Mie scattering by an anisotropic object. Part II. Arbitrary-shaped object: differential theory

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The differential theory of diffraction by an arbitrary-shaped body made of arbitrary anisotropic material is developed. The electromagnetic field is expanded on the basis of vector spherical harmonics, and the Maxwell equations in spherical coordinates are reduced to a first-order differential set. When discontinuities of permittivity exist, we apply the fast numerical factorization to find the link between the electric field vector and the vector of electric induction, developed in a truncated basis. The diffraction problem is reduced to a boundary-value problem by using a shooting method combined with the S-matrix propagation algorithm, formulated for the field components instead of the amplitudes. © 2006 Optical Society of America

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1. INTRODUCTION

Light diffraction and scattering by arbitrary three-dimensional (3D) objects is a problem of interest in many domains of science and technology, such as astrophysics, atmospheric physics, remote detection, radar scattering, and photonics. In a previous paper[1] we developed a differential theory to analyze the problem in the case of isotropic materials. However, in both nature and technology, diffracting particles are more complicated. Two examples are that interstellar dust can include crystalline particles[2] and that high-frequency light modulation can be performed by using electro-optical effects in anisotropic crystals such as $LiNbO_3$.[3]

Although a great amount of work has been devoted to the problem during the past 15 years, it seems that a general theory that could handle arbitrary shaped objects made of arbitrary anisotropic lossless or lossy material needs to be formulated. Published studies address particular shapes or kinds of anisotropy. For example, Ref. 4 deals with dielectric ellipsoids, and Ref. 5 considers rotationally symmetric anisotropy with geometries conformal to spherical coordinates; Ref. 6 deals with perfectly conducting cylinders coated with an anisotropic layer, while Ref. 7 is restricted to spherical scatterers including an annular layer of anisotropic material.

The aim of this paper is to take advantage of the flexibility of the differential theory of light diffraction,[8] recently extended to 3D optically isotropic objects described in spherical coordinates,[1] in order to develop the theory for an arbitrary anisotropy. This has become possible thanks to the possibility of representing the field in an anisotropic material in the basis of vector spherical harmonics, described in Part I.[9]

2. PRESENTATION OF THE PROBLEM

The diffracting object is represented schematically in Fig. 1. It has an arbitrary shape limited by a surface S, described in spherical coordinates by the equation

$$f(r,\theta,\varphi)=0, \tag{1}$$

or by

$$r=g(\theta,\varphi), \qquad \theta\in[0,\pi]. \tag{2}$$

The tensor of relative permittivity in Cartesian coordinates has the form

$$\bar{\bar{\epsilon}}=\begin{bmatrix}\epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz}\\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz}\\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz}\end{bmatrix}, \tag{3}$$

and we assume that its elements do not depend on (x,y,z). Its elements in any coordinate system with unit vectors $(\hat{\mathbf{i}},\hat{\mathbf{j}},\hat{\mathbf{l}})$ can be obtained using the formula $\tilde{\bar{\epsilon}}=\mathfrak{R}\bar{\bar{\epsilon}}\mathfrak{R}^{\mathrm{T}}$, where T stands for transpose and $\mathfrak{R}$ is the corresponding transformation matrix:

$$\mathfrak{R}=\begin{bmatrix}\hat{\mathbf{i}}\cdot\hat{\mathbf{x}} & \hat{\mathbf{i}}\cdot\hat{\mathbf{y}} & \hat{\mathbf{i}}\cdot\hat{\mathbf{z}}\\ \hat{\mathbf{j}}\cdot\hat{\mathbf{x}} & \hat{\mathbf{j}}\cdot\hat{\mathbf{y}} & \hat{\mathbf{j}}\cdot\hat{\mathbf{z}}\\ \hat{\mathbf{l}}\cdot\hat{\mathbf{x}} & \hat{\mathbf{l}}\cdot\hat{\mathbf{y}} & \hat{\mathbf{l}}\cdot\hat{\mathbf{z}}\end{bmatrix}. \tag{4}$$

