Reflection and Transmission of Electromagnetic Waves at a Rough Interface Between Two Different Media

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Abstract—An iterative technique is developed to rigorously compute the electromagnetic wave reflection and transmission at a rough interface between two media. The method is based upon a wave-function expansion technique in which the electromagnetic field equations and the radiation condition are satisfied analytically, while the boundary conditions at the interface are satisfied numerically. The latter is accomplished by an iterative minimization of the integrated square error in the boundary conditions. In each step of the iteration, only Fourier transforms of the spectral and spatial variables occur. As starting value, the Sommerfeld—Weyl plane interface results can be employed.

I. Introduction

HEN studying wave reflection and transmission in geophysical configurations one is almost invariably confronted with roughness of the interfaces between the different geological structures. Only for fairly simple models (mostly perfectly conducting cylindrical interfaces that are periodic in one direction) exact solutions have been constructed. Solutions of an approximate nature have been put forward to handle those cases where an exact solution seems beyond the reach of even present-day's powerful computers. Among these are: the Kirchhoff approximation and the physical-optics approximation for short wavelengths. By using the latter type of approxi-

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mation, surface-roughness effects can also be treated stochastically in a direct manner. When applying exact techniques, the stochastic aspects have to be deduced from proper averages over deterministically treated emsembles.

The literature on this subject is vast, and therefore we only mention the most important reviews: Beckmann and Spizzichino [1], Beckmann [2], Fortuin [3], Barrick and Peake [4], Barrick [5], Bass and Fuks [6], Shmelev [7], Hurdle, Flowers, and DeSanto [8], Trinkaus [9]. Further, we mention the comprehensive thesis by Rosich [10], in which an excellent historical introduction to rough-surface scattering theory as well as to many related theories is included. The first treatment of scattering from rough surfaces was by Rayleigh [11], who used a perturbation method to calculate the reflection of acoustic waves from a surface with a sinusoidal profile, while Rice [12] generalized the method to calculate the reflection of electromagnetic waves from any surface, whose profile could be represented by a two-dimensional Fourier series. The solution was limited only by the assumption that the variations in slope of the surface were small compared to the wavelength (see also Schouten and de Hoop [13]). Within the realm of the Rayleigh-Rice work we also mention the papers [14] - [24].

In this paper we develop an exact theory for the reflection and transmission of electromagnetic waves at a rough interface between two different media. Once the solution to this problem has been obtained, it can serve as a building block in electro-

magnetic wave propagation problems in layered configurations where the interfaces between any two successive layers may show roughness. The theory has to be implemented numerically on a computer. With this in mind, we stress the importance of iterative techniques. Here, storage requirements are minimized, although sometimes at the cost of an increase in computation time. The basic idea behind the method is that by expressing the electromagnetic field quantities in terms of suitable expansion functions, the electromagnetic field equations and the radiation condition are satisfied analytically, leaving the boundary conditions to be satisfied numerically. The latter is achieved by minimizing the integrated square error in the electromagnetic boundary conditions at the rough interface. The convergence of the iteration scheme is proved and it is shown that as a consequence at any interior point of the two media, the field values converge towards the exact ones. The major limitation of the method is put by the actual interval over which the (infinite) Fourier integrals have to be computed. How this turns out in practice, is the subject of investigation of a future paper.

The iteration scheme can be regarded as a continuous version of the conjugate-gradient plus the steepest descent technique for solving systems of linear algebraic equations iteratively [25], [26], [27]. We give, however, an independent presentation in which, from first principles, it is shown how to obtain optimum convergence. Experience with some two-dimensional scattering problems has shown [28] that the iterative technique is very efficient and could indeed handle configurations that are beyond the reach of a direct, i.e., noniterative, method.

The configuration under investigation is assumed to be a deviation from the one with a plane interface and this suggests the use of the well-known Sommerfeld-Weyl type solution [29], [30], [31], [32] of the plane interface problem as a starting value in the iterative technique applied to the rough interface. Since the Sommerfeld-Weyl representation is simple in the spatial Fourier (or spectral) domain, this also suggests the use of (uniform and nonuniform) plane waves as expansion functions. It is to be noted, however, that other starting values for the initial guess could be used as well (for example, the Kirchhoff or the physical-optics approximation). Since the theory is fully three-dimensional, the amplitude, phase, and polarization properties of the reflected and transmitted fields follow from it. For a discussion on the importance of the latter we refer to Boerner [33]. Finally, the iteration is stopped once the prescribed accuracy is arrived at.

II. FORMULATION OF THE PROBLEM

The configuration under investigation consists of a rough interface between two media with different electromagnetic properties (Fig. 1). A point in space is specified by its right-handed, orthogonal coordinates x, y, z. We assume that the roughness of the interface is a local deformation of an otherwise plane boundary z=0. The analysis is carried out in the frequency domain; the spectral field component with angular frequency ω has the complex time factor $\exp(-i\omega t)$. The two media occupy the domains D_1 and D_2 , respectively, and are assumed to be electromagnetically linear, homogeneous and isotropic with respective permittivities $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$, and permeabilities $\mu_1(\omega)$ and $\mu_2(\omega)$. We further assume that both

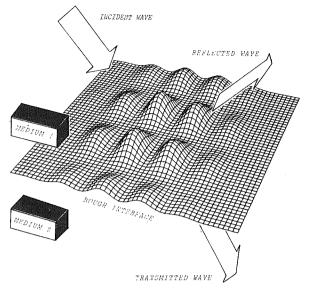


Fig. 1. Geometry of the configuration.

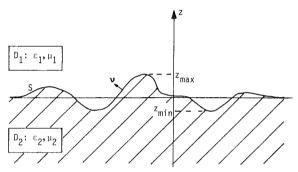


Fig. 2. Definition of the different domains in the configuration.

media exhibit some losses and that the real and imaginary parts of ϵ and μ satisfy the Kramers-Kronig causality relations [34]. The interface is denoted by S (Fig. 2).

In D_1 , an electromagnetic wave is incident upon S. This wave is generated by a source of finite extent. The incident wave is denoted by $\{\underline{E}^i, \underline{H}^i\}$. The total field in D_1 is written as the superposition of the incident field and the reflected field $\{\underline{E}^r, \underline{H}^r\}$. The reflected field satisfies the source-free Maxwell equations

$$\underline{\nabla} \times \underline{H}^r + i\omega \epsilon_1 \underline{E}^r = \underline{0},
\underline{\nabla} \times \underline{E}^r - i\omega \mu_1 \underline{H}^r = \underline{0},$$
 when $\underline{r} \in D_1$. (2.1)

In (2.1), $\underline{r} = (x, y, z)$ denotes the position vector. The field in D_2 is denoted as the transmitted field $\{\underline{E}^t, \underline{H}^t\}$. It satisfies the source-free Maxwell equations

$$\frac{\nabla \times \underline{H}^t + i\omega \epsilon_2 \underline{E}^t = \underline{0}}{\nabla \times \underline{E}^t - i\omega \mu_2 \underline{H}^t = \underline{0}}, \quad \text{when } \underline{r} \in D_2.$$
(2.2)

Further, the fields satisfy the boundary conditions on S, and at infinity $\{\underline{E}^r, \underline{H}^r\}$ and $\{\underline{E}^t, \underline{H}^t\}$ should consist of waves traveling away from S. Across S the tangential components of the electric field intensity and the tangential components of the magnetic field intensity must be continuous, i.e.,

$$\underline{\nu} \times \underline{E}^{t} + \underline{\nu} \times \underline{E}^{r} = \underline{\nu} \times \underline{E}^{t}, \\
\underline{\nu} \times \underline{H}^{t} + \underline{\nu} \times H^{r} = \underline{\nu} \times H^{t}, \quad \text{when } \underline{r} \in S$$
(2.3)

in which $\underline{\nu}$ is the unit vector in the direction of the normal to S, pointing into D_1 .

