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Rayleigh methods applied to electromagnetic scattering from gratings in general homogeneous media

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The application of the Rayleigh-Fourier and Rayleigh least-squares methods to reflection and transmission of electromagnetic waves at periodic rough interfaces between general homogeneous media is considered. For the calculation of the reflected and transmitted amplitudes, it is shown that the Rayleigh-Fourier method converges when the Waterman-Fourier method does and is therefore not limited by the validity of the Rayleigh hypothesis. It is also shown that the Rayleigh least-squares method applied to boundary-value problems is numerically convergent if the solution exists uniquely. A numerical application of both methods to the case of a sinusoidal interface between a perfectly conducting medium and a bi-isotropic medium corroborates these results. We indicate very general conditions under which the Rayleigh-Fourier and Rayleigh least-squares methods have the properties indicated above; they include anisotropic elastic solid media in particular. [S1063-651X(96)02811-5]

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I. INTRODUCTION

Among the various methods classically used to deal with reflection and transmission of waves at rough interfaces [1–3], the Rayleigh methods are particularly simple to implement. They are based on the hypothesis, postulated by Rayleigh [4], that the field scattered from a rough surface is representable as a sum of outgoing and evanescent waves everywhere on and above the surface. The determination of the amplitudes of those waves is achieved numerically by projecting the boundary conditions on a given set of basis functions; there are therefore as many Rayleigh methods as sets of basis functions used to project the boundary conditions on.

The Rayleigh hypothesis, regarded by some authors as dubious, gave rise to a debate, some accounts of which are given by Fortuin [5] and Bolomey and Wirgin [6]. Necessary and/or sufficient conditions of the validity of the Rayleigh hypothesis were established by Petit and Cadilhac [7], Nevière and Cadilhac [8], Millar [9,10] and van den Berg and Fokkema [11,12] for extended interfaces. The case of cylindrical obstacles has also been studied [13].

It has been found, however, that the Rayleigh-Fourier method and the Rayleigh least-squares method could yield accurate numerical results well beyond the domain of validity of the Rayleigh hypothesis [14–16]. In the Rayleigh least-squares method, which is applied to boundary-value problems, the scattered mode amplitudes are calculated by minimizing the integrated-square error on the boundary condition, which is equivalent to projecting the boundary condition expressed with the Rayleigh hypothesis on a certain set of functions [17]. In the case of two-dimensional scalar diffraction from a periodic rough surface, Millar [18] has shown that this method leads to a sequence that uniformly converges to the exact diffracted field in any closed subset of the medium of propagation provided that the problem has a unique solution; as a consequence, the numerical scattered mode amplitudes tend to their exact values as the number of equations solved tends to infinity. These remarkable properties hold regardless of the validity of the Rayleigh hypothesis; however, it has been noted that, in practice, the Rayleigh least-squares method is not the most efficient method of computation of the scattered mode amplitudes. The Rayleigh-Fourier method, in which the scattered mode amplitudes are found by projecting the boundary condition in the Fourier space, shows a faster convergence and gives remarkably good results [14–16,19,20]; Chesneaux and Wirgin have found, however, that this method cannot in general be used to compute the near field [21]. In addition, Jackson, Winebrenner, and Ishimaru [22] have carried out numerical and analytical calculations that tend to indicate that, in the case of diffraction of an acoustic plane wave from a surface with a Dirichlet condition, the perturbation series of the Rayleigh-Fourier method is identical to the perturbation series of the Waterman-Fourier method [14], which is not limited by the validity of the Rayleigh hypothesis; the authors conjecture that this identity holds for more general boundary conditions.

The behavior of the Rayleigh-Fourier method may seem surprising [15,16,21,22] since the convergence of the representation of the scattered field does not hold in general. In demonstrations that parallel that of Burrows for finite obstacles [23], it has been shown in Refs. [24,25] for fluid and isotropic solid media that if the Rayleigh-Fourier formalism and the Waterman-Fourier formalism have unique solutions in terms of the T matrix these solutions are connected by the reciprocity relationships and are therefore identical (since the Waterman-Fourier solution, which is exact, verifies the reciprocity relationships). This equality may seem formal, but, as we will see, it holds in terms of numerical results if specific truncations of the equations are made [25]; this apparently formal equality can also be used to show that the Waterman-Fourier and Rayleigh-Fourier perturbation series [22] are identical for a large class of surfaces. Another demonstration of the identity of the two perturbation series for scalar diffraction and the Dirichlet problem has been proposed recently [26]. Since the Rayleigh-Fourier perturbation series are the same as those derived from the exact Waterman-Fourier formalism, they can be used as a computational approach; their use, along with various enhanced convergence techniques, has turned out to be successful [22,27–31].

All the debate about the Rayleigh methods has so far mainly dealt with interfaces between simple isotropic media. The study of periodic rough interfaces between more general media has recently attracted some attention and has been addressed with integral-equation methods [32,33], Waterman methods [34–36], and differential methods [37]. In a recent article, Depine and Gigli [38] pointed out the practical interest of Rayleigh methods in dealing with anisotropic gratings; they showed numerically on specific problems that these methods give good results well beyond the domain of validity of the Rayleigh hypothesis. The purpose of this paper is to demonstrate that the Rayleigh-Fourier and Rayleigh least-squares methods can indeed be adequate, regardless of the validity of the Rayleigh hypothesis, to calculate reflection and transmission coefficients at periodic rough interfaces separating general homogeneous media and, for the Rayleigh least-squares method, to calculate the electric field at any point.

The plan of the paper is as follows. In Sec. II, we describe the problem, our notations, and some properties of the eigenwaves and of the free-space dyadic Green's functions of the Maxwell equations in general homogeneous media. In Sec. III, we give a justification of the use of the Rayleigh-Fourier method. In Sec. IV, we demonstrate that the Rayleigh least-squares results obtained for boundary-value problems converge to the exact results as the number of equations solved tends to infinity. In Sec. V, we illustrate the properties of both methods with a numerical application. Section VI presents our conclusions.

II. PROBLEM DESCRIPTION

We define an orthonormal basis $(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)$. We consider a periodic rough interface S, separating two homogeneous media, defined by the relation $z=f(\mathbf{R})$, where $\mathbf{R}$ is the component of the three-dimensional position vector $\mathbf{r}$ in the $(\mathbf{e}_1,\mathbf{e}_2)$ plane and z is the coordinate of $\mathbf{r}$ along $\mathbf{e}_3$; $\mathbf{a}_1$ and $\mathbf{a}_2$ are the two periods of f and the reciprocal vectors $\mathbf{R}_1$ and $\mathbf{R}_2$ are such that $\mathbf{a}_i\cdot\mathbf{R}_j=2\pi\delta_{ij}$, where δ_{ij} is the Kronecker delta symbol ($i,j=1$ or 2). f is assumed to be continuous. Except perhaps on a discrete set of points, it is possible to define a unit normal $\mathbf{n}$ to S pointing towards the above medium (say, medium 1) and two surface vector fields $\mathbf{t}_1$ and $\mathbf{t}_2$ in the plane tangent to S such that $(\mathbf{t}_1,\mathbf{t}_2,\mathbf{n})$ is an orthonormal basis at each point of S and, in particular, $\mathbf{t}_1\times\mathbf{t}_2=\mathbf{n}$, $\mathbf{t}_2\times\mathbf{n}=\mathbf{t}_1$, and $\mathbf{n}\times\mathbf{t}_1=\mathbf{t}_2$.

Boldface characters are used to designate vectors. All field quantities are time harmonic and classically expressed as complex quantities with time dependence $\exp(-i\omega t)$ suppressed. The electric and magnetic fields $\mathbf{D}$,$\mathbf{E}$ and $\mathbf{H}$,$\mathbf{B}$ (with classical notations) in each medium satisfy the Maxwell equations

$$\nabla\times\mathbf{E}=i\omega\mathbf{B}, \tag{1a}$$

$$\nabla\times\mathbf{H}=-i\omega\mathbf{D}. \tag{1b}$$

The interface conditions express the continuity of the tangential components of $\mathbf{E}$ and $\mathbf{H}$ on S,

$$\mathbf{n}\times\mathbf{E}^{+}=\mathbf{n}\times\mathbf{E}^{-}, \tag{2a}$$

$$\mathbf{n}\times\mathbf{H}^{+}=\mathbf{n}\times\mathbf{H}^{-}, \tag{2b}$$

where $\mathbf{E}^{\pm}$ and $\mathbf{H}^{\pm}$ designate the electric and magnetic fields at S above $(+)$ and below $(-)$ the interface. In addition, the reflected and transmitted electric and magnetic fields satisfy the radiation condition at infinity.

The constitutive relationships connecting $\mathbf{D}$ and $\mathbf{B}$ to $\mathbf{E}$ and $\mathbf{H}$ are

$$\mathbf{D}=\epsilon^{(j)}\cdot\mathbf{E}+\alpha^{(j)}\cdot\mathbf{H}, \tag{3a}$$

$$\mathbf{B}=\beta^{(j)}\cdot\mathbf{E}+\mu^{(j)}\cdot\mathbf{H}, \tag{3b}$$

where the superscripts (j) correspond to the medium j ($j=1$ or 2) and $\epsilon^{(j)}$, $\alpha^{(j)}$, $\beta^{(j)}$, and $\mu^{(j)}$ are 3×3 matrices. The constitutive relationships may be frequency dependent. $\mu^{(j)}$ is assumed to have an inverse $\mu^{(j)-1}$. For each medium j, we define a complementary medium [39], denoted jC, by the following constitutive relationships: $\epsilon^{(jC)}={}^{t}\epsilon^{(j)}$, $\alpha^{(jC)}=-{}^{t}\beta^{(j)}$, $\beta^{(jC)}=-{}^{t}\alpha^{(j)}$, and $\mu^{(jC)}={}^{t}\mu^{(j)}$, where the superscript t designates the transpose of a 3×3 matrix. The complementary medium of medium jC is the medium j.

In a medium designated by j, the homogeneous equation for $\mathbf{E}$ can be written

$$\mathcal{L}^{(j)}(\mathbf{E})=\mathbf{0}, \tag{4}$$

with the operator $\mathcal{L}^{(j)}$ being defined by its application to a vector field $\mathbf{V}$,

$$\mathcal{L}^{(j)}(\mathbf{V})=i\omega\nabla\times\mathbf{H}^{(j)}(\mathbf{V})-\omega^2[\epsilon^{(j)}\cdot\mathbf{V}+\alpha^{(j)}\cdot\mathbf{H}^{(j)}(\mathbf{V})], \tag{5a}$$

$$\mathbf{H}^{(j)}(\mathbf{V})=(i\omega)^{-1}\mu^{(j)-1}\cdot(\nabla\times\mathbf{V})-\mu^{(j)-1}\cdot(\beta^{(j)}\cdot\mathbf{V}). \tag{5b}$$

The eigenwaves are of the form $\mathbf{V}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})$, where $\mathbf{k}$ is a wave vector. Substitution of such a field into Eq. (4) leads to the vector equation $L^{(j)}(\mathbf{k},\omega)\cdot\mathbf{V}(\mathbf{k})=\mathbf{0}$, where $L^{(j)}(\mathbf{k},\omega)$ is a 3×3 matrix that depends on the medium j, $\mathbf{k}$, and ω. We designate the adjoint of $L^{(j)}(\mathbf{k},\omega)$ by $M^{(j)}(\mathbf{k},\omega)$; we note that for the values of $\mathbf{k}$ such that the determinant of $L^{(j)}(\mathbf{k},\omega)$ is equal to 0, the vectors $M^{(j)}(\mathbf{k},\omega)\cdot\mathbf{e}_1$, $M^{(j)}(\mathbf{k},\omega)\cdot\mathbf{e}_2$, and $M^{(j)}(\mathbf{k},\omega)\cdot\mathbf{e}_3$ are eigenvectors.