We divide the space into three regions by introducing two spheres S_1 and S_2 with radii R_1 and R_2, respectively. The first sphere S_1 is inscribed in the object, and the second sphere S_2 is circumscribed around the object (Fig. 1). Regions inside S_1 and outside S_2 are homogeneous. The intermediate region is inhomogeneous and will be called the modulated region. In this region, for any value of r ($R_1<r<R_2$) each tensorial component $\tilde{\bar{\epsilon}}_{ij}$, $i,\ j=(r,\theta,\varphi)$, of the permittivity is a periodic function of φ with period 2π and can furthermore be expressed on the basis of scalar spherical harmonics:

$$\tilde{\bar{\epsilon}}_{ij}(r,\theta,\varphi)=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\epsilon_{ij,nm}(r)Y_{nm}(\theta,\varphi), \tag{5}$$

where

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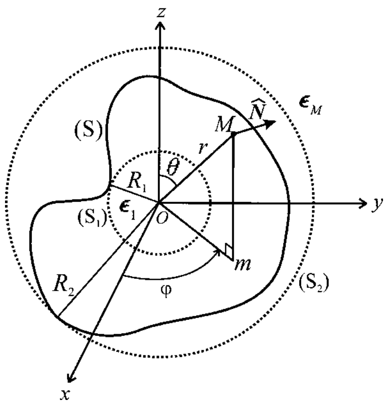

Fig. 1. Depiction of the diffracting object and notation.

$$\epsilon_{ij,nm}(r) = \int_0^{2\pi} \mathrm{d}\varphi \int_0^{\pi} \tilde{\bar{\epsilon}}_{ij}(r,\theta,\varphi) Y^*_{nm}(\theta,\varphi) \sin\theta \mathrm{d}\theta$$

$$\equiv \int_0^{4\pi} \tilde{\bar{\epsilon}}_{ij}(r,\theta,\varphi) Y^*_{nm}(\theta,\varphi) \mathrm{d}\Omega. \tag{6}$$

It is important to notice that the elements of $\bar{\epsilon}$ in Cartesian coordinates are piecewise-constant with respect to φ and θ.

3. FIELD EXPANSION ON VECTOR SPHERICAL HARMONICS

In spherical coordinates, several different basis sets are available to represent the electromagnetic field in any isotropic or anisotropic material. As already discussed in detail in Ref. 1, we shall use the basis of vector spherical harmonic functions $\mathbf{Y}_{nm}(\theta,\varphi)$, $\mathbf{X}_{nm}(\theta,\varphi)$, and $\mathbf{Z}_{nm}(\theta,\varphi)$, which allows the electric field to be expressed as

$$\mathbf{E}(r,\theta,\varphi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} [E_{Ynm}(r)\mathbf{Y}_{nm}(\theta,\varphi) + E_{Xnm}(r)\mathbf{X}_{nm}(\theta,\varphi) + E_{Znm}(r)\mathbf{Z}_{nm}(\theta,\varphi)]. \tag{7}$$

A numerical treatment requires truncation of the infinite sum in n, Eq. (7), to a value denoted by n_{Max}. We define a single summation index p to replace the two integers n and m through the relation $p=n(n+1)+m+1$ so that $p_{\mathrm{Max}}=(n_{\mathrm{Max}}+1)^2$. The inverse relations permit the determination of n and m from the values of p:

$$n = \mathrm{Int}\sqrt{p-1},$$

$$m = p - 1 - n(n+1). \tag{8}$$

In addition, we introduce a generic notation for the vector spherical harmonic functions, using a Greek letter superscript:

$$\mathbf{W}_p^{(\eta)} = \begin{cases} \mathbf{Y}_p, & \eta=1 \\ \mathbf{X}_p, & \eta=2 \\ \mathbf{Z}_p, & \eta=3 \end{cases}. \tag{9}$$

Using Eqs. (8) and (9), we can represent the electric field in a form more compact than Eq. (7):

$$\mathbf{E}(r,\theta,\varphi) = \sum_{p=1}^{p_{\mathrm{Max}}} \sum_{\eta=1}^{3} E_{\eta p}(r) \mathbf{W}_p^{(\eta)}(\theta,\varphi). \tag{10}$$