In the subdomain $z > z_{\text{max}}$ of D_1 , where z_{max} denotes the maximum value of z on S, the reflected field admits the representation

$$\{\underline{E}^r,\underline{H}^r\} = \iint_{-\infty}^{\infty} \{\underline{e}^r,\underline{h}^r\} \exp(i\underline{k}_1^*\cdot\underline{r}) d\alpha d\beta,$$

 $(z > z_{\text{max}}) \quad (2.4)$

in which

$$\underline{k}_1^+ = (\alpha, \beta, +\gamma_1) \tag{2.5}$$

where

$$\gamma_1 = (\omega^2 \epsilon_1 \mu_1 - \alpha^2 - \beta^2)^{1/2}$$
 with Re $(\gamma_1) > 0$,
Im $(\gamma_1) > 0$. (2.6)

From (2.1) and (2.4) it follows that the spectral amplitudes $\underline{e}^r = \underline{e}^r(\alpha, \beta)$ and $\underline{h}^r = \underline{h}^r(\alpha, \beta)$ satisfy the relations

$$i\underline{k}_{1}^{+} \times \underline{h}^{r} + i\omega\epsilon_{1} \underline{e}^{r} = \underline{0}$$

$$i\underline{k}_{1}^{+} \times \underline{e}^{r} - i\omega\mu_{1} \underline{h}^{r} = \underline{0}.$$
(2.7)

Equation (2.4) is a plane-wave representation for the reflected field in $z>z_{\rm max}$. In the subdomain $z< z_{\rm min}$ of D_2 , where $z_{\rm min}$ is the minimum value of z on S, the transmitted field admits the representation

$$\{\underline{E}^t, \underline{H}^t\} = \iint_{-\infty}^{\infty} \{\underline{e}^t, \underline{h}^t\} \exp(i\underline{k}_2^- \cdot \underline{r}) \, d\alpha \, d\beta,$$

in which

$$\underline{k}_{2}^{-} = (\alpha, \beta, -\gamma_{2}) \tag{2.9}$$

where

$$\gamma_2 = (\omega^2 \epsilon_2 \mu_2 - \alpha^2 - \beta^2)^{1/2}$$
 with Re $(\gamma_2) > 0$,
Im $(\gamma_2) > 0$. (2.10)

From (2.2) and (2.8) it follows that the spectral amplitudes $\underline{e}^t = \underline{e}^t(\alpha, \beta)$ and $\underline{h}^t = \underline{h}^t(\alpha, \beta)$ satisfy the relations

$$i\underline{k}_{2}^{-} \times \underline{h}^{t} + i\omega\epsilon_{2} \underline{e}^{t} = \underline{0}$$

$$i\underline{k}_{2}^{-} \times \underline{e}^{t} - i\omega\mu_{2} \underline{h}^{t} = \underline{0}.$$
(2.11)

Equation (2.8) is a plane-wave representation for the transmitted field in $z < z_{min}$.

It is noted that the representations (2.4) and (2.8) can in general not be continued analytically [35], [36] into the domain $z_{\min} < z < z_{\max}$ and thus they can not directly be used to satisfy pointwise the boundary conditions at S. How representations of this type can, nevertheless, be used to solve the reflection/transmission problem will be discussed in the next section.

III. THE INTEGRATED SQUARE ERROR CRITERION

In order to solve the reflection/transmission problem at hand, we approximate computationally the reflected field in D_1 and the transmitted field in D_2 by plane-wave representations that satisfy the corresponding source-free electromagnetic field equations and consist of constituents that travel in the direction of increasing z in D_1 and in the direction of decreasing z in D_2 . In fact, we take expressions of the type

$$\{\underline{\widetilde{E}}^r, \underline{\widetilde{H}}^r\} = \iint_{-\infty}^{\infty} \{\underline{\widetilde{e}}^r, \underline{\widetilde{h}}^r\} \exp(i\underline{k}_1^+ \cdot \underline{r}) \, d\alpha \, d\beta$$
when $r \in D_1$ (3.1)

and

$$\{\underline{\widetilde{E}}^t,\underline{\widetilde{H}}^t\} = \iint_{-\infty}^{\infty} \{\underline{\widetilde{e}}^t,\underline{\widetilde{h}}^t\} \exp(i\underline{k}_2^-\cdot\underline{r}) \,d\alpha \,d\beta$$

when $\underline{r} \in D_2$ (3.2)

where

$$\frac{\widetilde{e}^r = \underline{k}_1^+ \times \underline{b}_1}{\widetilde{\underline{h}}^r = (\omega \mu_1)^{-1} \underline{k}_1^+ \times (\underline{k}_1^+ \times \underline{b}_1)}$$
(3.3)

and

$$\frac{\underline{e}^t}{\underline{e}^t} = \underline{k}_2^- \times \underline{b}_2
\underline{h}^t = (\omega \mu_2)^{-1} \underline{k}_2^- \times (\underline{k}_2^- \times \underline{b}_2).$$
(3.4)

In view of (3.3), (3.1) satisfies (2.1), and in view of (3.4), (3.2) satisfies (2.2), provided that the right-hand sides of (3.1) and (3.2) converge in a certain sense.

From Appendix III, the theory of which is based upon the reciprocity relation discussed in Appendix I and the existence of Green's state of the two-media problem discussed in Appendix II, we know that, if \underline{b}_1 and \underline{b}_2 are constructed such that

$$ERR = \iint_{S} (|\underline{F}_{E}|^{2} + |\underline{F}_{H}|^{2} dA \to 0$$
(3.5)

where

$$\underline{F}_{E} = Y_{0}^{1/2} (\underline{\nu} \times \underline{E}^{i} + \underline{\nu} \times \underline{\widetilde{E}}^{r} - \underline{\nu} \times \underline{\widetilde{E}}^{t})
\underline{F}_{H} = Z_{0}^{1/2} (\underline{\nu} \times \underline{H}^{i} + \underline{\nu} \times \underline{\widetilde{H}}^{r} - \underline{\nu} \times \underline{\widetilde{H}}^{t})$$
(3.6)

we have

$$\{\underline{E}^r(\underline{r}), \underline{H}^r(\underline{r})\} \to \{\underline{E}^r(\underline{r}), \underline{H}^r(\underline{r})\} \quad \text{for any } \underline{r} \in D_1$$

$$(3.7)$$

and

$$\{\underline{\widetilde{E}}^t(\underline{r}), \underline{\widetilde{H}}^t(\underline{r})\} \to \{\underline{E}^t(\underline{r}), \underline{H}^t(\underline{r})\} \quad \text{for any } \underline{r} \in D_2.$$
(3.8)

In (3.6), $Y_0 = (\epsilon_0/\mu_0)^{1/2}$ is the wave admittance in free space and $Z_0 = (\mu_0/\epsilon_0)^{1/2}$ is the wave impedance in free space, which have been taken as reference values in the expressions for \underline{F}_E

and \underline{F}_H . (An alternative choice would be the values of the wave admittance and wave impedance of the medium in which the incident wave is traveling.) In the next section, we shall show how, in an iterative way, we can minimize ERR in (3.5) and enforce its convergence to zero.