We now give the plane-wave expansion of the free-space dyadic Green's functions. The free-space Green's vector fields $\mathbf{G}_{k_0}^{(j)}(\mathbf{r};\mathbf{r}_0)$ corresponding to the problem described in Sec. II satisfy, apart from the radiation condition,

$$\mathcal{L}^{(j)}[\mathbf{G}_{k_0}^{(j)}(\mathbf{r};\mathbf{r}_0)]=\mathbf{e}_{k_0}\delta(\mathbf{r}-\mathbf{r}_0) \tag{6}$$

where $\delta(\mathbf{r}-\mathbf{r}_0)$ is the classical delta function, $k_0=1$, 2, or 3, and $\mathcal{L}^{(j)}$ is the operator defined by Eq. (5a). $\mathbf{G}_{k_0}^{(j)}$, which is defined as a generalized function, is classically assumed to have a sense as a vector field (when $\mathbf{r}\neq\mathbf{r}_0$) whose plane-wave expansion can be written

$$\mathbf{G}_{k_0}^{(j)}(\mathbf{r};\mathbf{r}_0)=\pm\frac{i}{4\pi^2}\sum_{n=1}^{2}\int a_n^{(j)\pm}(\mathbf{K})\times[\mathbf{e}_{k_0}\cdot\mathbf{V}_n^{(jC)\mp}(-\mathbf{K})]\Delta_n^{(j)\pm}(\mathbf{K},\omega)\mathbf{V}_n^{(j)\pm}(\mathbf{K})\times\exp[i\mathbf{k}_n^{(j)\pm}(\mathbf{K})\cdot(\mathbf{r}-\mathbf{r}_0)]d^2K, \tag{7}$$

where the upper sign applies if $(z-z_0)>0$ and the lower sign applies if $(z-z_0)<0$ (z and z_0 are the coordinates of $\mathbf{r}$ and $\mathbf{r}_0$ along $\mathbf{e}_3$). The $\mathbf{k}_n^{(j)\pm}$'s are such that

$$\mathbf{k}_n^{(j)\pm}(\mathbf{K})=\mathbf{K}+k_{nz}^{(j)\pm}(\mathbf{K})\mathbf{e}_3, \tag{8}$$

$$\det L^{(j)}(\mathbf{k}_n^{(j)\pm}(\mathbf{K}),\omega)=0, \tag{9}$$

where n indicates the type of eigenwave considered ($n=1$ or 2), $\mathbf{K}$ is the transverse component of $\mathbf{k}_n^{(j)\pm}(\mathbf{K})$ in the $(\mathbf{e}_1,\mathbf{e}_2)$ plane, $k_{nz}^{(j)\pm}(\mathbf{K})$ is defined by Eq. (9) and the radiation condition $\pm\mathrm{Im}[k_{nz}^{(j)\pm}(\mathbf{K})]>0$ if $k_{nz}^{(j)\pm}(\mathbf{K})$ is not strictly real (Im designates the imaginary part of the argument) and $\pm\partial k_{nz}^{(j)\pm}/\partial\omega>0$ if $k_{nz}^{(j)\pm}(\mathbf{K})$ is real. $\det L^{(j)}$ is the determinant of $L^{(j)}$. The other elements in Eq. (7) are defined by

$$\mathbf{V}_n^{(j)\pm}(\mathbf{K})=M^{(j)}(\mathbf{k}_n^{(j)\pm}(\mathbf{K}),\omega)\cdot\mathbf{e}_1, \tag{10}$$

$$\Delta_n^{(j)\pm}(\mathbf{K},\omega)=\left(\frac{\partial\det L^{(j)}(\mathbf{k},\omega)}{\partial k_z}\right)^{-1}_{\mathbf{k}=\mathbf{k}_n^{(j)\pm}(\mathbf{K})}, \tag{11}$$

$$M^{(j)}(\mathbf{k}_n^{(j)\pm}(\mathbf{K}),\omega)\cdot\mathbf{e}_{k_0}=a_n^{(j)\pm}(\mathbf{K})[\mathbf{e}_{k_0}\cdot\mathbf{V}_n^{(jC)\mp}(-\mathbf{K})]\mathbf{V}_n^{(j)\pm}(\mathbf{K}). \tag{12}$$

Equation (7) is obtained by solving Eq. (6) in the Fourier space and evaluating the resulting integral for $\mathbf{G}_{k_0}^{(j)}(\mathbf{r};\mathbf{r}_0)$ in the k_z complex plane by the residue theorem. We have assumed that $\det L^{(j)}(\mathbf{k},\omega)$ has, for all $\mathbf{K}$, two proper single roots in k_z with each root corresponding to a one-dimensional space of eigenvectors. Then, when $\mathbf{k}=\mathbf{k}_n^{(j)\pm}(\mathbf{K})$ and therefore $\det L^{(j)}=0$, the three vectors $M^{(j)}\cdot\mathbf{e}_{k_0}$, which are as already indicated eigenvectors in this case, are collinear with $\mathbf{V}_n^{(j)\pm}(\mathbf{K})$; the equality $M^{(jC)}(-\mathbf{k},\omega)={}^tM^{(j)}(\mathbf{k},\omega)$, which stems from the definition of medium jC, allows us to write Eq. (12) with the scalar $a_n^{(j)\pm}(\mathbf{K})$ being independent of k_0.

It can be verified that the definition of medium jC also implies

$$L^{(jC)}(-\mathbf{k},\omega)={}^tL^{(j)}(\mathbf{k},\omega), \tag{13}$$

where the superscript t designates the transpose of a matrix, so that

$$\det L^{(jC)}(-\mathbf{k},\omega)=\det L^{(j)}(\mathbf{k},\omega). \tag{14}$$

As a consequence of Eq. (14) and the radiation condition, we can write

$$k_{nz}^{(j)\pm}(-\mathbf{K})=-k_{nz}^{(jC)\mp}(\mathbf{K}), \tag{15}$$

so that

$$\mathbf{k}_n^{(j)\pm}(-\mathbf{K})=-\mathbf{k}_n^{(jC)\mp}(\mathbf{K}). \tag{16}$$

Equations (16) and (12) and the equality $M^{(jC)}(-\mathbf{k},\omega)={}^tM^{(j)}(\mathbf{k},\omega)$ imply that

$$a_n^{(j)\pm}(-\mathbf{K})=a_n^{(jC)\mp}(\mathbf{K}) \tag{17}$$

and Eq. (14) leads to

$$\Delta_n^{(j)\pm}(-\mathbf{K},\omega)=-\Delta_n^{(jC)\mp}(\mathbf{K},\omega). \tag{18}$$

Equations (7) and (16)–(18) are essential to the arguments developed in this paper. It can be noted that they all stem from Eq. (13).

We now define the unknowns of the problem. The general expression of the free-space Green's vector fields shows that, in view of the linearity of the problem, reflection and transmission at S are completely described by reflection and transmission of two types of incident eigenwaves (say, coming from medium 1) of the form $\mathbf{V}_{n_0}^{(1)-}(\mathbf{K}_{\mathrm{inc}})\exp[i\mathbf{k}_{n_0}^{(1)-}(\mathbf{K}_{\mathrm{inc}})\cdot\mathbf{r}]$. With such incident electric fields, the reflected and transmitted electric fields $\mathbf{E}_{\mathrm{ref}}^{(1)}$ and $\mathbf{E}^{(2)}$ beyond the maximum excursions of the interface can be expressed as an expansion on two types of Bloch eigenwaves whose amplitudes define the T-matrix coefficients $t_{nn_0}^{(1)}(\mathbf{K}_{\mathrm{inc}\,MN},\mathbf{K}_{\mathrm{inc}})$ and $t_{nn_0}^{(2)}(\mathbf{K}_{\mathrm{inc}\,MN},\mathbf{K}_{\mathrm{inc}})$,

$$\mathbf{E}_{\mathrm{ref}}^{(1)}(\mathbf{r})=\sum_{n=1}^{2}\sum_{M,N}t_{nn_0}^{(1)}(\mathbf{K}_{\mathrm{inc}\,MN},\mathbf{K}_{\mathrm{inc}})\mathbf{V}_n^{(1)+}(\mathbf{K}_{\mathrm{inc}\,MN})\times\exp[i\mathbf{k}_n^{(1)+}(\mathbf{K}_{\mathrm{inc}\,MN})\cdot\mathbf{r}], \tag{19a}$$

$$\mathbf{E}^{(2)}(\mathbf{r})=\sum_{n=1}^{2}\sum_{M,N}t_{nn_0}^{(2)}(\mathbf{K}_{\mathrm{inc}\,MN},\mathbf{K}_{\mathrm{inc}})\mathbf{V}_n^{(2)-}(\mathbf{K}_{\mathrm{inc}\,MN})\times\exp[i\mathbf{k}_n^{(2)-}(\mathbf{K}_{\mathrm{inc}\,MN})\cdot\mathbf{r}], \tag{19b}$$

where M and N are integers, the sum is over all integers, and

$$\mathbf{K}_{\mathrm{inc}\,MN}=\mathbf{K}_{\mathrm{inc}}+M\mathbf{R}_1+N\mathbf{R}_2. \tag{20}$$

For a given $\mathbf{K}_{\mathrm{inc}}$, the problem of reflection and transmission at S is to determine the $t_{nn_0}^{(j)}(\mathbf{K}_{\mathrm{inc}\,MN},\mathbf{K}_{\mathrm{inc}})$ for all M,N,n,n_0,j. In general, we are mainly interested in the values of M and N such that $k_{nz}^{(1)+}(\mathbf{K}_{\mathrm{inc}\,MN})$ and $k_{nz}^{(2)-}(\mathbf{K}_{\mathrm{inc}\,MN})$ are real.

It can be noted that the $t_{nn_0}^{(j)}$'s and $t_{nn_0}^{(jC)}$'s are connected by specific relationships. When S separates media 1 and 2, we define the scattering Green's vector field $\mathbf{G}_{\mathrm{sc},k_0}(\mathbf{r};\mathbf{r}_0)$ to be the electric field at point $\mathbf{r}$ due to a unit source along $\mathbf{e}_{k_0}$ at point $\mathbf{r}_0$. When S separates media $1C$ and $2C$, we designate the analogous scattering Green's vector field by $\mathbf{G}_{\mathrm{sc},k_0}^{(C)}(\mathbf{r};\mathbf{r}_0)$. It can be classically shown with Green's theorem that

$$G_{\mathrm{sc},k_0k_1}^{(C)}(\mathbf{r}_1;\mathbf{r}_0)=G_{\mathrm{sc},k_1k_0}(\mathbf{r}_0;\mathbf{r}_1) \tag{21}$$

for all k_0 and k_1, with the notation $G_{\mathrm{sc},k_0k_1}=\mathbf{e}_{k_1}\cdot\mathbf{G}_{\mathrm{sc},k_0}$. Let $\mathbf{r}_0$ and $\mathbf{r}_1$ be two vector points located beyond the maximum excursions of S. We proceed, as Jackson, Winebrenner, and Ishimaru did for scalar diffraction [22], by expressing the incident electric field due to each unit point source with Eq. (7) as a superposition of plane waves, each of which gives rise to a diffracted field determined by the T-matrix coefficients; then, if $\mathbf{r}_0$ and $\mathbf{r}_1$ are both located above S, Eq. (21) leads to

$$-a_n^{(1)-}(\mathbf{K})\Delta_n^{(1)-}(\mathbf{K},\omega)t_{mn}^{(1)}(\mathbf{K}_{MN},\mathbf{K}) = a_m^{(1)+}(\mathbf{K}_{MN})\Delta_m^{(1)+}(\mathbf{K}_{MN},\omega)t_{nm}^{(1C)}(-\mathbf{K},-\mathbf{K}_{MN}) \tag{22}$$

for all $\mathbf{K}$, all m,n $(=1$ or 2), and all integers M and N, which generalizes the relationship for scalar diffraction in a simple isotropic medium [22]. If $\mathbf{r}_0$ is located above S and $\mathbf{r}_1$ is located below S, Eq. (21) leads to

$$a_n^{(1)-}(\mathbf{K})\Delta_n^{(1)-}(\mathbf{K},\omega)t_{mn}^{(2)}(\mathbf{K}_{MN},\mathbf{K}) = a_m^{(2)-}(\mathbf{K}_{MN})\Delta_m^{(2)-}(\mathbf{K}_{MN},\omega)t_{nm(B)}^{(1C)}(-\mathbf{K},-\mathbf{K}_{MN}) \tag{23}$$

for all $\mathbf{K}$, all m,n and all integers M and N. The subscript (B) refers to the case of illumination of S by an eigenwave coming from medium 2 (see Sec. III B). Equations (17) and (18) have been used to establish Eqs. (22) and (23).