Similar expansions will be used for the magnetic field **H** and electric induction **D**. In addition, Eq. (5) takes the form

$$\tilde{\bar{\epsilon}}_{ij}(r,\theta,\varphi) = \sum_{p=1}^{p_{\mathrm{Max}}} \epsilon_{ij,p}(r) Y_p(\theta,\varphi). \tag{11}$$

One of the advantages of using vector spherical harmonics is that the Maxwell equations take a simple form[1]:

$$a_p \frac{E_{X,p}}{r} = i\omega\mu_0 H_{Y,p}, \tag{12}$$

$$a_p \frac{E_{Y,p}}{r} - \frac{E_{Z,p}}{r} - \frac{\mathrm{d}E_{Z,p}}{\mathrm{d}r} = i\omega\mu_0 H_{X,p}, \tag{13}$$

$$\frac{E_{X,p}}{r} + \frac{\mathrm{d}E_{X,p}}{\mathrm{d}r} = i\omega\mu_0 H_{Z,p}, \tag{14}$$

$$a_p \frac{H_{X,p}}{r} = -i\omega D_{Y,p}, \tag{15}$$

$$a_p \frac{H_{Y,p}}{r} - \frac{H_{Z,p}}{r} - \frac{\mathrm{d}H_{Z,p}}{\mathrm{d}r} = -i\omega D_{X,p}, \tag{16}$$

$$\frac{H_{X,p}}{r} + \frac{dH_{X,p}}{dr} = -i\omega D_{Z,p}, \tag{17}$$

where $a_p = \sqrt{n(n+1)}$ and n is given in Eq. (8).

As we have done in the isotropic case,[1] we introduce a matrix Q_ϵ that links the components of **E** and **D**:

$$\begin{pmatrix} [D_Y] \\ [D_X] \\ [D_Z] \end{pmatrix} = \epsilon_0 Q_\epsilon \begin{pmatrix} [E_Y] \\ [E_X] \\ [E_Z] \end{pmatrix}, \tag{18}$$

where each column denoted by square brackets contains the $\mathrm{p}_{\mathrm{Max}}-1$ elements of each vector component. For example,

$$[E_X] = \begin{pmatrix} E_{X,2} \\ \vdots \\ E_{X,p_{\mathrm{Max}}} \end{pmatrix}. \tag{19}$$

Then the set of Eqs. (12)–(17) can be written in the form of a first-order differential set,

$$\frac{\mathrm{d}}{\mathrm{d}r}[F] = M(r)[F], \tag{20}$$

where the column $[F]$ has four blocks:

$$[F]=\begin{pmatrix}[E_X]\\ [E_Z]\\ [\tilde{H}_X]\\ [\tilde{H}_Z]\end{pmatrix} \tag{21}$$

with $\tilde{\mathbf{H}}=\sqrt{\mu_0/\epsilon_0}\mathbf{H}$, and the matrix M is a square matrix having 16 blocks, each having dimension $p_{\mathrm{Max}}-1$ and equal to

$$M_{11}=-\frac{\mathbb{I}}{r},\qquad M_{12}=M_{13}=0,\qquad M_{14}=i\mu k_0\mathbb{I},$$

$$M_{21}=-\frac{a}{r}Q^{-1}_{\epsilon,YY}Q_{\epsilon,YX},\qquad M_{22}=-\frac{\mathbb{I}}{r}-\frac{a}{r}Q^{-1}_{\epsilon,YY}Q_{\epsilon,YZ},$$

$$M_{23}=i\left(\frac{aQ^{-1}_{\epsilon,YY}a}{k_0r^2}-\mu k_0\mathbb{I}\right),\qquad M_{24}=0,$$

$$M_{31}=ik_0(Q_{\epsilon,ZY}Q^{-1}_{\epsilon,YY}Q_{\epsilon,YX}-Q_{\epsilon,ZX}),$$

$$M_{32}=ik_0(Q_{\epsilon,ZY}Q^{-1}_{\epsilon,YY}Q_{\epsilon,YZ}-Q_{\epsilon,ZZ}),$$

$$M_{33}=\frac{1}{r}(Q_{\epsilon,ZY}Q^{-1}_{\epsilon,YY}a-\mathbb{I}),\qquad M_{34}=0,$$