IV. ITERATIVE MINIMIZATION OF THE INTEGRATED SQUARE ERROR

In this section we outline an iterative minimization of the integrated square error which leads to the solution of the reflection/transmission problem. The tilde over the different symbols to denote the approximating procedure will henceforth be omitted. We assume the existence of an iterative procedure, in which n steps have been carried out, and that this has led to the values $\underline{b}_1^{(n)}$ and $\underline{b}_2^{(n)}$ which can be used in (3.3) and (3.4). The corresponding "approximate" field values are

$$\{\underline{E}^{r(n)}, \underline{H}^{r(n)}\} = \iint_{-\infty}^{\infty} \{\underline{e}^{r(n)}, \underline{h}^{r(n)}\} \exp(i\underline{k}_{1}^{+} \cdot \underline{r}) d\alpha d\beta$$

when $\underline{r} \in D_1$

$$\{\underline{E}^{t(n)},\underline{H}^{t(n)}\} = \iint_{-\infty}^{\infty} \{\underline{e}^{t(n)},\underline{h}^{t(n)}\} \exp(i\underline{k}_{2}^{-}\cdot\underline{r}) \,d\alpha \,d\beta$$

when $\underline{r} \in D_2$ (4.1)

where

$$\underline{e}^{r(n)} = \underline{k}_{1}^{+} \times \underline{b}_{1}^{(n)}, \qquad \underline{h}^{r(n)} = (\omega \mu_{1})^{-1} \underline{k}_{1}^{+} \times (\underline{k}_{1}^{+} \times \underline{b}_{1}^{(n)})
\underline{e}^{t(n)} = \underline{k}_{2}^{-} \times \underline{b}_{2}^{(n)}, \qquad \underline{h}^{t(n)} = (\omega \mu_{2})^{-1} \underline{k}_{2}^{-} \times (\underline{k}_{2}^{-} \times \underline{b}_{2}^{(n)}).$$
(4.2)

The integrated square error $ERR^{(n)}$ after n steps of iteration is

$$ERR^{(n)} = \iint_{C} (|\underline{F}_{E}^{(n)}|^{2} + |\underline{F}_{H}^{(n)}|^{2}) dA$$
 (4.3)

in which the deviations $\underline{F}_E^{(n)} = \underline{F}_E^{(n)}(\underline{r}), \ \underline{F}_H^{(n)} = \underline{F}_H^{(n)}(\underline{r})$ are given by

$$\underline{F}_{E}^{(n)} = Y_0^{1/2} (\underline{\nu} \times \underline{E}^i + \underline{\nu} \times \underline{E}^{r(n)} - \underline{\nu} \times \underline{E}^{t(n)})$$

$$F_{E}^{(n)} = Z_0^{1/2} (\underline{\nu} \times H^i + \underline{\nu} \times H^{r(n)} - \underline{\nu} \times \underline{H}^{t(n)}). \tag{4.4}$$

In going from the (n-1)st step to the nth, we take

$$\underline{b}_{1,2}^{(n)} = \underline{b}_{1,2}^{(n-1)} + \eta^{(n)} \underline{g}_{1,2}^{(n)} \tag{4.5}$$

where $\eta^{(n)}$ is a variational parameter and $\underline{g}_{1,2}^{(n)} = \underline{g}_{1,2}^{(n)}(\alpha, \beta)$ are suitably chosen variational vector functions (how they actually are constructed will be discussed in Sections V and VI). Upon using (4.3), the deviations become

$$\underline{F}_{E,H}^{(n)} = \underline{F}_{E,H}^{(n-1)} - \eta^{(n)} f_{E,H}^{(n)} \tag{4.6}$$

in which

$$\underline{f}_E^{(n)} = -Y_0^{1/2} \underline{\nu} \times \iint_{-\infty}^{\infty} \underline{k}_1^+ \times \underline{g}_1^{(n)} \exp(i\underline{k}_1^+ \cdot \underline{r}) \, d\alpha \, d\beta$$

$$+Y_0^{1/2}\underline{\nu} \times \iint_{-\infty}^{\infty} \underline{k}_2^- \times \underline{g}_2^{(n)} \exp(i\underline{k}_2^- \cdot \underline{r}) d\alpha d\beta$$
 (4.7)

$$\underline{f}_{H}^{(n)} = -Z_{0}^{1/2} (\omega \mu_{1})^{-1} \underline{\nu} \times \iint_{-\infty}^{\infty} \underline{k}_{1}^{+} \times (\underline{k}_{1}^{+} \times \underline{g}_{1}^{(n)})$$

$$\cdot \exp(i\underline{k}_{1}^{+} \cdot \underline{r}) d\alpha d\beta$$

$$+Z_0^{1/2}(\omega\mu_2)^{-1}\underline{\nu}\times\iint_{-\infty}^{\infty}\underline{k}_2^{-1}\times(\underline{k}_2^{-1}\times\underline{g}_2^{(n)})$$

$$\cdot\exp(i\underline{k}_2^{-1}\cdot\underline{r})\,d\alpha\,d\beta. \tag{4.8}$$

The expression for $ERR^{(n)}$ can be written as

$$\operatorname{ERR}^{(n)} = \operatorname{ERR}^{(n-1)} - 2 \operatorname{Re} (\eta^{(n)} A^{(n)}) + |\eta^{(n)}|^2 B^{(n)}$$

$$= \operatorname{ERR}^{(n-1)} - |A^{(n)}|^2 / B^{(n)} + |\eta^{(n)} - A^{(n)}|^2 / B^{(n)}$$
(4.9)

in which

$$A^{(n)} = \iint_{S} \left(\underline{F}_{E}^{(n-1)^*} \cdot \underline{f}_{E}^{(n)} + \underline{F}_{H}^{(n-1)^*} \cdot \underline{f}_{H}^{(n)} \right) dA \qquad (4.10)$$

and

$$B^{(n)} = \iint_{S} (|\underline{f}_{E}^{(n)}|^{2} + |\underline{f}_{H}^{(n)}|^{2}) dA$$
 (4.11)

where the asterisk denotes the complex conjugate. (Note, that $B^{(n)}$ is real.) The right-hand side of (4.9) has, as a function of $n^{(n)}$, a minimum at

$$\eta^{(n)} = A^{(n)*}/B^{(n)}. (4.12)$$

Taking $\eta^{(n)}$ to be this value in (4.9), we have that ERR⁽ⁿ⁾ < ERR⁽ⁿ⁻¹⁾, provided $A^{(n)} \neq 0$. This latter condition puts some restriction on the choice of the variational functions $\underline{g}_{1,2}^{(n)}$. Substitution of (4.12) in (4.9) leads to

$$ERR^{(n)} = ERR^{(n-1)} - |A^{(n)}|^2 / B^{(n)}$$
(4.13)

from which it follows that, if $A^{(n)} \neq 0$, an improvement in the satisfaction of the boundary conditions is arrived at, although it is in a "mean" sense.

Substitution of (4.12) in (4.6) leads to

$$\underline{F}_{E,H}^{(n)} = \underline{F}_{E,H}^{(n-1)} - (A^{(n)*}/B^{(n)}) \underline{f}_{E,H}^{(n)}. \tag{4.14}$$

From this, it follows that

$$\iint_{S} \left(\underline{F}_{E}^{(n)*} \cdot \underline{f}_{E}^{(n)} + \underline{F}_{H}^{(n)*} \cdot \underline{f}_{H}^{(n)} \right) dA = 0$$
 (4.15)

an orthogonality property on S that will be of later use. For later purposes we also want to bring out the dependence of $A^{(n)}$ on $g_1^{(n)}$ and $g_2^{(n)}$. To this end, we write

$$A^{(n)} = \iint_{-\infty}^{\infty} (\underline{s}_{1}^{(n-1)^{*}} \cdot \underline{g}_{1}^{(n)} + \underline{s}_{2}^{(n-1)^{*}} \cdot \underline{g}_{2}^{(n)}) \, d\alpha \, d\beta \quad (4.16)$$

where

$$\underline{\underline{s}}_{1}^{(n-1)^{*}} = -Y_{0}^{1/2} \underline{k}_{1}^{+} \times \iint_{S} \underline{\underline{\nu}} \times \underline{F}_{E}^{(n-1)^{*}} \exp\left(i\underline{k}_{1}^{+} \cdot \underline{r}\right) dA$$

$$+Z_{0}^{1/2} (\omega \mu_{1})^{-1} \underline{k}_{1}^{+} \times \left(\underline{k}_{1}^{+} \times \iint_{S} \underline{\underline{\nu}} \times \underline{F}_{H}^{(n-1)^{*}}\right)$$

$$\cdot \exp\left(i\underline{k}_{1}^{+} \cdot \underline{r}\right) dA \qquad (4.17)$$

$$\underline{\underline{s}}_{2}^{(n-1)^{*}} = +Y_{0}^{1/2} \underline{k}_{2}^{-} \times \iint_{S} \underline{\underline{\nu}} \times \underline{F}_{E}^{(n-1)^{*}} \exp\left(i\underline{k}_{2}^{-} \cdot \underline{r}\right) dA$$

$$-Z_{0}^{1/2} (\omega \mu_{2})^{-1} \underline{k}_{2}^{-} \times \left(\underline{k}_{2}^{-} \times \iint_{S} \underline{\underline{\nu}} \times \underline{F}_{H}^{(n-1)^{*}}\right)$$

$$\cdot \exp\left(i\underline{k}_{2}^{-} \cdot \underline{r}\right) dA \qquad (4.18)$$