III. RAYLEIGH-FOURIER METHOD

A. Formalism description

In the Rayleigh-Fourier method, the T-matrix coefficients are determined by formally writing the interface conditions with the expressions (19a) and (19b) of the reflected and transmitted electric fields in each medium and projecting them on the sets of surface vector fields $\mathbf{t}_1\exp(-i\mathbf{K}_{\mathrm{inc}PQ}\cdot\mathbf{R})$ and $\mathbf{t}_2\exp(-i\mathbf{K}_{\mathrm{inc}PQ}\cdot\mathbf{R})$, where P and Q are integers. For reasons that will appear in Sec. III B, we choose to express the Rayleigh-Fourier formalism in the case where S separates medium $1C$, located above, and medium $2C$. In the case of illumination of S by an eigenwave of type n_0 coming from medium $1C$, we obtain

$$\begin{aligned}X^{(1C)-}(\mathbf{K}_{\mathrm{inc}},l,n_0,0,0,P,Q)&+\sum_{n=1}^{2}\sum_{M=-M_{\max}}^{M_{\max}}\sum_{N=-N_{\max}}^{N_{\max}} t_{nn_0,R}^{(1C)}(\mathbf{K}_{\mathrm{inc}MN},\mathbf{K}_{\mathrm{inc}})X^{(1C)+}(\mathbf{K}_{\mathrm{inc}},l,n,M,N,P,Q)\\ &=\sum_{n=1}^{2}\sum_{M=-M_{\max}}^{M_{\max}}\sum_{N=-N_{\max}}^{N_{\max}} t_{nn_0,R}^{(2C)}(\mathbf{K}_{\mathrm{inc}MN},\mathbf{K}_{\mathrm{inc}})X^{(2C)-}(\mathbf{K}_{\mathrm{inc}},l,n,M,N,P,Q),\end{aligned} \tag{24a}$$

$$\begin{aligned}Y^{(1C)-}(\mathbf{K}_{\mathrm{inc}},l,n_0,0,0,P,Q)&+\sum_{n=1}^{2}\sum_{M=-M_{\max}}^{M_{\max}}\sum_{N=-N_{\max}}^{N_{\max}} t_{nn_0,R}^{(1C)}(\mathbf{K}_{\mathrm{inc}MN},\mathbf{K}_{\mathrm{inc}})Y^{(1C)+}(\mathbf{K}_{\mathrm{inc}},l,n,M,N,P,Q)\\ &=\sum_{n=1}^{2}\sum_{M=-M_{\max}}^{M_{\max}}\sum_{N=-N_{\max}}^{N_{\max}} t_{nn_0,R}^{(2C)}(\mathbf{K}_{\mathrm{inc}MN},\mathbf{K}_{\mathrm{inc}})Y^{(2C)-}(\mathbf{K}_{\mathrm{inc}},l,n,M,N,P,Q)\end{aligned} \tag{24b}$$

for all l $(l=1$ or 2), P,Q (with $-M_{\max}\leq P\leq M_{\max}$ and $-N_{\max}\leq Q\leq N_{\max}$), where

$$X^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}},l,n,M,N,P,Q) = \int_{S_0}(\mathbf{t}_l\times\mathbf{n})\cdot\mathbf{V}_n^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}MN})e^{i\mathbf{k}_n^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}MN})\cdot\mathbf{r}_S}\times e^{-i\mathbf{K}_{\mathrm{inc}PQ}\cdot\mathbf{R}}d^2R, \tag{25a}$$

$$Y^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}},l,n,M,N,P,Q) = \int_{S_0}(\mathbf{t}_l\times\mathbf{n})\cdot\mathbf{HV}_n^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}MN})e^{i\mathbf{k}_n^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}MN})\cdot\mathbf{r}_S}\times e^{-i\mathbf{K}_{\mathrm{inc}PQ}\cdot\mathbf{R}}d^2R, \tag{25b}$$

where $\mathbf{HV}_n^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}MN})$ is defined by

$$\mathbf{H}^{(jC)}[\mathbf{V}_n^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}MN})e^{i\mathbf{k}_n^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}MN})\cdot\mathbf{r}}] = \mathbf{HV}_n^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}MN})e^{i\mathbf{k}_n^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}MN})\cdot\mathbf{r}}. \tag{26}$$

In Eqs. (25a) and (25b), S_0 is a given unit cell of S and $\mathbf{r}_S=\mathbf{R}+f(\mathbf{R})\mathbf{e}_3$. The Rayleigh-Fourier equations (24a) and (24b) have been truncated for numerical applications so that they form a linear system of $4(2N_{\max}+1)(2M_{\max}+1)$ equations with $4(2N_{\max}+1)(2M_{\max}+1)$ unknowns. The subscript R indicates that the solution is obtained with the Rayleigh-Fourier method and the truncation chosen.

There are as many Rayleigh-Fourier methods as possible definitions of $\mathbf{t}_1$ and $\mathbf{t}_2$. In this paper, we suppose that one definition is chosen once and for all to implement both the Rayleigh-Fourier method and the Waterman-Fourier method.

B. Connection between the Rayleigh-Fourier and Waterman-Fourier numerical results

In the Appendix, we have established the Waterman-Fourier equations in the case where S, separating media 1 and 2, is illuminated from either medium with a transverse incident wave vector equal to $-\mathbf{K}_{\mathrm{inc}M_0N_0}$, where M_0 and N_0 are two given integers; it must be noted that a certain type of truncation, depending on M_0 and N_0, has been applied and is implicit in the definition of the Waterman-Fourier numerical results (designated by the subscript W).

First we consider Eqs. (A18)–(A21) written in the case where the incident plane wave is $\mathbf{V}_{n_0}^{(1)-}(-\mathbf{K}_{\mathrm{inc}M_0N_0})\exp[i\mathbf{k}_{n_0}^{(1)-}(-\mathbf{K}_{\mathrm{inc}M_0N_0})\cdot\mathbf{r}]$ $(\delta_1=1$ and $\delta_2=0$ in the Appendix). In view of the type of truncation chosen, we can express each $X^{(1C)-}$ and $Y^{(1C)-}$ in Eq. (A21) with Eqs. (24a) and (24b), respectively; by doing so, we find

$$-\frac{4\pi^2}{\omega a_n^{(1)+}(-\mathbf{K}_{\text{inc}})}[\Delta_n^{(1)+}(-\mathbf{K}_{\text{inc}},\omega)]^{-1} \times t_{nn_0,W}^{(1)}(-\mathbf{K}_{\text{inc}},-\mathbf{K}_{\text{inc}M_0N_0}) = -\sum_{n'=1}^{2}\sum_{M'=-M_{\max}}^{M_{\max}}\sum_{N'=-N_{\max}}^{N_{\max}} \times t_{n'n,R}^{(1C)}(\mathbf{K}_{\text{inc}M'N'},\mathbf{K}_{\text{inc}})B^{(1C)+}(n',M',N';M_0,N_0) + \sum_{n'=1}^{2}\sum_{M'=-M_{\max}}^{M_{\max}}\sum_{N'=-N_{\max}}^{N_{\max}} \times t_{n'n,R}^{(2C)}(\mathbf{K}_{\text{inc}M'N'},\mathbf{K}_{\text{inc}})B^{(2C)-}(n',M',N';M_0,N_0), \tag{27}$$

where $B^{(1C)+}$ and $B^{(2C)-}$ are defined in the Appendix. By taking Eqs. (A18) and (A19) into account in Eq. (27), we get, with $N_{\max}>|N_0|$ and $M_{\max}>|M_0|$,

$$-a_{n_0}^{(1)-}(-\mathbf{K}_{\text{inc}M_0N_0})\Delta_{n_0}^{(1)-}(-\mathbf{K}_{\text{inc}M_0N_0},\omega) \times t_{nn_0,W}^{(1)}(-\mathbf{K}_{\text{inc}},-\mathbf{K}_{\text{inc}M_0N_0}) = a_n^{(1)+}(-\mathbf{K}_{\text{inc}})\Delta_n^{(1)+}(-\mathbf{K}_{\text{inc}},\omega)t_{n_0n,R}^{(1C)}(\mathbf{K}_{\text{inc}M_0N_0},\mathbf{K}_{\text{inc}}). \tag{28}$$

Then we consider Eqs. (A18)–(A21) in the case where the incident plane wave is

$$\mathbf{V}_{n_0}^{(2)+}(-\mathbf{K}_{\text{inc}M_0N_0})\exp[i\mathbf{k}_{n_0}^{(2)+}(-\mathbf{K}_{\text{inc}M_0N_0})\cdot\mathbf{r}]$$

($\delta_1=0$ and $\delta_2=1$ in the Appendix); the subscript (B) is added to indicate this type of illumination of S. By expressing each $X^{(1C)-}$ and $Y^{(1C)-}$ in Eq. (A21) with Eqs. (24a) and (24b) and taking Eqs. (A18) and (A19) into account as above, we get, with $N_{\max}>|N_0|$ and $M_{\max}>|M_0|$,

$$a_{n_0}^{(2)+}(-\mathbf{K}_{\text{inc}M_0N_0})\Delta_{n_0}^{(2)+}(-\mathbf{K}_{\text{inc}M_0N_0},\omega) \times t_{nn_0,W(B)}^{(1)}(-\mathbf{K}_{\text{inc}},-\mathbf{K}_{\text{inc}M_0N_0}) = a_n^{(1)+}(-\mathbf{K}_{\text{inc}})\Delta_n^{(1)+}(-\mathbf{K}_{\text{inc}},\omega)t_{n_0n,R}^{(2C)}(\mathbf{K}_{\text{inc}M_0N_0},\mathbf{K}_{\text{inc}}). \tag{29}$$

It appears in Eqs. (28) and (29) that the numerical results of the Rayleigh-Fourier and Waterman-Fourier methods are connected by the equalities (22) and (23) (when Eq. (23) is applied to media $1C$ and $2C$ and Eqs. (17) and (18) are used). These relationships are strictly verified by the exact values of the T-matrix coefficients. Therefore, if it is admitted that the Waterman-Fourier numerical results converge to the exact values of the T-matrix coefficients as $M_{\max}$ and $N_{\max}$ tend to infinity (this is implicitly the case when the method is used), the Rayleigh-Fourier numerical results also converge to the exact values. Furthermore, since the domain of validity of the Rayleigh hypothesis is not involved in the quality of the Waterman-Fourier results, it does not intervene either in the quality of the Rayleigh-Fourier results. This conclusion has been found above when the Rayleigh-Fourier method is applied to the physical problem of wave propagation in media $1C$ and $2C$; since there is no constraint on the choice of these media, it is of course also valid for wave propagation in media 1 and 2.

Therefore the use of the Rayleigh-Fourier method is not *a priori* less justified than the use of the Waterman-Fourier method and, in particular, it is not limited by the validity of the Rayleigh hypothesis. Like the Waterman-Fourier method, it can be regarded as a computational tool for the evaluation of the T-matrix coefficients in the kind of problem considered. This method has already been numerically investigated by Depine and Gigli [38] in the case of a corrugated interface (sinusoidal or cycloidal) between a uniaxial crystal and an isotropic dielectric. They found that the Rayleigh-Fourier method gives good results for the T-matrix coefficients well beyond the domain of validity of the Rayleigh hypothesis, which can be explained by the arguments developed in this section. It must be noted, however, that the Rayleigh-Fourier method has been shown to be adequate only for the computation of the T-matrix coefficients; Chesneaux and Wirgin [21] have found it to be inadequate for evaluating the near field in general. We confirm these results in the numerical application of Sec. V.

We have found that, more generally, it is possible to associate with each Rayleigh method (characterized by a set of projection basis functions) a Waterman method (characterized by a set of expansion basis functions) such that the equalities (28) and (29) hold. We have focused on the Rayleigh-Fourier and Waterman-Fourier methods because they are simple and frequently used.

IV. RAYLEIGH LEAST-SQUARES METHOD

We now return to the general problem described in Sec. II. Here S is the boundary of a semi-infinite homogeneous medium located above S and the electric field satisfies $\mathbf{n}\times\mathbf{E}=\mathbf{0}$ at S; S is such that this boundary-value problem has a unique solution for $\mathbf{E}$. We show that, with the expression (A10) of the free-space pseudoperiodic Green's vector fields, the rationale of Millar applied to scalar diffraction in a simple isotropic medium [18] can be extended to diffraction in a general medium so that the Rayleigh least-squares method is also numerically convergent in the latter case. We use the notations of Sec. II with the now unnecessary superscript (j) omitted. The superscript (C) now indicates the complementary medium defined in Sec. II.