$$M_{41}=i\left(k_0Q_{\epsilon,XX}-k_0Q_{\epsilon,XY}Q^{-1}_{\epsilon,YY}Q_{\epsilon,YX}-\frac{a^2}{\mu k_0r^2}\right),$$

$$M_{42}=ik_0(Q_{\epsilon,XZ}-Q_{\epsilon,XY}Q^{-1}_{\epsilon,YY}Q_{\epsilon,YZ}),$$

$$M_{43}=-Q_{\epsilon,XY}Q^{-1}_{\epsilon,YY}\frac{a}{r},\qquad M_{44}=-\frac{\mathbb{I}}{r}. \tag{22}$$

Here $\mathbb{I}$ is a unit matrix and a is a diagonal matrix with diagonal elements equal to a_p.

These equations are valid for both isotropic and anisotropic materials. The difference between isotropic and anisotropic cases is contained in the form of both the matrix Q_ϵ and the field expansion inside the homogeneous anisotropic region ($r<R_1$). In the following sections we deal consecutively with these two topics.

4. DETERMINATION OF THE Q_ϵ MATRIX USING THE FAST NUMERICAL FACTORIZATION

As in the isotropic case, the components of Q_ϵ are determined by obtaining the link between $\mathbf{E}$ and $\mathbf{D}$, projected onto the same truncated basis. The truncation requires applying special factorization rules, one for the tangential (subscript T) components, the other for the normal (subscript N) ones.[10,11] However, in contrast to the isotropic case,[1] the tensorial character of $\tilde{\tilde{\epsilon}}$ complicates the relation between $\mathbf{E}$ and $\mathbf{D}$, so D_N depends on both E_N and E_T, and likewise for D_T. This requires applying an approach quite different from the one used in Ref. 1 but similar to that followed in Cartesian coordinates to analyze anisotropic diffraction gratings.[8]

Let us consider the unit vector $\hat{\mathbf{N}}$, normal to the surface S of the object, defined on the surface:

$$\hat{\mathbf{N}}(\theta,\varphi)=\mathbf{grad}\,f/|\mathbf{grad}\,f|_{f=0}. \tag{23}$$

We need to extend the definition of $\hat{\mathbf{N}}$ to the entire modulated region; we state

$$\hat{\mathbf{N}}(r,\theta,\varphi)\equiv\hat{\mathbf{N}}(\theta,\varphi),\qquad \forall\, r\in[R_1,R_2]. \tag{24}$$

As previously stated, the circumflex denotes unit vectors. We then construct two unit tangential vectors $\hat{\mathbf{T}}_1$ and $\hat{\mathbf{T}}_2$, defined by

$$\hat{\mathbf{T}}_1=\frac{\hat{\mathbf{N}}\times\hat{\boldsymbol{\varphi}}}{|\hat{\mathbf{N}}\times\hat{\boldsymbol{\varphi}}|}\equiv\frac{N_\theta}{\sqrt{N_r^2+N_\theta^2}}\hat{\mathbf{r}}-\frac{N_r}{\sqrt{N_r^2+N_\theta^2}}\hat{\boldsymbol{\theta}}, \tag{25}$$

$$\hat{\mathbf{T}}_2=\hat{\mathbf{T}}_1\times\hat{\mathbf{N}}\equiv-\frac{N_rN_\theta}{\sqrt{N_r^2+N_\theta^2}}\hat{\mathbf{r}}-\frac{N_\theta N_\varphi}{\sqrt{N_r^2+N_\theta^2}}\hat{\boldsymbol{\theta}}+\frac{1-N_\varphi^2}{\sqrt{N_r^2+N_\theta^2}}\hat{\boldsymbol{\varphi}}, \tag{26}$$

if $\hat{\mathbf{N}}$ is not parallel to $\hat{\boldsymbol{\varphi}}$. If they are parallel, then

$$\hat{\mathbf{T}}_1=\hat{\mathbf{r}}, \tag{27}$$

$$\hat{\mathbf{T}}_2=\hat{\mathbf{T}}_1\times\hat{\mathbf{N}}\equiv-\hat{\boldsymbol{\theta}}. \tag{28}$$