With this, (4.15) leads to

$$\iint_{-\infty}^{\infty} \left(\underline{s}_{1}^{(n)*} \cdot \underline{g}_{1}^{(n)} + \underline{s}_{2}^{(n)*} \cdot \underline{g}_{2}^{(n)} \right) d\alpha \, d\beta = 0$$
 (4.19)

which exhibits that $\{\underline{s}_1^{(n)}, \underline{s}_2^{(n)}\}$ is orthogonal to $\{\underline{g}_1^{(n)}, \underline{g}_2^{(n)}\}$ in the spectral domain.

In subsequent sections, some particular choices of $g_{1,2}^{(n)}$, which up to now have been completely arbitrary, will be discussed.

V. A SECOND MINIMIZATION STEP

In this section we will investigate how, during the *n*th iteration, we can decrease the right-hand side of (4.13) still further by manipulating the variational vector functions $\underline{g}_{1,2}^{(n)}$. This will be done in such a manner that $B^{(n)}$ is minimized, while keeping $A^{(n)}$ constant. In view of (4.19), the value of $A^{(n)}$ remains unchanged if, in the right-hand side of (4.16), for given n, the functions $\underline{g}_{1,2}^{(n)}$ are replaced by $\underline{g}_{1,2}^{(n)} - \underline{\xi}^{(n)} \underline{g}_{1,2}^{(n-1)}$, where $\underline{\xi}^{(n)}$ is a second variational parameter. Carrying out this replacement in (4.7) and (4.8), we are led to new values $\underline{f}_{E,H}^{(n)}$ that are given by

$$\underline{f}_{E,H}^{(n)} = \underline{f}_{E,H}^{(n)} - \xi^{(n)} \underline{f}_{E,H}^{(n-1)}. \tag{5.1}$$

Using this in (4.11), a new value $\underline{B}^{(n)}$ of $B^{(n)}$ is constructed, that follows as

$$\overline{B}^{(n)} = B^{(n)} - |C^{(n)}|^2 / B^{(n-1)} + |\xi^{(n)} - C^{(n)*} / B^{(n-1)}|^2 B^{(n-1)}$$

(5.2)

where

$$C^{(n)} = \iint_{S} \left(\underline{f}_{E}^{(n)^{*}} \cdot \underline{f}_{E}^{(n-1)} + \underline{f}_{H}^{(n)^{*}} \cdot \underline{f}_{H}^{(n-1)} \right) dA.$$
 (5.3)

The right-hand side of (5.2) has, as a function of $\xi^{(n)}$, a minimum at

$$\xi^{(n)} = C^{(n)*}/B^{(n-1)}. (5.4)$$

Taking, in (5.2), $\xi^{(n)}$ to be this value, we arrive at

$$\bar{B}^{(n)} = B^{(n)} - |C^{(n)}|^2 / B^{(n-1)}. \tag{5.5}$$

First of all, this shows that $\overline{B}^{(n)} < B^{(n)}$, if $C^{(n)} \neq 0$. Further, it follows by substituting (5.4) in (5.1), that

$$\iint_{S} \left(\underline{f}_{E}^{(n)*} \cdot \underline{f}_{E}^{(n-1)} + \underline{f}_{H}^{(n)*} \cdot \underline{f}_{H}^{(n-1)} \right) dA = 0.$$
 (5.6)

If the original sequence of functions $\{\underline{f}_{E,H}^{(n)}\}$ was already such that the right-hand side of (5.3) vanished, then no improvement will be attained in this second minimization step. Note that this is consistent with (5.6)! Hence, the second minimization automatically stops after being carried out once. The resulting expression for the improved integrated square error follows as

$$\overline{ERR}^{(n)} = ERR^{(n-1)} - |A^{(n)}|^2 / (B^{(n)} - |C^{(n)}|^2 / B^{(n-1)})$$
 (5.7)

in which $A^{(n)}$, $B^{(n)}$, and $C^{(n)}$ are given by (4.10), (4.11), and (5.3), respectively.

In the next section we shall discuss a procedure that leads, in each iteration, to the generation of a particular value of $\underline{g}_{1,2}^{(n)}$. Once $\xi^{(n)}$ has been determined, we then replace $g_{1,2}^{(n)}$ by

$$\underline{\overline{g}}_{1,2}^{(n)} = g_{1,2}^{(n)} - \xi^{(n)} g_{1,2}^{(n-1)}$$
(5.8)

where $\xi^{(n)}$ is given by (5.4).

Now, with $\overline{g}_{1,2}^{(n)}$, we again carry out the procedure of Section IV. The result is that (4.14) and (4.15) are replaced by

$$\overline{F}_{E,H}^{(n)} = \underline{F}_{E,H}^{(n-1)} - (A^{(n)*}/\overline{B}^{(n)}) \underline{f}_{E,H}^{(n)}$$
(5.9)

and

$$\iint_{S} \left(\overline{\underline{F}}_{E}^{(n)*} \cdot \underline{\overline{f}}_{E}^{(n)} + \overline{\underline{F}}_{H}^{(n)*} \cdot \underline{\overline{f}}_{H}^{(n)} \right) dA = 0$$
 (5.10)

respectively. In the latter, $\overline{F}_{E,H}^{(n)}$ (c.f., (4.4)) results from the $\overline{b}_{1,2}^{(n)}$ that follow from (4.5).

From now on, we assume that this entire procedure has been carried out in all iterations. (Note that the second minimization step can only be carried out from n = 2 onward, since $g_{1,2}^{(0)}$ is not defined). On this assumption, (5.9) can be replaced by

$$\overline{F}_{E,H}^{(n)} = \overline{F}_{E,H}^{(n-1)} - (A^{(n)*}/\overline{B}^{(n)}) \, \overline{f}_{E,H}^{(n)}$$
(5.11)

with

$$\overline{F}_{E,H}^{(0)} = F_{E,H}^{(0)}$$
 and $\overline{F}_{E,H}^{(1)} = F_{E,H}^{(1)}$

while (4.10) can be replaced by

$$A^{(n)} = \iint_{S} \left(\overline{F}_{E}^{(n-1)*} \cdot \underline{f}_{E}^{(n)} + \overline{F}_{H}^{(n-1)*} \cdot \underline{f}_{H}^{(n)} \right) dA. \tag{5.12}$$

