Sov. Phys. JETP **19**, 494 (1964)].
[2] Yu. A. Ryzhov, V. V. Tamoĭkin, and V. I. Tatarskiĭ, Zh. Eksp. Teor. Fiz. **48**, 656 (1965) [Sov. Phys. JETP **21**, 433 (1965)].
[3] Yu. A. Ryzhov, Zh. Eksp. Teor. Fiz. **55**, 567 (1968) [Sov. Phys. JETP **1**, 475 (1955)].
[4] J. C. Garland and D. B. Tanner (eds.), *Electrical, Transport, and Optical Properties of Inhomogeneous Media*, New York, 1978.
[5] D. E. Aspnes, J. B. Theetin, and F. Hottier, Phys. Rev. B **20**, 3292 (1979).
[6] A. V. Rzhanov, K. K. Svitashev, A. I. Semenenko *et al.*, *Basic Ellipsometry* [in Russian], Nauka, Novosibirsk, 1979.
[7] R. M. Azzam and N. M. Bashara, *Ellipsometry and Polarized Light*, Elsevier, New York, 1977.
[8] A. V. Rzhanov, S. N. Svitasheva, and K. K. Svitashev, Dokl. Akad. Nauk SSSR **273**, 1123 (1983) [Sov. Phys. Dokl. **28**, 1059 (1983)].
[9] F. G. Bass and J. M. Fuks, *Wave Scattering by a Statistically Irregular Surface*, Pergamon Press, Oxford, 1977.
[10] R. G. Newton, *Scattering Theory of Waves and Particles*, McGraw-Hill, New York, 1966.
[11] L. M. Brekhovskikh, *Waves in Layered Media*, Nauka, Moscow, 1973 [translation of earlier edition, Academic, 1970].
[12] G. V. Rozhnov, Zh. Eksp. Teor. Fiz. **96**, 1137 (1989) [Sov. Phys. JETP **69**, 646 (1989)].
[13] A. A. Maradudin and D. L. Mills, Phys. Rev. B **11**, 1392 (1975).
[14] D. L. Mills and A. A. Maradudin, Phys. Rev. B **12**, 2943 (1975).
[15] J. M. Elson, Appl. Opt. **16**, 2872 (1977).

Translated by D. Parsons