We first show that the set of vector functions

$$\mathbf{W}_n^{(C)+}(-\mathbf{K}_{\text{inc}PQ})(\mathbf{r}_S)=\mathbf{n}\times\mathbf{V}_n^{(C)+}(-\mathbf{K}_{\text{inc}PQ}) \times\exp[i\mathbf{k}_n^{(C)+}(-\mathbf{K}_{\text{inc}PQ})\cdot\mathbf{r}_S],$$

where $\mathbf{r}_S=\mathbf{R}+f(\mathbf{R})\mathbf{e}_3$, $\mathbf{K}_{\text{inc}}$ and $\mathbf{R}$ are vectors in the $(\mathbf{e}_1,\mathbf{e}_2)$ plane, $n=1$ or 2, and P and Q are integers, forms a complete basis of $L_\perp^2(-\mathbf{K}_{\text{inc}})$, which we define as the space of pseudoperiodic (with pseudoperiodicity characterized by $-\mathbf{K}_{\text{inc}}$) vector fields defined on S, tangent to S at all points, and square integrable on a given unit cell S_0 of S. In order to do so, we classically show that a vector field $\mathbf{g}$ of $L_\perp^2(-\mathbf{K}_{\text{inc}})$, which is orthogonal to every $\mathbf{W}_n^{(C)+}(-\mathbf{K}_{\text{inc}PQ})$, is necessarily the null element of $L_\perp^2(-\mathbf{K}_{\text{inc}})$. Let $\mathbf{g}$ be such an element; for all integers P and Q and for $n=1$ or 2 we can write

$$\int_{S_0}[\mathbf{n}\times\mathbf{g}^*(\mathbf{r}_S)]\cdot\mathbf{V}_n^{(C)+}(-\mathbf{K}_{\text{inc}PQ}) \times\exp[i\mathbf{k}_n^{(C)+}(-\mathbf{K}_{\text{inc}PQ})\cdot\mathbf{r}_S]dS=0, \tag{30}$$

where $\mathbf{g}^*$ denotes the conjugate of $\mathbf{g}$.

Let $\mathbf{r}_0$ be a vector point in the region defined by $z<\min f(\mathbf{R})$. By multiplying Eq. (30) for each n,P,Q,k_0 ($k_0=1$, 2, or 3) by

$$a_n^-(\mathbf{K}_{\mathrm{inc}PQ})\Delta_n^-(\mathbf{K}_{\mathrm{inc}PQ},\omega)[\mathbf{e}_{k_0}\cdot\mathbf{V}_n^-(\mathbf{K}_{\mathrm{inc}PQ})]$$
$$\times\exp[-i\mathbf{k}_n^{(C)+}(-\mathbf{K}_{\mathrm{inc}PQ})\cdot\mathbf{r}_0]$$

and summing on n, P, and Q, we find, for all k_0,

$$\int_{S_0}[\mathbf{n}\times\mathbf{g}^*(\mathbf{r}_S)]\cdot\mathbf{G}_{k_0}^{(C)(\mathrm{PP})}(\mathbf{r}_S;\mathbf{r}_0)dS=0, \qquad (31)$$

where $\mathbf{G}_{k_0}^{(C)(\mathrm{PP})}$ is the pseudoperiodic Green's vector field defined by Eq. (A10). Uniform convergence on S_0 of the series in Eq. (A10) has been assumed for all $\mathbf{r}_0$ located below the lowest point of S in order to interchange the integration and the discrete sum.

We now set, for all $\mathbf{r}_0$ not located on S and all k_0,

$$\mathbf{e}_{k_0}\cdot\mathbf{\Phi}(\mathbf{r}_0)=\int_{S_0}[\mathbf{n}\times\mathbf{g}^*(\mathbf{r}_S)]\cdot\mathbf{G}_{k_0}^{(C)(\mathrm{PP})}(\mathbf{r}_S;\mathbf{r}_0)dS. \qquad (32)$$

Equation (31) shows that $\mathbf{\Phi}(\mathbf{r}_0)=\mathbf{0}$ for all $\mathbf{r}_0$ below the lowest point of S. We now show that $\mathbf{\Phi}(\mathbf{r}_0)=\mathbf{0}$ for all $\mathbf{r}_0$ below S.

It has been assumed in the Appendix that $\mathbf{G}_{k_0}^{(C)(\mathrm{PP})}(\mathbf{r}_S;\mathbf{r}_0)$ is a holomorphic function of the Cartesian coordinates of $\mathbf{r}_0$. Since $\mathbf{n}\times\mathbf{g}^*(\mathbf{r}_S)$ is square integrable on S_0, it can be approximated in the mean-square sense as closely as wanted by a continuous function so that differentiation under the integral sign in Eq. (32) is possible [40]; consequently, $\mathbf{\Phi}(\mathbf{r}_0)$ is also a holomorphic function of the Cartesian coordinates of $\mathbf{r}_0$ and is therefore analytic [40]. Since $\mathbf{\Phi}$ is analytic and $\mathbf{\Phi}(\mathbf{r}_0)=\mathbf{0}$ for all $\mathbf{r}_0$ below the lowest point of S, $\mathbf{\Phi}(\mathbf{r}_0)=\mathbf{0}$ for all $\mathbf{r}_0$ below S.

Equations (A7) and (A9) indicate the jump properties at S of potentials defined like $\mathbf{\Phi}(\mathbf{r}_0)$ when $\mathbf{g}^*$ is continuous; in the present case, $\mathbf{n}\times\mathbf{\Phi}$ is continuous across S. Since $\mathbf{\Phi}(\mathbf{r}_S-\lambda\mathbf{n})$ tends to $\mathbf{0}$ as λ tends to 0 (with $\lambda>0$), $\mathbf{n}\times\mathbf{\Phi}$ is the null vector at S above the interface. In the more general case where $\mathbf{g}^*$ is square integrable, $\mathbf{n}\times\mathbf{g}^*$ can be approximated in the mean-square sense as closely as wanted by a continuous surface vector field, say, $\mathbf{n}\times\mathbf{g}_c^*(\mathbf{r}_S)$, which generates a pseudoperiodic vector potential $\mathbf{\Phi}_c$ (the subscript c should not be confused with the superscript C, which designates the complementary medium). With the aid of the Schwarz inequality, it can be shown that $\max\|\mathbf{\Phi}-\mathbf{\Phi}_c\|$ can be made as small as wanted on either side of S. Since in addition $\mathbf{\Phi}=\mathbf{0}$ below the interface and $\mathbf{n}\times\mathbf{\Phi}_c$ is continuous across S, $\mathbf{n}\times\mathbf{\Phi}=\mathbf{0}$ at S above the interface (as in the case where $\mathbf{g}$ is continuous). Therefore $\mathbf{\Phi}$ satisfies the general equations of propagation (in the original medium), the radiation condition, and $\mathbf{n}\times\mathbf{\Phi}=\mathbf{0}$ at S. Since the boundary-value problem considered here is assumed to have a unique solution, $\mathbf{\Phi}(\mathbf{r}_0)=\mathbf{0}$ at all $\mathbf{r}_0$ above S so that

$$\mathbf{\Phi}(\mathbf{r}_0)=\mathbf{0} \qquad (33)$$

at all $\mathbf{r}_0$ not located on S.

Equation (33) indicates that $\mathbf{H}[\mathbf{\Phi}(\mathbf{r}_S\pm\lambda\mathbf{n})]$ tends to $\mathbf{0}$ as λ tends to 0. Then

$$\int_{S_0}\|\mathbf{n}\times\mathbf{g}^*(\mathbf{r}_S)\|^2dS=0. \qquad (34)$$

Equations (A7) and (A9) and the existence of the limit indicated before Eq. (34) show that if $\mathbf{g}^*$ is continuous, this result holds without the square integration. Equation (34) is an extension to the case where $\mathbf{g}^*$ is square integrable; it is analogous to the extension made in Ref. [41] in a simpler case. This equation can be demonstrated by noting that $\max\|\mathbf{n}\times\mathbf{H}^{(\mathrm{C})}(\mathbf{\Phi}_c)\|$ can, as $\max\|\mathbf{\Phi}_c\|$, be made as small as wanted on either side of S; then Eq. (34) can be shown with the Minkowski inequality involving $\mathbf{n}\times\mathbf{g}^*$, $\mathbf{n}\times\mathbf{g}_c^*$, and the jumps of $\mathbf{n}\times\mathbf{H}(\mathbf{\Phi})$ and $\mathbf{n}\times\mathbf{H}(\mathbf{\Phi}_c)$ across S. The rationale leading to Eq. (34) is quite similar to that of Millar [18].

Since, by definition of $\mathbf{g}$, $\mathbf{n}\cdot\mathbf{g}^*(\mathbf{r}_S)=0$ for all $\mathbf{r}_S$, Eq. (34) implies

$$\int_{S_0}\|\mathbf{g}^*(\mathbf{r}_S)\|^2dS=0, \qquad (35)$$

which indicates that $\mathbf{g}(\mathbf{r}_S)=\mathbf{0}$ almost everywhere on S and ends the proof of completeness of the $\mathbf{W}_n^{(C)+}(-\mathbf{K}_{\mathrm{inc}PQ})$ in $L_\perp^2(-\mathbf{K}_{\mathrm{inc}})$.

It can be noted that since there is no constraint on $\mathbf{K}_{\mathrm{inc}}$ and on the medium, the completeness of the $\mathbf{W}_n^{(C)+}(-\mathbf{K}_{\mathrm{inc}PQ})$ in $L_\perp^2(-\mathbf{K}_{\mathrm{inc}})$ implies the completeness of the $\mathbf{W}_n^+(\mathbf{K}_{\mathrm{inc}PQ})$ in $L_\perp^2(\mathbf{K}_{\mathrm{inc}})$. We are now in a position to deduce the numerical convergence of the Rayleigh least-squares method from the completeness of the $\mathbf{W}_n^+(\mathbf{K}_{\mathrm{inc}PQ})$ by again proceeding as Millar [18]. The incident electric field is assumed to be $\mathbf{E}_{\mathrm{inc}}(\mathbf{r}_0)=\mathbf{V}_{n_0}^-(\mathbf{K}_{\mathrm{inc}})\exp[i\mathbf{k}_{n_0}^-(\mathbf{K}_{\mathrm{inc}})\cdot\mathbf{r}_0]$. Let $\boldsymbol{\mathcal{G}}_{k_0}^{(C)(\mathrm{PP})}(\mathbf{r}_S;\mathbf{r}_0)$ be the radiative pseudoperiodic Green's vector field in the complementary medium, with the source along $\mathbf{e}_{k_0}$, such that $\mathbf{n}\times\boldsymbol{\mathcal{G}}_{k_0}^{(C)(\mathrm{PP})}(\mathbf{r}_S;\mathbf{r}_0)=\mathbf{0}$ for all $\mathbf{r}_s$ on S. The classical application of Green's theorem yields

$$\mathbf{e}_{k_0}\cdot\mathbf{E}_{\mathrm{ref}}(\mathbf{r}_0)=i\omega\int_{S_0}[\mathbf{n}\times\mathbf{E}_{\mathrm{ref}}(\mathbf{r}_S)]\cdot\mathbf{H}^{(C)}[\boldsymbol{\mathcal{G}}_{k_0}^{(C)(\mathrm{PP})}(\mathbf{r}_S;\mathbf{r}_0)]dS, \qquad (36)$$

where $\mathbf{E}_{\mathrm{ref}}$ is the reflected field, $\mathbf{r}_0$ is any vector point not located on S, and the operator $\mathbf{H}^{(C)}$ applies to the dependence in $\mathbf{r}_S$. Likewise, since the eigenwaves verify the general equations of propagation and the radiation condition, we can write for all P, Q, and n

$$\mathbf{e}_{k_0}\cdot\mathbf{V}_n^+(\mathbf{K}_{\mathrm{inc}PQ})\exp[i\mathbf{k}_n^+(\mathbf{K}_{\mathrm{inc}PQ})\cdot\mathbf{r}_0]$$
$$=i\omega\int_{S_0}\mathbf{W}_n^+(\mathbf{K}_{\mathrm{inc}PQ})(\mathbf{r}_S)\cdot\mathbf{H}^{(C)}[\boldsymbol{\mathcal{G}}_{k_0}^{(C)(\mathrm{PP})}(\mathbf{r}_S;\mathbf{r}_0)]dS. \qquad (37)$$

Since the $\mathbf{W}_n^+(\mathbf{K}_{\mathrm{inc}PQ})$ with $-M_{\max}\le P\le M_{\max}$ and $-N_{\max}\le Q\le N_{\max}$ are independent vector functions, there exists a single set of coefficients $A_{nPQ}(M_{\max},N_{\max})$ that minimizes the positive quantity err $(M_{\max},N_{\max})$ defined by

$$\mathrm{err}^2(M_{\max},N_{\max})=\int_{S_0}\Big\|-\mathbf{n}\times\mathbf{E}_{\mathrm{inc}}(\mathbf{r}_S)-\sum_{n=1}^{2}\sum_{P,Q}A_{nPQ}(M_{\max},N_{\max})\times\mathbf{W}_n^{+}(\mathbf{K}_{\mathrm{inc}PQ})(\mathbf{r}_S)\Big\|^2 dS, \tag{38}$$

where it is henceforth implicit that $-M_{\max}\leqslant P\leqslant M_{\max}$ and $-N_{\max}\leqslant Q\leqslant N_{\max}$ and it can be noted that $\mathbf{n}\times\mathbf{E}_{\mathrm{ref}}=-\mathbf{n}\times\mathbf{E}_{\mathrm{inc}}$ at S.