Further, (5.1), (5.3), (5.4), and (5.6) are then replaced by

$$\underline{f}_{E,H}^{(n)} = \underline{f}_{E,H}^{(n)} - \xi^{(n)} \underline{f}^{(n-1)}$$

$$(5.13)$$

$$C^{(n)} = \iint_{S} \left(\underline{f}_{E}^{(n)*} \cdot \underline{\overline{f}}_{E}^{(n-1)} + \underline{f}_{H}^{(n)*} \cdot \underline{\overline{f}}_{H}^{(n-1)} \right) dA \qquad (5.14)$$

$$\xi^{(n)} = C^{(n)*}/\overline{B}^{(n-1)} \tag{5.15}$$

$$\iint_{S} \left(\underline{\overline{f}}_{E}^{(n)^{*}} \cdot \underline{\overline{f}}_{E}^{(n-1)} + \underline{\overline{f}}_{H}^{(n)^{*}} \cdot \underline{\overline{f}}_{H}^{(n-1)} \right) dA = 0$$
 (5.16)

respectively. Multiplying the complex conjugate of (5.11) by $\overline{f}_{E,H}^{(n-1)}$, integrating over S, applying (5.16) and using (5.10) with n replaced by n-1, we obtain the result

$$\iint_{S} \left(\underline{\overline{F}}_{E}^{(n)*} \cdot \underline{\overline{f}}_{E}^{(n-1)} + \underline{\overline{F}}_{H}^{(n)*} \cdot \underline{\overline{f}}_{H}^{(n-1)} \right) dA = 0$$
 (5.17)

which shows that $\{\bar{F}_E^{(n)}, \bar{F}_H^{(n)}\}$ is orthogonal to $\{\bar{f}_E^{(n-1)}, \bar{f}_H^{(n-1)}\}$. In the spectral domain, the replaced values of $\bar{E}_{E,H}^{(n-1)}$ lead, via (4.17) and (4.18), to replaced values of $\bar{g}_{1,2}^{(n-1)}$. In order to arrive at an orthogonality relation between $\{\bar{g}_1^{(n)}, \bar{g}_2^{(n)}\}$ and $\{g_1^{(n)}, g_2^{(n)}\}$, we observe that, by substituting (5.13) in (5.10), and using (5.17), we arrive at

$$\iint_{S} \left(\overline{\underline{F}}_{E}^{(n)*} \cdot \underline{f}_{E}^{(n)} + \overline{\underline{F}}_{H}^{(n)*} \cdot \underline{f}_{H}^{(n)} \right) dA = 0.$$
 (5.18)

By substituting (4.7), (4.8), and the replaced versions of (4.17) and (4.18) with n-1 replaced by n, into (5.18), we obtain the desired orthogonality relation in the spectral domain

$$\iint_{-\infty}^{\infty} \left(\underline{\underline{s}}_{1}^{(n)*} \cdot \underline{g}_{1}^{(n)} + \underline{\underline{s}}_{2}^{(n)*} \cdot \underline{g}_{2}^{(n)} \right) d\alpha d\beta = 0.$$
 (5.19)

Equation (5.19) is the replaced form of (4.19) and will be of later use in Section VI.

VI. GENERATION OF THE VARIATIONAL FUNCTIONS

As we have seen in Section IV, an iterative improvement in the satisfaction of the boundary conditions at the interface is only arrived at if, in each iteration, $A^{(n)} \neq 0$. The spectral-domain equivalent of (5.12) shows that this can be guaranteed, if we take

$$g_{1,2}^{(n)} = \underline{\overline{s}}_{1,2}^{(n-1)}. \tag{6.1}$$

Substituting (6.1) in the spectral domain equivalent of (5.12) we obtain

$$A^{(n)} = \iint_{-\infty}^{\infty} (|\underline{s}_{1}^{(n-1)}|^{2} + |\underline{s}_{2}^{(n-1)}|^{2}) d\alpha d\beta.$$
 (6.2)

Substitution of (6.1) in (5.19) leads to

$$\iint_{-\infty}^{\infty} \left(\underline{\underline{s}}_{1}^{(n)*} \cdot \underline{\underline{s}}_{1}^{(n-1)} + \underline{\underline{s}}_{2}^{(n)*} \cdot \underline{\underline{s}}_{2}^{(n-1)} \right) d\alpha d\beta = 0. \tag{6.3}$$

The choice (6.1) has another advantage. As we have seen in Section V, the value of $\xi^{(n)}$ can only be determined after the minimization of Section IV has been carried out. However, if we could calculate $\xi^{(n)}$ beforehand, it would not be necessary to return to the iteration of Section IV a second time, since the minimization of Section IV could then be carried out with $\overline{g}_{1,2}^{(n)}$. We shall now show that the choice (6.1) does yield possibility of calculating $\xi^{(n)}$ beforehand. To this end, we substitute into (5.15) the value

$$C^{(n)} = (\overline{B}^{(n-1)}/A^{(n-1)^*}) \left(\iint_{S} \left(\underline{f}_{E}^{(n)^*} \cdot \overline{\underline{F}}_{E}^{(n-2)} + \underline{f}_{H}^{(n)^*} \cdot \overline{\underline{F}}_{H}^{(n-2)} \right) dA - \iint_{S} \left(\underline{f}_{E}^{(n)^*} \cdot \overline{\underline{F}}_{E}^{(n-1)} + \underline{f}_{H}^{(n)^*} \cdot \overline{\underline{F}}_{H}^{(n-1)} \right) dA \right)$$

$$(6.4)$$

which follows from (5.14) and (5.11) with n replaced by n-1. However, we also have

TABLE I THE ITERATION SCHEME; $\underline{b}_1^{(0)}$ and $\underline{b}_2^{(0)}$ are Input Data (Initial Values)

$$\iint_{S} \left(\underline{f}_{E}^{(n)^{*}} \cdot \underline{F}_{E}^{(n-2)} + \underline{f}_{H}^{(n)^{*}} \cdot \underline{F}_{H}^{(n-2)} \right) dA$$

$$= \iint_{-\infty}^{\infty} \left(\underline{\underline{s}}_{1}^{(n-1)^{*}} \cdot \underline{\underline{s}}_{1}^{(n-2)} + \underline{\underline{s}}_{2}^{(n-1)^{*}} \cdot \underline{\underline{s}}_{2}^{(n-2)} \right) d\alpha d\beta \quad (6.5)$$

in which (4.7), (4.8), the replaced versions of (4.17) and (4.18), and (6.1) have been used. In view of (5.19) and (6.1) with n replaced by n-1, the right-hand side of (6.5) vanishes. Hence, from (5.12), (5.15), (6.4), and (6.5) it follows that

$$\xi^{(n)} = -A^{(n)}/A^{(n-1)}. (6.6)$$

Consequently, $\xi^{(n)}$ can be computed in advance, provided the value of $A^{(n-1)}$ is available. Finally, $\underline{\underline{g}}_{1,2}^{(n)}$ is obtained as follows

$$\underline{\underline{g}}_{1,2}^{(n)} = \underline{\underline{s}}_{1,2}^{(n-1)} + (A^{(n)}/A^{(n-1)}) \underline{\underline{g}}_{1,2}^{(n-1)}, \quad n \ge 2$$
 (6.7)

while

$$\underline{g}_{1,2}^{(1)} = \underline{s}_{1,2}^{(0)}. \tag{6.8}$$

The complete iteration scheme is shown in Table I, where the bars over the symbols have been omitted.

In Appendix IV it is shown that the sequence of functions $\{\underline{\overline{s}}_{1,2}^{(n)}, n=0,1,2,\cdots\}$ and the sequence $\{\overline{f}_{E,H}^{(n)}, n=1,2,3,\cdots\}$ are orthogonal sequences. As such, the former can be used to expand any spectral field amplitude $\underline{b}_{1,2}$, while the latter can be used to expand any tangential surface field $F_{E,H}$. Of course, the actual use of such expansions requires the storage of the two sequences for all values of the variables that are needed in a numerical integration and up to some order which is large enough to lead to sufficiently small integrated square errors. In practice, the relevant storage will have to be done on peripheral storage (e.g., disk files, tape).

VII. CONCLUDING REMARKS

A scheme has been developed by which the electromagnetic field that is reflected and transmitted at a rough interface between two different media can be computed in an iterative way. The method uses a wave-function expansion technique, where the electromagnetic field equations and the radiation condition are satisfied analytically, while the boundary conditions at the interface are satisfied numerically. In two steps, the integrated square error in the boundary conditions is minimized, after which a particular choice of the variational functions in the spectral domain leads to a relatively simple scheme. The convergence of the iterative scheme is proved. Experience with some two-dimensional scattering problems [28] has shown that the technique is a very efficient one. Some final remarks will be made.

Initial Guess

In the preceding sections, we arrived at values of \underline{b}_1 and \underline{b}_2 that in their turn determine the reflected and transmitted fields. The only freedom we still have is the choice of the initial values $\underline{b}_1^{(0)}$ and $\underline{b}_2^{(0)}$. In our case, where the roughness is considered as a deviation from an otherwise plane interface, a natural choice for $\underline{b}_1^{(0)}$ and $\underline{b}_2^{(0)}$ are the Sommerfeld-Weyl plane interface values of these quantities. However, other values for the initial guess could be used as well (for example, the Kirchhoff or the physical-optics approximation).

Computation of the Integrals

In each iteration step we only have to compute direct and inverse Fourier transforms. This is efficiently accomplished with the aid of the fast Fourier transform algorithm. The remaining integrals leading to the values of $A^{(n)}$ and $B^{(n)}$ are computed with the aid of linear interpolation. Further, the integrands in the Fourier integrals contain the exponential functions $\exp(i\gamma_1 z)$ and $\exp(i\gamma_2 z)$, which remain unaltered in the iteration process. Hence, if sufficient storage capacity is available, these functions can be stored for the interface under consideration and for the values of α and β in the integration.

Periodic Interface

In case we are dealing with a two-dimensional periodic interface, we replace the spectral integrations $\iint_{-\infty}^{\infty} d\alpha \ d\beta$ by double Fourier series $\sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty}$ while the spatial integrations $\iint_{\mathcal{S}} dA$ reduce to integrations over a single period.

APPENDIX I RECIPROCITY RELATION

The frequency-domain reciprocity relation interrelates two nonidentical, admissible electromagnetic states "A" and "B"

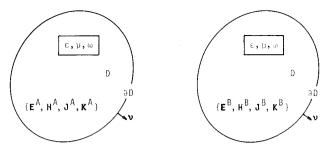


Fig. 3. States "A" and "B" in the bounded domain D.

of the same angular frequency ω , that are present in the same bounded domain D (Fig. 3). Using Maxwell's equations with source distributions J and K

$$\underline{\nabla} \times \underline{H} + i\omega \epsilon \underline{E} = \underline{J}$$

$$\underline{\nabla} \times \underline{E} - i\omega \mu \underline{H} = -\underline{K}$$
(A1)

we arrive at

$$\underline{\nabla} \cdot (\underline{E}^A \times \underline{H}^B - \underline{E}^B \times \underline{H}^A) = -\underline{E}^A \cdot \underline{J}^B + \underline{E}^B \cdot \underline{J}^A - \underline{H}^B \cdot \underline{K}^A + \underline{H}^A \cdot \underline{K}^B \quad (A2)$$

being the local form of the reciprocity relation. Integration of (A2) over D and application of Gauss' divergence theorem yield the global form of the reciprocity relation

$$\iint_{\partial D} \underline{\nu} \cdot (\underline{E}^A \times \underline{H}^B - \underline{E}^B \times \underline{H}^A) dA$$

$$= \iiint_{D} (-\underline{E}^A \cdot \underline{J}^B + \underline{E}^B \cdot \underline{J}^A - \underline{H}^B \cdot \underline{K}^A + \underline{H}^A \cdot \underline{K}^B) dV.$$
(A3)

In (A3), ∂D denotes the boundary surface of D and $\underline{\nu}$ denotes the unit vector in the direction of the outward normal to ∂D .

APPENDIX II GREEN'S STATE OF THE TWO-MEDIA PROBLEM

In this appendix we derive surface source-integral representations for the reflected and transmitted fields in the two-media problem of Fig. 4. The configuration is excited by an incident field $\{\underline{E}^i,\underline{H}^i\}$, the sources of which are located in D_1 . The reflected and transmitted fields satisfy the homogeneous Maxwell's equations in D_1 and D_2

$$\underline{\nabla} \times \underline{H} + i\omega e \, \underline{E} = \underline{0}$$

$$\underline{\nabla} \times E - i\omega \mu \underline{H} = \underline{0}$$
(B1)

where in D_1 : $\epsilon = \epsilon_1$, $\mu = \mu_1$ and in D_2 : $\epsilon = \epsilon_2$, $\mu = \mu_2$. Further, in D_1 , $\{\underline{E},\underline{H}\} = \{\underline{E}^r,\underline{H}^r\}$ denotes the reflected field, while, in D_2 , $\{\underline{E},\underline{H}\} = \{\underline{E}^t,\underline{H}^t\}$ denotes the transmitted field. In addition, the reflected field satisfies at infinity the radiation condition. In \mathbb{R}^3 , we define the electric-current Green's state as the field $\{\underline{E}^j,\underline{H}^j\}$ that satisfies the conditions

$$\underline{\nabla} \times \underline{H}^{j} + i\omega\epsilon \, \underline{E}^{j} = \underline{j} \, \delta(\underline{r} - \underline{r}'),$$

$$\underline{r} \in D_{1} \cup D_{2}, \ \underline{r}' \in \mathbb{R}^{3}, \quad (B2)$$

$$\underline{\nabla} \times \underline{E}^{j} - i\omega\mu \, \underline{H}^{j} = \underline{0},$$
where $\epsilon = \epsilon_{1}$, $\mu = \mu_{1}$ in D_{1} and $\epsilon = \epsilon_{2}$, $\mu = \mu_{2}$ in D_{2} , while

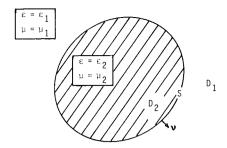


Fig. 4. The configuration of the two-media problem.

 $\underline{\nu} \times \underline{E}^{j} = \text{continuous across } S$ $\nu \times H^{j} = \text{continuous across } S$ (B3)

and in which $\underline{\nu}$ is the unit vector along the outward normal to S. Further, the field $\{\underline{E}^{j}, \underline{H}^{j}\}$ satisfies the radiation condition at infinity. Application of (A3) to the domain D_1 and to the fields $\{\underline{E}^{A}, \underline{H}^{A}\} = \{\underline{E}^{r}, \underline{H}^{r}\}$ and $\{\underline{E}^{B}, \underline{H}^{B}\} = \{\underline{E}^{j}, \underline{H}^{j}\}$ yields

$$\iint_{S} \left[(\underline{\nu} \times \underline{E}^{r}) \cdot \underline{H}^{j} + (\underline{\nu} \times \underline{H}^{r}) \cdot \underline{E}^{j} \right] dA = \left\{ \underline{j} \cdot \underline{E}^{r} (\underline{r}'), 0 \right\}$$
when $r' \in \{D_{1}, D_{2}\}$. (B4)

Application of (A3) to the domain D_2 and to the fields

$$\{\underline{E}^A, \underline{H}^A\} = \{\underline{E}^t, \underline{H}^t\}$$
 and $\{\underline{E}^B, \underline{H}^B\} = \{\underline{E}^j, \underline{H}^j\}$

yields

$$\iint_{S} \left[(\underline{\nu} \times \underline{E}^{t}) \cdot \underline{H}^{j} + (\underline{\nu} \times \underline{H}^{t}) \cdot \underline{E}^{j} \right] \, dA = \{0, -\underline{j} \cdot \underline{E}^{t}(\underline{r}')\}$$

when
$$\underline{r}' \in \{D_1, D_2\}$$
. (B5)

Subtraction of (B5) from (B4), and use of (B3) leads to the expression

$$\iint_{S} \left[(\underline{\nu} \times \underline{E}^{r} - \underline{\nu} \times \underline{E}^{t}) \cdot \underline{H}^{j} + (\underline{\nu} \times \underline{H}^{r} - \underline{\nu} \times \underline{H}^{t}) \cdot \underline{E}^{j} \right] dA$$

$$= \{ \underline{j} \cdot \underline{E}^{r}(\underline{r}'), \underline{j} \cdot \underline{E}^{t}(\underline{r}') \}, \text{ when } \underline{r}' \in \{D_{1}, D_{2}\}.$$
(B6)

Note that for $\underline{\underline{j}}$ we can successively take the Cartesian unit vectors and that $\{\underline{E}^j, \underline{H}^j\}$ depends linearly on $\underline{\underline{j}}$. The field $\{\underline{E}^j, \underline{H}^j\}$ is just the electromagnetic field excited by a point source with electric current density $\underline{\underline{J}} = j \delta(r - r')$.