In the Rayleigh least-squares method, the reflected field $\mathbf{E}_{\mathrm{ref}}(\mathbf{r}_0)$ is taken to be equal to $\mathbf{\Lambda}(\mathbf{r}_0;M_{\max},N_{\max})$, with

$$\mathbf{\Lambda}(\mathbf{r}_0;M_{\max},N_{\max})=\sum_{n=1}^{2}\sum_{P,Q}A_{nPQ}(M_{\max},N_{\max})\mathbf{V}_n^{+}(\mathbf{K}_{\mathrm{inc}PQ})\times\exp[i\mathbf{k}_n^{+}(\mathbf{K}_{\mathrm{inc}PQ})\cdot\mathbf{r}_0], \tag{39}$$

where the A_{nPQ} are those scalars that minimize the right-hand side of Eq. (38).

With Eqs. (36) and (37) and the Schwarz inequality, we can write for all $\mathbf{r}_0$ not located on S and for all $M_{\max}$ and $N_{\max}$

$$|\mathbf{e}_{k_0}\cdot\mathbf{E}_{\mathrm{ref}}(\mathbf{r}_0)-\mathbf{e}_{k_0}\cdot\mathbf{\Lambda}(\mathbf{r}_0;M_{\max},N_{\max})|\leqslant\omega\ \mathrm{err}(M_{\max},N_{\max})\times\left(\int_{S_0}\|\mathbf{H}^{(C)}[\boldsymbol{\mathcal{G}}_{k_0}^{(C)(\mathrm{PP})}(\mathbf{r}_S;\mathbf{r}_0)]\|^2 dS\right)^{1/2}. \tag{40}$$

Because of the completeness of the $\mathbf{W}_n^{+}(\mathbf{K}_{\mathrm{inc}PQ})$ in $L_\perp^2(\mathbf{K}_{\mathrm{inc}})$, $\mathrm{err}(M_{\max},N_{\max})$ can be made as small as wanted by increasing $M_{\max}$ and $N_{\max}$; thus Eq. (40) shows that, for all k_0 (k_0=1, 2, or 3),

$$\lim_{M_{\max},N_{\max}\to+\infty}|\mathbf{e}_{k_0}\cdot\mathbf{E}_{\mathrm{ref}}(\mathbf{r}_0)-\mathbf{e}_{k_0}\cdot\mathbf{\Lambda}(\mathbf{r}_0;M_{\max},N_{\max})|=0 \tag{41}$$

in all closed subsets of the medium above S. Therefore $\mathbf{\Lambda}(\mathbf{r}_0;M_{\max},N_{\max})$ uniformly converges to the exact solution in all closed subsets of the medium of propagation.

By writing that uniform convergence holds in particular above the highest point of S, it readily follows [18] that, for given integers P and Q, and $n=1$ or 2,

$$\lim_{M_{\max},N_{\max}\to+\infty}A_{nPQ}(M_{\max},N_{\max})=t_{nn_0}(\mathbf{K}_{\mathrm{inc}PQ},\mathbf{K}_{\mathrm{inc}}). \tag{42}$$

Equations (41) and (42) have been established for a particular case of boundary condition. As noted by Millar [18] for scalar diffraction, these equations can be extended to the case of linear boundary conditions combining $\mathbf{n}\times\mathbf{E}$ and $\mathbf{n}\times\mathbf{H}$, which ensure the existence and uniqueness of a solution to the problem.

As indicated at the end of Sec. III, the Rayleigh least-squares numerical results can also be connected by the equalities (22) and (23) to a Waterman method numerical results. However, the above conclusions yield still firmer ground for the application of the Rayleigh least-squares method and more information (in particular about the evaluation of the near field).

V. NUMERICAL APPLICATION

A. Statement of the problem

We consider the case of a sinusoidal interface S between an isotropic chiral medium, above S, and a perfectly conducting medium, below S. The interface S is defined by $z=hf(x)$ with $f(x)=\cos(2\pi x/\mathrm{D})$, where x is an horizontal coordinate (say, along $\mathbf{e}_1$); the constitutive relationships in the chiral medium are [34]

$$\mathbf{D}=\epsilon(\mathbf{E}+\beta\nabla\times\mathbf{E}), \tag{43a}$$

$$\mathbf{B}=\mu(\mathbf{H}+\beta\nabla\times\mathbf{H}), \tag{43b}$$

where ϵ, μ, and β are real scalars.

The interface S is illuminated by the electric field $\mathbf{E}_{\mathrm{inc}}$ [34]

$$\mathbf{E}_{\mathrm{inc}}(\mathbf{r})=\sum_{j=1}^{2}A_j\frac{\gamma_j}{\xi_{j,0}}\mathbf{e}_{j,0}^{-}\exp[i\mathbf{k}_j^{-}(K_{\mathrm{inc}})\cdot\mathbf{r}], \tag{44}$$

where, with $k=\omega(\epsilon\mu)^{1/2}$ and for any integer N,

$$\gamma_1=\frac{k}{1-k\beta}, \tag{45}$$

$$\gamma_2=\frac{k}{1+k\beta}, \tag{46}$$

$$\mathbf{k}_j^{\pm}(K_{\mathrm{inc}N})=K_{\mathrm{inc}N}\mathbf{e}_1\pm\xi_{j,N}\mathbf{e}_3, \tag{47}$$

$$\xi_{j,N}=(\gamma_j^2-K_{\mathrm{inc}N}^2)^{1/2}, \tag{48}$$

$$K_{\mathrm{inc}N}=K_{\mathrm{inc}}+2\pi\frac{N}{D}, \tag{49}$$

$$\mathbf{e}_{1,N}^{\pm}=\frac{1}{\sqrt{2}}\left[\mathbf{e}_2-\frac{i}{\gamma_1}(\pm\xi_{1,N}\mathbf{e}_1-K_{\mathrm{inc}N}\mathbf{e}_3)\right], \tag{50}$$

$$\mathbf{e}_{2,N}^{\pm}=\frac{1}{\sqrt{2}}\left[\mathbf{e}_2+\frac{i}{\gamma_2}(\pm\xi_{2,N}\mathbf{e}_1-K_{\mathrm{inc}N}\mathbf{e}_3)\right], \tag{51}$$

where $j=1$ or 2, and the square root in Eq. (48) is taken to be positive if $\gamma_j^2>K_{\mathrm{inc}N}^2$ and positive imaginary if $\gamma_j^2<K_{\mathrm{inc}N}^2$. The reflected electric field $\mathbf{E}_{\mathrm{ref}}$ is numerically sought as [34]

$$\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r})=\sum_{N=-N_{\max}}^{N_{\max}}\sum_{j=1}^{2}\frac{\gamma_j}{\xi_{j,N}}C_{j,N}\mathbf{e}_{j,N}^{+}\exp[i\mathbf{k}_j^{+}(K_{\mathrm{inc}N})\cdot\mathbf{r}]. \tag{52}$$

B. Application of the Rayleigh least-squares method

In the Rayleigh least-squares method, the scattered mode amplitudes are calculated by minimizing the integrated-square error on the boundary condition $\mathbf{n}\times\mathbf{E}=\mathbf{0}$, which amounts to writing, for all M such that $-N_{\max}\leqslant M\leqslant N_{\max}$ and for $j=1$ or 2,

$$\int_0^D\{(\mathbf{n}'\times\mathbf{e}_{j,M}^{+})\exp[i\mathbf{k}_j^{+}(K_{\mathrm{inc}M})\cdot\mathbf{r}_S]\}^*\cdot[\mathbf{n}'\times\mathbf{E}_{\mathrm{inc}}(\mathbf{r}_S)+\mathbf{n}'\times\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r}_S)]dx=0, \tag{53}$$

where $\mathbf{r}_s = x\mathbf{e}_1 + hf(x)\mathbf{e}_3$, $\mathbf{n}' = -hf'(x)\mathbf{e}_1 + \mathbf{e}_3$, and $\mathbf{E}_{\mathrm{inc}}$ and $\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}$ are expressed by (44) and (52).

The $C_{j,N}$'s are obtained by solving the linear system (53), which can be written, for all M such that $-N_{\max} \leqslant M \leqslant N_{\max}$ and for $I=1$ or 2,

$$\sum_{J=1}^{2} \sum_{N=-N_{\max}}^{N_{\max}} U_{\mathrm{RLS}}(M,N,I,J) C_{J,N} = \sum_{J=1}^{2} A_J Z_{\mathrm{RLS}}(M,I,J), \tag{54}$$

where the dependence of the $C_{J,N}$'s on $N_{\max}$ is implicit and, for $I,J=1$ or 2,

$$\begin{aligned}\frac{\xi_{J,N}}{\gamma_J} U_{\mathrm{RLS}}(M,N,I,J) &= \left[1+(-1)^{I+J}\frac{\xi_{I,M}^{*}\xi_{J,N}}{\gamma_I\gamma_J} + \frac{1}{2}\left(2\pi\frac{h}{D}\right)^2 \times \left(1+(-1)^{I+J}\frac{K_{\mathrm{inc}N}K_{\mathrm{inc}M}}{\gamma_I\gamma_J}\right)\right] I_{N,M}^{(I,J)} - (-1)^{I+J} \\ &\quad\times \frac{i}{2\gamma_I\gamma_J}\left(2\pi\frac{h}{D}\right)(\xi_{I,M}^{*}K_{\mathrm{inc}N} + \xi_{J,N}K_{\mathrm{inc}M}) \\ &\quad\times (I_{N+1,M}^{(I,J)} - I_{N-1,M}^{(I,J)}) - \frac{1}{4}\left(2\pi\frac{h}{D}\right)^2 \left[1+(-1)^{I+J} \times \frac{K_{\mathrm{inc}N}K_{\mathrm{inc}M}}{\gamma_I\gamma_J}\right](I_{N+2,M}^{(I,J)} + I_{N-2,M}^{(I,J)}),\end{aligned} \tag{55}$$

$$\begin{aligned}-\frac{\xi_{J,0}}{\gamma_J} Z_{\mathrm{RLS}}(M,I,J) &= \left[1-(-1)^{I+J}\frac{\xi_{I,M}^{*}\xi_{J,0}}{\gamma_I\gamma_J} + \frac{1}{2}\left(2\pi\frac{h}{D}\right)^2 \times \left(1+(-1)^{I+J}\frac{K_{\mathrm{inc}}K_{\mathrm{inc}M}}{\gamma_I\gamma_J}\right)\right] K_M^{(I,J)} - (-1)^{I+J} \\ &\quad\times \frac{i}{2\gamma_I\gamma_J}\left(2\pi\frac{h}{D}\right)(\xi_{I,M}^{*}K_{\mathrm{inc}} - \xi_{J,0}K_{\mathrm{inc}M}) \\ &\quad\times (K_{M-1}^{(I,J)} - K_{M+1}^{(I,J)}) - \frac{1}{4}\left(2\pi\frac{h}{D}\right)^2 \\ &\quad\times \left[1+(-1)^{I+J}\frac{K_{\mathrm{inc}}K_{\mathrm{inc}M}}{\gamma_I\gamma_J}\right](K_{M-2}^{(I,J)} + K_{M+2}^{(I,J)}),\end{aligned} \tag{56}$$

with the notations

$$I_{K,L}^{(j,k)} = (-i)^{|K-L|} J_{|K-L|}[h(\xi_{j,M}^{*} - \xi_{k,N})], \tag{57}$$

$$K_L^{(j,k)} = (-i)^{|L|} J_{|L|}[h(\xi_{j,M}^{*} + \xi_{k,0})], \tag{58}$$

where $j,k=1$ or 2 and J_L is the cylindrical Bessel function of order L. Equations (22a) and (23a) of Ref. [34] have been used to establish Eqs. (55) and (56) here. Once the amplitudes of the incident electric field are given, the problem is completely described by $K_{\mathrm{inc}}D$, kD, h/D, and β/D.

For all the real positive $\xi_{1,N}$ and $\xi_{2,N}$, we set, with $j=1$ or 2,

$$R_{1j,N} = \frac{\gamma_1}{\gamma_j}\frac{\xi_{j,0}}{\xi_{1,N}}\frac{|C_{1,N}|^2}{|A_j|^2}, \tag{59}$$

$$R_{2j,N} = \frac{\gamma_2}{\gamma_j}\frac{\xi_{j,0}}{\xi_{2,N}}\frac{|C_{2,N}|^2}{|A_j|^2}. \tag{60}$$

The exact values of the reflected efficiencies $R_{1j,N}$ and $R_{2j,N}$ verify the law of conservation of energy $\mathcal{E}_j=1$ with

$$\mathcal{E}_j = \sum_N (R_{1j,N} + R_{2j,N}), \tag{61}$$

where only the real positive values of $\xi_{1,N}$ and $\xi_{2,N}$ are retained.

The performance of the Rayleigh least-squares method for the calculation of the reflected efficiencies defined above is illustrated in Table I, where some of them and their complete sum are indicated. For these results $A_1=1$ and $A_2=0$, the angle of incidence θ_i is 0, $\beta/D=0.025$, and $kD=10$. Up to $h/D=0.10$ (the Rayleigh hypothesis is valid up to $h/D \simeq 0.072$), a good convergence of the reflected efficiencies is found. As noted by Wirgin for isotropic achiral media [42], despite the fact that the Rayleigh least-squares method is theoretically always convergent, the matrix of the linear system (54) tends to become numerically singular for large $N_{\max}$ (all the larger as h/D is smaller) so that its inversion is unreliable. Beyond $h/D \simeq 0.10$, this situation occurs before $N_{\max}$ can get large enough for the method to give satisfactory results; thus, while incidence is normal for the results of Table I, we find that $R_{21,-1} \neq R_{21,1}$, $R_{11,-2} \neq R_{11,2}$, and $R_{11,-1} \neq R_{11,1}$ instead of equality for $N_{\max}=20$ and $h/D=0.15$ or 0.25 (as indicated by the presence of an asterisk).

We have found about the same limit of numerical applicability in h/D with other values of angle of incidence and a different polarization of the incident electric field; this limit decreases somewhat when kD increases (simply because there are more reflected efficiencies to be determined). It may be greater for isotropic achiral media [17] because then only one type of polarization may be involved and the linear system to be solved may be smaller. As in the case of isotropic achiral media, the Rayleigh least-squares method is characterized by a slow and monotonic convergence of the reflected efficiencies with a systematic deficit of energy in the energy balance check as $N_{\max}$ increases [20].

Since we expect the results of the Rayleigh least-squares method to converge to the exact value of $\mathbf{E}$ in the near field, it is interesting to observe how the results obtained in this region behave numerically, in particular whether the boundary condition is verified and whether the electric field in the grooves converges. We set $\mathbf{r}_1 = 0.5D\mathbf{e}_1 - h\mathbf{e}_3$, $\mathbf{r}_2 = 0.5D\mathbf{e}_1 - 0.5h\mathbf{e}_3$, and

$$\delta^{(N_{\max})}(\mathbf{r}_1) = \frac{\|\mathbf{n}(\mathbf{r}_1)\times\mathbf{E}_{\mathrm{inc}}(\mathbf{r}_1) + \mathbf{n}(\mathbf{r}_1)\times\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r}_1)\|}{\|\mathbf{n}(\mathbf{r}_1)\times E_{\mathrm{inc}}(\mathbf{r}_1)\|}. \tag{62}$$

TABLE I. Reflected efficiencies calculated with the Rayleigh least-squares method for a sinusoidal grating defined by $z=h\cos(2\pi x/D)$. The problem parameters are $\theta_i=0$, $\beta/D=0.025$, and $kD=10$ and the incident wave is defined by $A_1=1$ and $A_2=0$. The sum of the reflected efficiencies corresponding to radiating eigenwaves is given in the column labelled SE. The presence of an asterisk indicates results that do not satisfy the expected symmetry properties.

h/D	N_{max}	$R_{21,0}$	$R_{21,1}$	$R_{11,0}$	$R_{11,1}$	SE
0.05	5	0.528 652	0.214 891	$0.155\,589\times10^{-1}$	$0.109\,421\times10^{-1}$	0.999 990
	10	0.528 648	0.214 886	$0.155\,620\times10^{-1}$	$0.109\,465\times10^{-1}$	1.000 000
	20	0.528 648	0.214 886	$0.155\,620\times10^{-1}$	$0.109\,465\times10^{-1}$	1.000 000
0.10	5	$0.147\,752\times10^{-1}$	0.372 937	0.158 648	$0.131\,651\times10^{-1}$	0.987 574
	10	$0.145\,894\times10^{-1}$	0.367 079	0.168 043	$0.151\,046\times10^{-1}$	0.999 682
	20	$0.145\,876\times10^{-1}$	0.366 953	0.168 243	$0.151\,478\times10^{-1}$	1.000 000
0.15	5	0.134 749	0.159 238	0.294 204	$0.124\,981\times10^{-1}$	0.820 821
	10	0.143 982	0.116 774	0.443 203	$0.159\,191\times10^{-1}$	0.954 889
	20	0.145 098	0.108 138*	0.479 079	$0.168\,333\times10^{-1}$*	0.998 558
0.25	5	$0.242\,000\times10^{-1}$	$0.763\,104\times10^{-1}$	0.347 921	$0.548\,537\times10^{-1}$	0.666 257
	10	$0.448\,660\times10^{-1}$	0.150 575	0.398 691	$0.863\,693\times10^{-1}$	0.951 101
	20	$0.609\,542\times10^{-1}$	0.177 420*	0.349 345	$0.993\,825\times10^{-1}$*	1.007 188

The values of $\delta^{(N_{\max})}(\mathbf{r}_1)$, $\|\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r}_2)\|$, and the components of $\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r}_2)$, obtained when $N_{\max}=5$, 10, or 20, $\theta_i=0$, $kD=10$, $h/D=0.10$, $\beta/D=0.025$, $A_1=1$, and $A_2=0$, are given in Table II [the component of $\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r}_2)$ along $\mathbf{e}_3$, of the order of 10^{-9}, is not indicated]. Since $\mathbf{r}_1$ is on S, $\delta^{(N_{\max})}(\mathbf{r}_1)$ is expected to converge to 0; we can note that this is so up to $N_{\max}=20$ after which value the linear system (54) becomes numerically singular, as explained above. This result is not obvious from the construction of the Rayleigh least-squares method, which requires verification of the boundary condition only in the mean-square sense. In addition, it also appears that $\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r}_2)$ converges up to $N_{\max}=20$. We have found that numerical convergence of $\delta^{(N_{\max})}(\mathbf{r}_1)$ and $\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r}_2)$ is observed for other choices of points on S and in the grooves, and that it is obtained under the same conditions as numerical convergence of reflected efficiencies (i.e., up to $h/D\simeq0.10$, beyond the domain of validity of the Rayleigh hypothesis).

C. Application of the Rayleigh-Fourier method

In the Rayleigh-Fourier method, the scattered mode amplitudes are calculated by projecting the boundary condition $\mathbf{n}\times\mathbf{E}=\mathbf{0}$ on the Fourier basis comprising the functions $\mathbf{t}_1\exp(-iK_{\mathrm{inc}M}x)$ and $\mathbf{t}_2\exp(-iK_{\mathrm{inc}M}x)$, where M is an integer such that $-N_{\max}\leqslant M\leqslant N_{\max}$ and $\mathbf{t}_1=\mathbf{e}_1+hf'(x)\mathbf{e}_3$ and $\mathbf{t}_2=\mathbf{e}_2$. As a result, the $C_{j,N}$'s are obtained by solving the linear system (54), where the U_{RLS} and Z_{RLS} are replaced by the U_{RF} and Z_{RF} defined by

$$\frac{\xi_{I,N}}{\gamma_I}U_{\mathrm{RF}}(M,N,1,I)=-\left[1+\frac{1}{2}\left(\frac{2\pi h}{D}\right)^2\right]I_{N,M}^{(I)}+\frac{1}{4}\left(\frac{2\pi h}{D}\right)^2\left(I_{N+2,M}^{(I)}+I_{N-2,M}^{(I)}\right),\tag{63}$$

$$(-1)^I U_{\mathrm{RF}}(M,N,2,I)=iI_{N,M}^{(I)}+\frac{1}{2}\frac{K_{\mathrm{inc}N}}{\xi_{I,N}}\left(\frac{2\pi h}{D}\right)\times\left(I_{N+1,M}^{(I)}-I_{N-1,M}^{(I)}\right),\tag{64}$$

$$\frac{\xi_{I,0}}{\gamma_I}Z_{\mathrm{RF}}(M,1,I)=\left[1+\frac{1}{2}\left(\frac{2\pi h}{D}\right)^2\right]K_M^{(I)}-\frac{1}{4}\left(\frac{2\pi h}{D}\right)^2\times\left(K_{M-2}^{(I)}+K_{M+2}^{(I)}\right),\tag{65}$$

$$(-1)^I Z_{\mathrm{RF}}(M,2,I)=iK_M^{(I)}-\frac{1}{2}\frac{K_{\mathrm{inc}}}{\xi_{I,0}}\left(\frac{2\pi h}{D}\right)\left(K_{M-1}^{(I)}-K_{M+1}^{(I)}\right),\tag{66}$$

with $I=1$ or 2 and the notations

TABLE II. Reflected electric field at $\mathbf{r}_2=0.5D\mathbf{e}_1-0.5h\mathbf{e}_3$ and verification of the boundary condition at $\mathbf{r}_1=0.5D\mathbf{e}_1-h\mathbf{e}_3$ obtained with the Rayleigh least-squares method for a sinusoidal grating defined by $z=h\cos(2\pi x/D)$. The problem parameters are $\theta_i=0$, $\beta/D=0.025$, $kD=10$, and $h/D=0.10$ and the incident wave is defined by $A_1=1$ and $A_2=0$. The component of $\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}$ along $\mathbf{e}_3$, of order 10^{-9}, is not given.

$N_{\max}$	5	10	20
$\mathbf{e}_1\cdot\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r}_2)$	$0.765\,354+0.163\,339i$	$0.782\,557+0.180\,184i$	$0.782\,927+0.180\,365i$
$\mathbf{e}_2\cdot\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r}_2)$	$-0.219\,248-0.778\,731i$	$-0.209\,574-0.763\,293i$	$-0.209\,346-0.763\,002i$
$\|\mathbf{E}_{\mathrm{ref}}^{(N_{\max})}(\mathbf{r}_2)\|$	1.125 583	1.127 564	1.127 610
$\delta^{(N_{\max})}(\mathbf{r}_1)$	0.75×10^{-1}	0.95×10^{-2}	0.20×10^{-3}

TABLE III. Reflected efficiencies calculated with the Rayleigh-Fourier method for a sinusoidal grating defined by $z=h\cos(2\pi x/D)$. The problem parameters are $\theta_i=0$, $\beta/D=0.025$, and $kD=10$ and the incident wave is defined by $A_1=1$ and $A_2=0$. The sum of the reflected efficiencies corresponding to radiating eigenwaves is given in the column labeled SE.

h/D	N_{max}	$R_{21,0}$	$R_{21,1}$	$R_{11,0}$	$R_{11,1}$	SE
0.05	5	0.528 648	0.214 886	$0.155\,619\times10^{-1}$	$0.109\,464\times10^{-1}$	1.000 000
	10	0.528 648	0.214 886	$0.155\,620\times10^{-1}$	$0.109\,465\times10^{-1}$	1.000 000
	15	0.528 648	0.214 886	$0.155\,620\times10^{-1}$	$0.109\,465\times10^{-1}$	1.000 000
0.10	5	$0.145\,952\times10^{-1}$	0.366 975	0.168 201	$0.151\,495\times10^{-1}$	1.000 032
	10	$0.145\,876\times10^{-1}$	0.366 953	0.168 243	$0.151\,478\times10^{-1}$	1.000 000
	15	$0.145\,876\times10^{-1}$	0.366 953	0.168 243	$0.151\,478\times10^{-1}$	1.000 000
0.15	5	0.143 976	0.108 696	0.478 696	$0.171\,248\times10^{-1}$	1.000 358
	10	0.145 261	0.107 774	0.480 290	$0.168\,681\times10^{-1}$	1.000 002
	15	0.145 263	0.107 771	0.480 296	$0.168\,671\times10^{-1}$	1.000 000
0.25	5	$0.571\,215\times10^{-1}$	0.169 627	0.271 784	$0.962\,951\times10^{-1}$	0.928 041
	10	$0.728\,799\times10^{-1}$	0.177 864	0.304 805	0.105 771	0.999 909
	15	$0.734\,226\times10^{-1}$	0.177 897	0.305 001	0.105 780	1.000 003

$$I^{(I)}_{K,L}=(-i)^{|K-L|}J_{|K-L|}(-h\xi_{I,N}), \tag{67}$$

$$K^{(I)}_{L}=(-i)^{|L|}J_{|L|}(h\xi_{I,0}). \tag{68}$$

Numerical results obtained for the reflected efficiencies with the Rayleigh-Fourier method with the same conditions as in Table I (except for N_{max}) are shown in Table III. As in the case of an achiral isotropic medium [20], the Rayleigh-Fourier method, compared to the Rayleigh least-squares method, can be used for greater values of h/D (up to 0.25) and converges faster. We have generally observed a monotonic convergence of the reflected efficiencies. We have found again that the angle of incidence and the polarization of the incident electric field do not significantly affect the domain or the rate of convergence; this domain decreases somewhat when kD increases.