Similarly, when the magnetic-current Green's state $\{\underline{E}^k, \underline{H}^k\}$ that is generated by the source distribution

$$\underline{K} = \underline{k} \, \delta(\underline{r} - \underline{r}') \tag{B7}$$

is introduced, we arrive at the expression

$$\iint_{S} \left[(\underline{\nu} \times \underline{E}^{r} - \underline{\nu} \times \underline{E}^{t}) \cdot \underline{H}^{k} + (\underline{\nu} \times \underline{H}^{r} - \underline{\nu} \times \underline{H}^{t}) \cdot \underline{E}^{k} \right] dA$$

$$= -\{ \underline{k} \cdot \underline{H}^{r}(\underline{r}'), \underline{k} \cdot \underline{H}^{t}(\underline{r}') \}, \quad \text{when } \underline{r}' \in \{D_{1}, D_{2}\}.$$
(B8)

It is obvious that $\{\underline{E}^k, \underline{H}^k\}$ depends linearly on \underline{k} .

$$\underline{\nu} \times \underline{E}^{i} + \underline{\nu} \times \underline{E}^{r} - \underline{\nu} \times \underline{E}^{t} = \underline{0}
\underline{\nu} \times \underline{H}^{i} + \underline{\nu} \times \underline{H}^{r} - \underline{\nu} \times \underline{H}^{t} = \underline{0}$$
when $\underline{r} \in S$
(B9)

we arrive at the result

$$\{\underline{j} \cdot \underline{E}^{r}(\underline{r}'), \underline{j} \cdot \underline{E}^{t}(\underline{r}')\} = \iint_{S} [(-\underline{\nu} \times \underline{E}^{i}) \cdot \underline{H}^{i} + (-\underline{\nu} \times \underline{H}^{i}) \cdot \underline{E}^{j}] dA \qquad (B10)$$

$$-\{\underline{k} \cdot \underline{H}^{r}(\underline{r}'), \underline{k} \cdot \underline{H}^{t}(\underline{r}')\} = \iint_{S} [(-\underline{\nu} \times \underline{E}^{i}) \cdot \underline{H}^{k} + (-\underline{\nu} \times \underline{H}^{i}) \cdot \underline{E}^{k}] dA \qquad \text{when } \underline{r}' \in \{D_{1}, D_{2}\}. \qquad (B11)$$

These are the desired surface-source representations for the reflected and the transmitted fields. If $\{\underline{E}^j, \underline{H}^j\}$ were known, (B10) would lead to $\underline{E}^{r,t}$ at any $\underline{r}' \in D_{1,2}$, while if $\{\underline{E}^k, \underline{H}^k\}$ were known, (B11) would lead to $\underline{H}^{r,t}$ at any $\underline{r}' \in D_{1,2}$.

APPENDIX III SUFFICIENCY OF AN ERROR CRITERION IN THE BOUNDARY CONDITIONS

In this appendix the existence is assumed of some field $\{\underline{\widetilde{E}}^r, \underline{\widetilde{H}}^r\}$ in D_1 and some field $\{\underline{\widetilde{E}}^t, \underline{\widetilde{H}}^t\}$ in D_2 , which satisfy Maxwell's equations (B1) and the radiation condition at infinity. It is also assumed that they violate the boundary conditions at S, i.e.,

$$\underline{\nu} \times \underline{E}^{t} + \underline{\nu} \times \underline{\widetilde{E}}^{r} \neq \underline{\nu} \times \underline{\widetilde{E}}^{t}$$

$$\text{when } \underline{r} \in S. \tag{C1}$$

$$\nu \times \underline{H}^{t} + \underline{\nu} \times \widetilde{H}^{r} \neq \underline{\nu} \times \widetilde{H}^{t}$$

It is then shown that a certain approximation in the boundary conditions leads to a certain degree of approximation in the reflected and transmitted fields. Since Maxwell's equations and the radiation condition are satisfied, relations of the type (B6) and (B8) also hold for $\{\underline{\widetilde{E}}^r, \underline{\widetilde{H}}^r\}$ in D_1 and $\{\underline{\widetilde{E}}^t, \underline{\widetilde{H}}^t\}$ in D_2 :

$$\{\underline{j} \cdot \underline{\widetilde{E}}^{r}(\underline{r}'), \underline{j} \cdot \underline{\widetilde{E}}^{t}(\underline{r}')\} = \iint_{\mathcal{S}} [(\underline{\nu} \times \underline{\widetilde{E}}^{r} - \underline{\nu} \times \underline{\widetilde{E}}^{t}) \cdot \underline{H}^{j} + (\underline{\nu} \times \underline{\widetilde{H}}^{r} - \underline{\nu} \times \underline{\widetilde{H}}^{t}) \cdot \underline{E}^{j}] dA$$
(C2)

$$-\{\underline{k}\cdot\widetilde{\underline{H}}^{r}(\underline{r}'),\underline{k}\cdot\widetilde{\underline{H}}^{t}(\underline{r}')\} = \iint_{S} \left[(\underline{\nu}\times\underline{\widetilde{E}}^{r}-\underline{\nu}\times\underline{\widetilde{E}}^{t})\cdot\underline{H}^{k} + (\underline{\nu}\times\widetilde{\underline{H}}^{r}-\underline{\nu}\times\widetilde{\underline{H}}^{t})\cdot\underline{E}^{k} \right] dA$$
(C3)

where $\underline{r}' \in \{D_1, D_2\}$. Combining (C2) with (B10), and (C3) with (B11), and applying Cauchy-Schwarz's inequality, we obtain the following inequalities

$$|\underline{j} \cdot \underline{E}^{r}(\underline{r}') - \underline{j} \cdot \underline{\widetilde{E}}^{r}(\underline{r}')|^{2} \leq (\text{ERR}_{E} + \text{ERR}_{H}) \iint_{S} (Z_{0} |\underline{H}^{j}|^{2} + Y_{0} |\underline{E}^{j}|^{2}) dA$$

$$(C4)$$

$$|\underline{k} \cdot \underline{H}^{r}(\underline{r}') - \underline{k} \cdot \underline{\widetilde{H}}^{r}(\underline{r}')|^{2} \leq (\text{ERR}_{E} + \text{ERR}_{H}) \iint_{S} (Z_{0} |\underline{H}^{k}|^{2})$$

 $+ Y_0 |E^k|^2 dA$

(C5)

$$|\underline{j}\cdot\underline{E}^t(\underline{r}')-\underline{j}\cdot\underline{\widetilde{E}}^t(\underline{r}')|^2 \leq (\mathrm{ERR}_E+\mathrm{ERR}_H)\iint_S (Z_0|\underline{H}^j|^2 \qquad A^{(t)}=\iint_{-\infty}^\infty |\underline{s}^{(t-1)}|^2 \ d\alpha \ d\beta \ .$$

$$+ Y_0 |\underline{E}^j|^2) dA \qquad (C6)$$

$$|\underline{k} \cdot \underline{H}^{t}(\underline{r}') - \underline{k} \cdot \underline{\widetilde{H}}^{t}(\underline{r}')|^{2} \leq (\text{ERR}_{E} + \text{ERR}_{H}) \iint_{S} (Z_{0} |\underline{H}^{k}|^{2}$$

$$(4.18)$$

where $\underline{r}' \in \{D_1, D_2\}$, and where the integrated square errors in the tangential electric and magnetic fields at S have been introduced as

$$ERR_{E} = \iint_{\Sigma} Y_{0} |\underline{\nu} \times \underline{E}^{i} + \underline{\nu} \times \underline{\widetilde{E}}^{r} - \underline{\nu} \times \underline{\widetilde{E}}^{t}|^{2} dA$$
 (C8)

$$ERR_{H} = \iint_{S} Z_{0} |\underline{\nu} \times \underline{H}^{i} + \underline{\nu} \times \underline{\widetilde{H}}^{r} - \underline{\nu} \times \underline{\widetilde{H}}^{t}|^{2} dA.$$
 (C9)