$\delta^{N_{max}}(\mathbf{r}_1)$, defined in Sec. V B, is found to converge to 0 only when the Rayleigh hypothesis is valid, which is in agreement with the computations presented by Chesneaux and Wirgin [21] for an achiral isotropic medium. The convergence of the near field is slower than it is with the Rayleigh least-squares method; the slow convergence of the Rayleigh-Fourier method for the computation of the near field has also been noted in Ref. [21].

VI. CONCLUSION

We have considered the problem of electromagnetic reflection and transmission at a periodic rough interface separating two semi-infinite general homogeneous media. The problem is assumed to have a unique solution. We have shown that numerical convergence of the Waterman-Fourier method for the calculation of the T-matrix coefficients implies numerical convergence of the Rayleigh-Fourier method. The latter must therefore not be regarded as limited by the validity of the Rayleigh hypothesis for the computation of the reflected and transmitted amplitudes; this is confirmed by the numerical results of Depine and Gigli [38]. This is also confirmed by the application to the case of a sinusoidal surface separating a perfectly conducting medium and a chiral medium; very good results are found for the reflected efficiencies up to $h/D=0.25$, which is more than 3 times the maximum slope of validity of the Rayleigh hypothesis. We have found, however, that the Rayleigh-Fourier method is either invalid (if the Rayleigh hypothesis does not hold) or inadequate to evaluate the near field.

In the case of a single semi-infinite medium bounded by a periodic rough surface, it has been shown that the Rayleigh least-squares method gives expansions that uniformly converge to the exact reflected field in all closed subsets of the medium; as a consequence, the Rayleigh least-squares method is also numerically convergent for the calculation of the reflected amplitudes. These convergence properties stem from completeness properties of the set of outgoing and evanescent eigenwaves. They have been corroborated by the application to the same case as for the Rayleigh-Fourier method; good results for the reflected efficiencies and for the near field have been found up to $h/D\simeq0.10$, which is about 1.5 times the maximum slope of validity of the Rayleigh hypothesis. Beyond this value of h/D, the method becomes inapplicable for numerical reasons [42].

The qualitative features of the Rayleigh least-squares method found by Wirgin with an achiral isotropic medium [20] and a sinusoidal surface, namely, a slow and monotonic convergence of the reflected efficiencies, are unchanged when the medium is chiral. It is not the case for the Rayleigh-Fourier method: it still converges faster, but in a monotonic (and not oscillatory) fashion. It seems reasonable to conjecture that, in anisotropic media as in isotropic chiral and achiral media, the Rayleigh-Fourier method is more suited (faster convergence and larger domain of validity) to compute the reflected efficiencies and the Rayleigh least-squares method is more suited to compute the near field.

For the demonstration of these results, it has been assumed that the dispersion equation (9) has only single roots in k_z with each root corresponding to a one-dimensional space of eigenvectors. This is not true in the limiting case of an achiral isotropic medium; however, the expression of the free-space Green's vector fields is still similar to Eq. (7) and it is possible to reach the conclusions indicated above. In addition, in Sec. IV, which deals with the Rayleigh least-squares method, we have made the classical assumptions of term by term differentiability and uniform convergence of the series in Eq. (A10); term by term differentiability has enabled us to regard the Green's vector fields as analytic.

We can try to further extend the conditions of validity of the conclusions reached. If there exists a complementary medium C such that the dispersion relationship governing plane waves propagation verifies, with the definitions of Sec. II, $L^{(C)}(-\mathbf{k},\omega)={}^tL(\mathbf{k},\omega)$ for all $\mathbf{k}$ and ω, and if the vector fields sought can be expressed by surface integrals with integrands of the form $\mathbf{A}(\mathbf{n},\mathbf{E})\cdot\mathbf{B}^{(C)}(\mathbf{n},\mathbf{G}_{k_0}^{(C)})-\mathbf{A}^{(C)}(\mathbf{n},\mathbf{G}_{k_0}^{(C)})\cdot\mathbf{B}(\mathbf{n},\mathbf{E})$, where $\mathbf{A}$ and $\mathbf{B}$ are surface vector fields expressing the interface conditions, then it is possible to reproduce the demonstrations of this paper. Such conditions include anisotropic elastic media; they also include media that do not necessarily satisfy the physical constraints of electromagnetic propagation [39]. We conjecture that Rayleigh methods can, as in the case of acoustic scattering in isotropic media [43], be applied to scattering from finite bodies under the same general conditions.

The conclusions of this paper broadly extend results progressively established in the case of simple isotropic media [18,24,25]. It can be noted that they focus on the numerical results obtained with the Rayleigh methods (and their relation to the exact results) so that they have a practical interest. These conclusions also indicate that approaches related to the Rayleigh methods discussed, and apparently not yet considered for general media, could be useful. One of them is a numerical method proposed by Matsuda and Okuno [44] to enhance the convergence of the Rayleigh least-squares method, which is rather slow in practice. Another is the perturbation method [22] possibly implemented with enhanced convergence techniques [27–31]. Indeed, for surface profiles that are finite linear combinations of sinusoids, the demonstration of either Sec. III or Ref. [25] (extended to general media) can be used (because then only finite sums intervene at each order) to show that the Rayleigh-Fourier perturbation series is identical to the Waterman-Fourier perturbation series so that the former, which is easier to implement, can be regarded as derived from an exact formalism.

APPENDIX: WATERMAN-FOURIER FORMALISM

The T-matrix formalism proposed by Waterman for electromagnetic scattering [45] involves two steps: solving the null-field equations [46] for the unknown surface fields and using the result to compute the reflected and transmitted fields with the classical integral representation. The unknown surface fields are represented by an expansion on a set of complete functions; when a Fourier expansion is used, the method is sometimes called the Waterman-Fourier method [14].

In the case where S separates media 1 and 2, a classical demonstration using Green's theorem leads to

$$E_{\mathrm{inc},k_0}^{(1)}(\mathbf{r}_0)+i\omega\int_S[(\mathbf{n}\times\mathbf{E})\cdot\mathbf{H}^{(1C)}(\mathbf{G}_{k_0}^{(1C)})+(\mathbf{n}\times\mathbf{H})\cdot\mathbf{G}_{k_0}^{(1C)}]dS=0 \tag{A1}$$

for all k_0 (k_0=1, 2, or 3), where $E_{\mathrm{inc},k_0}^{(1)}$ is the k_0^{th} component of the incident electric field coming from medium 1, $\mathbf{r}_0$ is any vector point located below S, and $\mathbf{G}_{k_0}^{(1C)}$ stands for $\mathbf{G}_{k_0}^{(1C)}(\mathbf{r}_S;\mathbf{r}_0)$, where $\mathbf{r}_S$ is a vector point on S. The extinction theorem yields a second equation

$$E_{\mathrm{inc},k_0}^{(2)}(\mathbf{r}_0)-i\omega\int_S[(\mathbf{n}\times\mathbf{E})\cdot\mathbf{H}^{(2C)}(\mathbf{G}_{k_0}^{(2C)})+(\mathbf{n}\times\mathbf{H})\cdot\mathbf{G}_{k_0}^{(2C)}]dS=0, \tag{A2}$$

where $E_{\mathrm{inc},k_0}^{(2)}$ is the k_0^{th} component of the incident electric field coming from medium 2, $\mathbf{r}_0$ is any vector point located above S, and $\mathbf{G}_{k_0}^{(2C)}$ stands for $\mathbf{G}_{k_0}^{(2C)}(\mathbf{r}_S;\mathbf{r}_0)$, where $\mathbf{r}_S$ is a vector point on S. In Eqs. (A1) and (A2), the operators $\mathbf{H}^{(jC)}$ apply to the dependence in $\mathbf{r}_S$.

The $\pm$ superscripts of $\mathbf{E}$ and $\mathbf{H}$ in the surface integrals have been omitted because of the interface conditions (2a) and (2b). Equations (A1) and (A2) form a system of two equations with the two unknown surface fields $\mathbf{n}\times\mathbf{E}$ and $\mathbf{n}\times\mathbf{H}$. Once these unknowns are determined, they can be used in the integral representation of the electric field in medium 1, which can be written as

$$E_{k_0}^{(1)}(\mathbf{r}_0)=E_{\mathrm{inc},k_0}^{(1)}(\mathbf{r}_0)+i\omega\int_S[(\mathbf{n}\times\mathbf{E})\cdot\mathbf{H}^{(1C)}(\mathbf{G}_{k_0}^{(1C)})+(\mathbf{n}\times\mathbf{H})\cdot\mathbf{G}_{k_0}^{(1C)}]dS, \tag{A3}$$

where $E_{k_0}^{(1)}$ is the k_0^{th} component of the electric field in medium 1, $\mathbf{r}_0$ is any vector point located above S, and $\mathbf{G}_{k_0}^{(1C)}$ stands for $\mathbf{G}_{k_0}^{(1C)}(\mathbf{r}_S;\mathbf{r}_0)$, where $\mathbf{r}_S$ is a vector point on S. A similar expression can be established for the electric field in medium 2, but only Eq. (A3) is necessary for the purpose of this paper.

We express the Waterman-Fourier formalism with the incident fields

$$E_{\mathrm{inc},k_0}^{(1)}(\mathbf{r}_0)=\delta_1[\mathbf{e}_{k_0}\cdot\mathbf{V}_{n_0}^{(1)-}(\mathbf{K}_{\mathrm{inc}})]\exp[i\mathbf{k}_{n_0}^{(1)-}(\mathbf{K}_{\mathrm{inc}})\cdot\mathbf{r}_0], \tag{A4}$$

$$E_{\mathrm{inc},k_0}^{(2)}(\mathbf{r}_0)=\delta_2[\mathbf{e}_{k_0}\cdot\mathbf{V}_{n_0}^{(2)+}(\mathbf{K}_{\mathrm{inc}})]\exp[i\mathbf{k}_{n_0}^{(2)+}(\mathbf{K}_{\mathrm{inc}})\cdot\mathbf{r}_0], \tag{A5}$$

where δ_1 and δ_2 are complex scalars. We write the reflected electric field in medium 1 above the highest point of S as

$$\mathbf{E}_{\mathrm{ref}}^{(1)}(\mathbf{r})=\sum_{n=1}^{2}\sum_{M,N}T_{nn_0}^{(1)}(\mathbf{K}_{\mathrm{inc}MN},\mathbf{K}_{\mathrm{inc}})\mathbf{V}_n^{(1)+}(\mathbf{K}_{\mathrm{inc}MN})\times\exp[i\mathbf{k}_n^{(1)+}(\mathbf{K}_{\mathrm{inc}MN})\cdot\mathbf{r}], \tag{A6}$$

where the $T_{nn_0}^{(1)}$'s are complex scalars.

By noting the pseudoperiodicity of the surface fields, using the expression (7) of the free-space Green's vector fields (applied to media $1C$ and $2C$) and Eqs. (16)–(18) and proceeding as Waterman [47], we can rewrite Eqs. (A1)–(A3) as

$$E^{(1)}_{\mathrm{inc},k_0}(\mathbf{r}_0)+i\omega\int_{S_0}[(\mathbf{n}\times\mathbf{E})\cdot\mathbf{H}^{(1C)}(\mathbf{G}^{(1C)(\mathrm{PP})}_{k_0})+(\mathbf{n}\times\mathbf{H})\cdot\mathbf{G}^{(1C)(\mathrm{PP})}_{k_0}]dS=0, \tag{A7}$$

$$E^{(2)}_{\mathrm{inc},k_0}(\mathbf{r}_0)-i\omega\int_{S_0}[(\mathbf{n}\times\mathbf{E})\cdot\mathbf{H}^{(2C)}(\mathbf{G}^{(2C)(\mathrm{PP})}_{k_0})+(\mathbf{n}\times\mathbf{H})\cdot\mathbf{G}^{(2C)(\mathrm{PP})}_{k_0}]dS=0, \tag{A8}$$

$$E^{(1)}_{k_0}(\mathbf{r}_0)=E^{(1)}_{\mathrm{inc},k_0}(\mathbf{r}_0)+i\omega\int_{S_0}[(\mathbf{n}\times\mathbf{E})\cdot\mathbf{H}^{(1C)}(\mathbf{G}^{(1C)(\mathrm{PP})}_{k_0})+(\mathbf{n}\times\mathbf{H})\cdot\mathbf{G}^{(1C)(\mathrm{PP})}_{k_0}]dS, \tag{A9}$$

where S_0 is the unit cell of S used in Sec. III and the pseudoperiodic Green's vector fields $\mathbf{G}^{(jC)(\mathrm{PP})}_{k_0}$ stand for $\mathbf{G}^{(jC)(\mathrm{PP})}_{k_0}(\mathbf{r}_S;\mathbf{r}_0)$ and are such that

$$\begin{aligned}\mathbf{G}^{(jC)(\mathrm{PP})}_{k_0}(\mathbf{r};\mathbf{r}_0)=&\pm\frac{i}{4\pi^2}\|\mathbf{R}_1\times\mathbf{R}_2\|\sum_{n=1}^{2}\sum_{P,Q}a_n^{(j)\pm}(\mathbf{K}_{\mathrm{inc}PQ})\\&\times[\mathbf{e}_{k_0}\cdot\mathbf{V}_n^{(j)\pm}(\mathbf{K}_{\mathrm{inc}PQ})]\Delta_n^{(j)\pm}(\mathbf{K}_{\mathrm{inc}PQ,}\omega)\\&\times\mathbf{V}_n^{(jC)\mp}(-\mathbf{K}_{\mathrm{inc}PQ})\\&\times\exp[i\mathbf{k}_n^{(jC)\mp}(-\mathbf{K}_{\mathrm{inc}PQ})\cdot(\mathbf{r}-\mathbf{r}_0)],\end{aligned} \tag{A10}$$

where the upper sign applies if $(z_0-z)>0$ and the lower sign applies if $(z_0-z)<0$.

Equation (A10) could also be obtained by seeking, in the space of generalized functions defined as in Ref. [1], the $\mathbf{G}^{(jC)}_{k_0}$'s in the form of a double Fourier series and by defining the $a_n^{(j)\pm}$'s and $\Delta_n^{(j)\pm}$'s as in Sec. II. We assume that $\mathbf{G}^{(jC)(\mathrm{PP})}_{k_0}$ has a sense as a vector field (when $\mathbf{r}\neq\mathbf{r}_0$) and that its differentiation with respect to the Cartesian coordinates of $\mathbf{r}_0$ can be carried out by term by term differentiation of the series in Eq. (A10). As a consequence, $\mathbf{G}^{(jC)(\mathrm{PP})}_{k_0}$ is a holomorphic function of the Cartesian coordinates of $\mathbf{r}_0$ and is therefore analytic [40].

With Eqs. (A4)–(A10) and Eq. (16), we find that

$$\begin{aligned}&\frac{4\pi^2\delta_1}{\omega a_{n_0}^{(1)-}(\mathbf{K}_{\mathrm{inc}})}[\Delta_{n_0}^{(1)-}(\mathbf{K}_{\mathrm{inc}},\omega)]^{-1}\delta_{nn_0}\delta_{P0}\delta_{Q0}\\&+\int_{S_0}[(\mathbf{n}\times\mathbf{H}')\cdot\mathbf{V}_n^{(1C)+}(-\mathbf{K}_{\mathrm{inc}PQ})]\\&\times\exp[i\mathbf{k}_n^{(1C)+}(-\mathbf{K}_{\mathrm{inc}PQ})\cdot\mathbf{r}]d^2R\\&+\int_{S_0}[(\mathbf{n}\times\mathbf{E}')\cdot\mathbf{H}\mathbf{V}_n^{(1C)+}(-\mathbf{K}_{\mathrm{inc}PQ})]\\&\times\exp[i\mathbf{k}_n^{(1C)+}(-\mathbf{K}_{\mathrm{inc}PQ})\cdot\mathbf{r}]d^2R=0,\end{aligned} \tag{A11}$$

$$\begin{aligned}&\frac{4\pi^2\delta_2}{\omega a_{n_0}^{(2)+}(\mathbf{K}_{\mathrm{inc}})}[\Delta_{n_0}^{(2)+}(\mathbf{K}_{\mathrm{inc}},\omega)]^{-1}\delta_{nn_0}\delta_{P0}\delta_{Q0}\\&+\int_{S_0}[(\mathbf{n}\times\mathbf{H}')\cdot\mathbf{V}_n^{(2C)-}(-\mathbf{K}_{\mathrm{inc}PQ})]\\&\times\exp[i\mathbf{k}_n^{(2C)-}(-\mathbf{K}_{\mathrm{inc}PQ})\cdot\mathbf{r}]d^2R\\&+\int_{S_0}[(\mathbf{n}\times\mathbf{E}')\cdot\mathbf{H}\mathbf{V}_n^{(2C)-}(-\mathbf{K}_{\mathrm{inc}PQ})]\\&\times\exp[i\mathbf{k}_n^{(2C)-}(-\mathbf{K}_{\mathrm{inc}PQ})\cdot\mathbf{r}]d^2R=0,\end{aligned} \tag{A12}$$

$$\begin{aligned}&-\frac{4\pi^2}{\omega a_n^{(1)+}(\mathbf{K}_{\mathrm{inc}PQ})}[\Delta_n^{(1)+}(\mathbf{K}_{\mathrm{inc}PQ},\omega)]^{-1}T^{(1)}_{nn_0}(\mathbf{K}_{\mathrm{inc}PQ},\mathbf{K}_{\mathrm{inc}})\\&=\int_{S_0}[(\mathbf{n}\times\mathbf{H}')\cdot\mathbf{V}_n^{(1C)-}(-\mathbf{K}_{\mathrm{inc}PQ})]\\&\times\exp[i\mathbf{k}_n^{(1C)-}(-\mathbf{K}_{\mathrm{inc}PQ})\cdot\mathbf{r}]d^2R\\&+\int_{S_0}[(\mathbf{n}\times\mathbf{E}')\cdot\mathbf{H}\mathbf{V}_n^{(1C)-}(-\mathbf{K}_{\mathrm{inc}PQ})]\\&\times\exp[i\mathbf{k}_n^{(1C)-}(-\mathbf{K}_{\mathrm{inc}PQ})\cdot\mathbf{r}]d^2R,\end{aligned} \tag{A13}$$

where the notations $\mathbf{H}'$ and $\mathbf{E}'$ stand for

$$\mathbf{H}'=[1+(\boldsymbol{\nabla}f)^2]^{1/2}\|\mathbf{R}_1\times\mathbf{R}_2\|\mathbf{H}, \tag{A14}$$

$$\mathbf{E}'=[1+(\boldsymbol{\nabla}f)^2]^{1/2}\|\mathbf{R}_1\times\mathbf{R}_2\|\mathbf{E}. \tag{A15}$$

Equations (A11)–(A13) hold for all $\mathbf{K}_{\mathrm{inc}}$, all integers P and Q, and all n and n_0 (n,n_0=1 or 2). When a numerical solution is sought, the unknown surface fields $\mathbf{n}\times\mathbf{E}'$ and $\mathbf{n}\times\mathbf{H}'$ are expanded on a set of complete functions and the equations are truncated. For the purpose of this paper, we choose to write the equations for a transverse incident wave vector equal to $-\mathbf{K}_{\mathrm{inc}M_0N_0}$ (where M_0 and N_0 are given integers) and a truncation such that $M_0-M_{\max}\leqslant P\leqslant M_0+M_{\max}$ and $N_0-N_{\max}\leqslant Q\leqslant N_0+N_{\max}$, where $M_{\max}$ and $N_{\max}$ are positive integers such that $M_{\max}>|M_0|$ and $N_{\max}>|N_0|$. For the pseudoperiodic surface fields $\mathbf{n}\times\mathbf{E}'$ and $\mathbf{n}\times\mathbf{H}'$, we set

$$\mathbf{n}\times\mathbf{E}'(\mathbf{r}_S)=\sum_{l=1}^{2}\sum_{K=M_0-M_{\max}}^{K=M_0+M_{\max}}\sum_{L=N_0-N_{\max}}^{L=N_0+N_{\max}}\alpha_{l,KL}\mathbf{t}_l(\mathbf{r}_S)\times\exp[-i\mathbf{K}_{\mathrm{inc}(M_0-K)(N_0-L)}\cdot\mathbf{R}], \tag{A16}$$

$$\mathbf{n}\times\mathbf{H}'(\mathbf{r}_S)=\sum_{l=1}^{2}\sum_{K=M_0-M_{\max}}^{K=M_0+M_{\max}}\sum_{L=N_0-N_{\max}}^{L=N_0+N_{\max}}\beta_{l,KL}\mathbf{t}_l(\mathbf{r}_S)\times\exp[-i\mathbf{K}_{\mathrm{inc}(M_0-K)(N_0-L)}\cdot\mathbf{R}], \tag{A17}$$

where $\mathbf{r}_S$ is a point of S_0 and $\mathbf{t}_1$ and $\mathbf{t}_2$ are the vectors tangent to S_0 chosen as in Sec. III (for the application of the Rayleigh-Fourier method).

Then Eqs. (A11) and (A12) yield, for n_0=1 or 2 and for all integers P and Q defined by the above truncation,

$$B^{(1C)+}(n,M_0-P,N_0-Q;M_0,N_0)=-\frac{4\pi^2\delta_1}{\omega a_{n_0}^{(1)-}(-\mathbf{K}_{\mathrm{inc}M_0N_0})}[\Delta_{n_0}^{(1)-}(-\mathbf{K}_{\mathrm{inc}M_0N_0},\omega)]^{-1}\delta_{nn_0}\delta_{P0}\delta_{Q0}, \tag{A18}$$

$$B^{(2C)-}(n,M_0-P,N_0-Q;M_0,N_0)=-\frac{4\pi^2\delta_2}{\omega a_{n_0}^{(2)+}(-\mathbf{K}_{\mathrm{inc}M_0N_0})}[\Delta_{n_0}^{(2)+}(-\mathbf{K}_{\mathrm{inc}M_0N_0},\omega)]^{-1}\delta_{nn_0}\delta_{P0}\delta_{Q0}, \tag{A19}$$

where, with $j=1$ or 2,

$$\begin{aligned}B^{(jC)\pm}(n,M_0-P,N_0-Q;M_0,N_0)=&\sum_{K,L}\alpha_{1,KL}Y^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}},2,n,M_0-P,N_0-Q,M_0-K,N_0-L)\\&-\sum_{K,L}\alpha_{2,KL}Y^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}},1,n,M_0-P,N_0-Q,M_0-K,N_0-L)\\&+\sum_{K,L}\beta_{1,KL}X^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}},2,n,M_0-P,N_0-Q,M_0-K,N_0-L)\\&-\sum_{K,L}\beta_{2,KL}X^{(jC)\pm}(\mathbf{K}_{\mathrm{inc}},1,n,M_0-P,N_0-Q,M_0-K,N_0-L).\end{aligned} \tag{A20}$$

For the scattered mode amplitude corresponding to a transverse component of the wave vector equal to $-\mathbf{K}_{\mathrm{inc}}$, Eq. (A13) yields

$$\begin{aligned}&-\frac{4\pi^2}{\omega a_n^{(1)+}(-\mathbf{K}_{\mathrm{inc}})}[\Delta_n^{(1)+}(-\mathbf{K}_{\mathrm{inc}},\omega)]^{-1}T_{nn_0,W}^{(1)}(-\mathbf{K}_{\mathrm{inc}},-\mathbf{K}_{\mathrm{inc}M_0N_0})\\&=\sum_{K,L}\alpha_{1,KL}Y^{(1C)-}(\mathbf{K}_{\mathrm{inc}},2,n,0,0,M_0-K,N_0-L)-\sum_{K,L}\alpha_{2,KL}Y^{(1C)-}(\mathbf{K}_{\mathrm{inc}},1,n,0,0,M_0-K,N_0-L)\\&\quad+\sum_{K,L}\beta_{1,KL}X^{(1C)-}(\mathbf{K}_{\mathrm{inc}},2,n,0,0,M_0-K,N_0-L)-\sum_{K,L}\beta_{2,KL}X^{(1C)-}(\mathbf{K}_{\mathrm{inc}},1,n,0,0,M_0-K,N_0-L).\end{aligned} \tag{A21}$$

$X^{(jC)\pm}$ and $Y^{(jC)\pm}$ are defined in Sec. III. In Eqs. (A20) and (A21), it is implicit that the sums on the integers K and L are such that $M_0-M_{\max}\leqslant K\leqslant M_0+M_{\max}$ and $N_0-N_{\max}\leqslant L\leqslant N_0+N_{\max}$. The subscript W in Eq. (A21) indicates that the results are obtained with the Waterman-Fourier method and the truncation chosen. Equations (A18)–(A21) are useful to establish the connection between the numerical results obtained with the Rayleigh-Fourier and Waterman-Fourier methods.

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