The factor $Y_0 = (\epsilon_0/\mu_0)^{1/2}$ is the wave admittance in free space, while $Z_0 = (\mu_0/\epsilon_0)^{1/2}$ is the wave impedance in free space. They have been included for dimensional convenience. Since the surface integrals containing the Green's states are bounded $(r' \notin S)$, it follows that if

$$(ERR_E + ERR_H) \to 0 \tag{C10}$$

then

$$\underline{j} \cdot \underline{E}^{r}(\underline{r}') \to \underline{j} \cdot \underline{E}^{r}(\underline{r}')$$

for any
$$\underline{r}' \in D_1$$
 (C11)

$$\underline{k} \cdot \underline{\widetilde{H}}^r(\underline{r}') \to \underline{k} \cdot \underline{H}^r(\underline{r}')$$

and

$$\underline{j} \cdot \underline{\widetilde{E}}^{t}(\underline{r}') \to \underline{j} \cdot \underline{E}^{t}(\underline{r}')$$
 for any $r' \in D_2$. (C12)

$$\underline{k} \cdot \widetilde{H}^{t}(r') \rightarrow k \cdot H^{t}(r')$$

Because of the arbitrariness of j and k, (C11) and (C12) lead to

$$\{\widetilde{E}^r, \widetilde{H}^r\} \to \{E^r, H^r\} \quad \text{when } r' \in D,$$
 (C13)

$$\{\widetilde{E}^t, \widetilde{H}^t\} \rightarrow \{E^t, H^t\} \quad \text{when } r' \in D_2.$$
 (C14)

The error criterion (C10) has been used in the main text.

APPENDIX IV ORTHOGONALITY PROPERTIES

In this appendix it is proved that the sequences of functions obtained from the minimization schemes developed in Sections V and VI are completely orthogonal. The bars over the relevant symbols will be omitted, as well as the subscripts E, H, 1, and 2, that refer to the E- and H-field contributions to the different field quantities. In this short-hand notation the following relations are needed

$$g^{(1)} = \underline{s}^{(0)} \tag{D1}$$

$$g^{(i)} = \underline{s}^{(i-1)} + (A^{(i)}/A^{(i-1)}) g^{(i-1)}$$
 when $i \ge 2$ (D2)

$$\underline{g}^{(i)} = \underline{s}^{(i-1)} + (A^{(i)}/A^{(i-1)})\underline{g}^{(i-1)} \quad \text{when } i \ge 2$$
 (D2)
$$\underline{F}^{(i)} = \underline{F}^{(i-1)} - (A^{(i)*}/B^{(i)})\underline{f}^{(i)} \quad \text{when } i \ge 1$$
 (D3)

in which

$$A^{(i)} = \iint_{-\infty}^{\infty} |\underline{s}^{(i-1)}|^2 d\alpha d\beta.$$
 (D4)

(C6) These follow from (6.8), (6.7), (5.11), and (6.2), respectively. Further, the following relation holds (c.f., (4.7), (4.8), (4.17),

$$\iint_{S} \underline{F}^{(i-1)^*} \cdot \underline{f}^{(j)} dA = \iint_{-\infty}^{\infty} \underline{s}^{(i-1)^*} \cdot \underline{g}^{(j)} d\alpha d\beta \qquad (D5)$$

when $\{i, j\} = 1, 2, 3, \cdots$. From (D1) and (D2), we can conclude that

$$\underline{g}^{(i)} = A^{(i)} \sum_{j=1}^{i} \underline{s}^{(j-1)} / A^{(j)}$$
 when $i \ge 1$. (D6)

The proof of the orthogonality relationships will be given by induction. To this end, assume that

$$\iint_{-\infty}^{\infty} \underline{s}^{(i-1)^*} \cdot \underline{s}^{(j-1)} d\alpha d\beta = 0 \quad \text{when } i \neq j$$
 (D7)

holds for $\{i, j\} = 1, 2, 3, \dots, k$, where $k \ge 3$. Now, from (6.3) it follows already that (D7) holds for $\{i, j\} = 1, 2$. Next, (D6) and (D7) lead to the relation

$$\iint_{-\infty}^{\infty} \underline{s}^{(i-1)^*} \cdot \underline{g}^{(k)} d\alpha d\beta = A^{(k)} \quad \text{when } i \leq k.$$
 (D8)

Multiplying the complex conjugate of (D3) by $f^{(k)}$, and using (D5), one arrives at the result

$$\iint_{-\infty}^{\infty} \underline{s}^{(i)*} \cdot \underline{g}^{(k)} d\alpha d\beta = \iint_{-\infty}^{\infty} \underline{s}^{(i-1)*} \cdot \underline{g}^{(k)} d\alpha d\beta$$
$$- (A^{(i)}/B^{(i)}) \iint_{S} \underline{f}^{(i)*} \cdot \underline{f}^{(k)} dA.$$
(D9)

When $i \le k - 1$, (D8) shows that the left-hand side and the first term on the right-hand side of (D9) are both equal to $A^{(k)}$, from which it follows that

$$\iint_{\mathbf{C}} \underline{f}^{(i)*} \cdot \underline{f}^{(k)} dA = 0 \quad \text{when } i \leq k-1.$$
 (D10)

Note that (D10) is one of the desired orthogonality relations. For the next step, one requires the relation

$$\iint_{S} \underline{F}^{(i)*} \cdot \underline{f}^{(j)} dA = 0 \quad \text{when } i = j \text{ or } i = j + 1.$$
(D11)

This follows from (5.10) and (5.17). Multiplying the expression that results from (D3) with i = k successively by $f^{(k-2)}$, $f^{(k-3)}$, \cdots , $f^{(1)}$, integrating over S, and using (D11), one successively obtains the conditions

$$\iint_{S} \underline{F}^{(k)*} \cdot \underline{f}^{(k-2)} dA = 0$$

$$\iint_{S} \underline{F}^{(k)*} \cdot \underline{f}^{(k-3)} dA = 0$$

 $\iint_{\mathcal{L}} \underline{F}^{(k)*} \cdot \underline{f}^{(1)} dA = 0.$ (D12)

Together with (D11) for i = k, j = k, and i = k, j = k - 1, (D12)

$$\iint_{S} \underline{F}^{(k)*} \cdot \underline{f}^{(j)} dA = 0 \quad \text{when } j \le k.$$
 (D13)

From (D13) and (D5) it follows that

$$\iint_{-\infty}^{\infty} \underline{s}^{(k)*} \cdot \underline{g}^{(j)} d\alpha d\beta = 0 \quad \text{when } j \leq k.$$
 (D14)

Upon substituting (D2) in (D14) and reusing (D14), one finally obtains

$$\iint_{-\infty}^{\infty} \underline{s}^{(k)*} \cdot \underline{s}^{(j-1)} d\alpha d\beta = 0 \quad \text{when } j \leq k.$$
 (D15)

Hence the subsequent member $\underline{s}^{(k)}$ of the sequence $\{\underline{s}^{(0)},\underline{s}^{(1)},\underline{s}^{(2)},\cdots,\underline{s}^{(k-1)}\}$ is orthogonal to all previous members. Induction then completes the proof of (D7) for all i and j. As a consequence, (D10) leads to

$$\iint_{S} \underline{f}^{(i)*} \cdot \underline{f}^{(j)} dA = 0 \quad \text{when } i \neq j$$
 (D16)

for all i and j.

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