The column

$$F_\epsilon\equiv\begin{pmatrix}F_{\epsilon,1}\\ F_{\epsilon,2}\\ F_{\epsilon,3}\end{pmatrix}=\begin{pmatrix}E_{T_1}\\ \frac{1}{\epsilon_0}D_N\\ E_{T_2}\end{pmatrix}\overset{\text{def}}{=}\begin{pmatrix}\mathbf{E}\cdot\hat{\mathbf{T}}_1\\ \frac{1}{\epsilon_0}\mathbf{D}\cdot\hat{\mathbf{N}}\\ \mathbf{E}\cdot\hat{\mathbf{T}}_2\end{pmatrix} \tag{29}$$

is continuous across the object surface S, where the permittivity is discontinuous. Let us underline the fact that F_ϵ is not a vector: each of its elements represents a scalar. The elements can be expressed through the components of $\mathbf{E}$ using a square matrix A_ϵ,

$$F_\epsilon=A_\epsilon\mathbf{E}, \tag{30}$$

which can be determined by taking into account that

$$\begin{aligned}\frac{1}{\epsilon_0}D_N=\frac{1}{\epsilon_0}\mathbf{D}\cdot\hat{\mathbf{N}}=\hat{\mathbf{N}}\cdot(\tilde{\tilde{\epsilon}}\mathbf{E})\\ =N_r(\epsilon_{rr}E_r+\epsilon_{r\theta}E_\theta+\epsilon_{r\varphi}E_\varphi)+N_\theta(\epsilon_{\theta r}E_r+\epsilon_{\theta\theta}E_\theta+\epsilon_{\theta\varphi}E_\varphi)\\ +N_\varphi(\epsilon_{\varphi r}E_r+\epsilon_{\varphi\theta}E_\theta+\epsilon_{\varphi\varphi}E_\varphi).\end{aligned} \tag{31}$$

As a result, one obtains

$$A_\epsilon = \begin{bmatrix} T_{1,r} & T_{1,\theta} & 0 \\ (N_r\epsilon_{rr}+N_\theta\epsilon_{\theta r}+N_\varphi\epsilon_{\varphi r}) & (N_r\epsilon_{r\theta}+N_\theta\epsilon_{\theta\theta}+N_\varphi\epsilon_{\varphi\theta}) & (N_r\epsilon_{r\varphi}+N_\theta\epsilon_{\theta\varphi}+N_\varphi\epsilon_{\varphi\varphi}) \\ T_{2,r} & T_{2,\theta} & T_{2,\varphi} \end{bmatrix}, \tag{32}$$

which can be written in a more compact form by introducing a dot product $(\mathbf{N}\cdot\tilde{\tilde{\epsilon}})$ denoting a contraction over the first tensorial subscript of $\tilde{\tilde{\epsilon}}$:

$$A_\epsilon = \begin{bmatrix} T_{1,r} & T_{1,\theta} & 0 \\ (\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}})_r & (\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}})_\theta & (\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}})_\varphi \\ T_{2,r} & T_{2,\theta} & T_{2,\varphi} \end{bmatrix}. \tag{33}$$

After tedious but elementary calculations, it can be shown that its inverse matrix has the form

$$C \overset{\text{def}}{=} A_\epsilon^{-1} = \frac{1}{\xi_0}\begin{bmatrix} [(\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}})\times\hat{\mathbf{T}}_2]_r & N_r & [\hat{\mathbf{T}}_1\times(\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}})]_r \\ [(\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}})\times\hat{\mathbf{T}}_2]_\theta & N_\theta & [\hat{\mathbf{T}}_1\times(\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}})]_\theta \\ [(\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}})\times\hat{\mathbf{T}}_2]_\varphi & N_\varphi & [\hat{\mathbf{T}}_1\times(\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}})]_\varphi \end{bmatrix}, \tag{34}$$

where $\xi_0=\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}}\cdot\hat{\mathbf{N}}$ is the determinant of A_ϵ. Using the mutual orthogonality of $\hat{\mathbf{N}}$, $\hat{\mathbf{T}}_1$, and $\hat{\mathbf{T}}_2$, and the fact that the mixed product of three vectors is null when two of the vectors are identical, one can easily verify that $A_\epsilon A_\epsilon^{-1}=\mathbb{I}$. In addition, due to the symmetry of $\tilde{\tilde{\epsilon}}$, the determinant ξ_0 of A_ϵ is a positive quadratic form and thus is never null. By using Eqs. (25) and (26), we can write matrix C in another form:

$$C = \begin{pmatrix} T_{1,r}-\frac{\xi_1}{\xi_0}N_r & \frac{1}{\xi_0}N_r & T_{2,r}-\frac{\xi_2}{\xi_0}N_r \\ T_{1,\theta}-\frac{\xi_1}{\xi_0}N_\theta & \frac{1}{\xi_0}N_\theta & T_{2,\theta}-\frac{\xi_2}{\xi_0}N_\theta \\ T_{1,\varphi}-\frac{\xi_1}{\xi_0}N_\varphi & \frac{1}{\xi_0}N_\varphi & T_{2,\varphi}-\frac{\xi_2}{\xi_0}N_\varphi \end{pmatrix} = (\mathbf{C}_1,\mathbf{C}_2,\mathbf{C}_3), \tag{35}$$

where $\xi_1=\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}}\cdot\hat{\mathbf{T}}_1$ and $\xi_2=\hat{\mathbf{N}}\cdot\tilde{\tilde{\epsilon}}\cdot\hat{\mathbf{T}}_2$ are scalars. As can be observed, the three vectors $(\mathbf{C}_1,\mathbf{C}_2,\mathbf{C}_3)$ representing the three columns of C consist of a linear combination of the normal $(\hat{\mathbf{N}})$ and tangential $(\hat{\mathbf{T}}_1,\hat{\mathbf{T}}_2)$ vectors, whatever the coordinated system used. In the anisotropic case, $\mathbf{C}_1,\mathbf{C}_2,\mathbf{C}_3$ are not mutually orthogonal, while they are orthogonal in isotropic media, with $\xi_1=\xi_2=0$.

Inversing Eq. (30) gives

$$\mathbf{E} = CF_\epsilon, \tag{36}$$

and thus

$$\mathbf{D} = \epsilon_0\tilde{\tilde{\epsilon}}\mathbf{E} = \epsilon_0\tilde{\tilde{\epsilon}}CF_\epsilon. \tag{37}$$

Let us recall that the aim is to express the components of the column $[\mathbf{D}]$, made of three block columns $[D_Y]$, $[D_X]$, and $[D_Z]$ in terms of the column $[\mathbf{E}]$, made of $[E_Y]$, $[E_X]$, and $[E_Z]$. To achieve this goal we have to pass through the column F_ϵ, which is composed of those components of the electric and induction field that are continuous across the diffractive object surface S.

A. Direct Factorization Rule

All the components of the column F_ϵ are continuous across S, while some of the components of $\mathbf{D}$ are discontinuous and some are continuous. We can then apply the direct factorization rule to Eq. (37) by projecting $\mathbf{D}$ onto the basis of vector spherical harmonics [see Eq. (10)] and projecting the scalar elements of F_ϵ onto the basis of scalar spherical harmonics. Then Eq. (37) takes the form

$$\sum_{p,\eta} D_{\eta,p}(r)\mathbf{W}_p^{(\eta)}(\theta,\varphi) = \epsilon_0\tilde{\tilde{\epsilon}}(r,\theta,\varphi)C(r,\theta,\varphi) \times\sum_p \begin{pmatrix} F_{\epsilon,1,p}(r) \\ F_{\epsilon,2,p}(r) \\ F_{\epsilon,3,p}(r)\end{pmatrix} Y_p(\theta,\varphi), \tag{38}$$

where $\tilde{\tilde{\epsilon}}$ is a square matrix of size 3×3 with elements $\tilde{\tilde{\epsilon}}_{ij}$. Matrix C is also a square matrix of size 3×3 with elements C_{iJ} representing the components of the three vectors $\mathbf{C}_J$, $J=1,2,3$, Eq. (35), expressed in the same coordinate system as $\tilde{\tilde{\epsilon}}$. Their product $(\tilde{\tilde{\epsilon}}C)$ has the same form with elements

$$(\tilde{\tilde{\epsilon}}C)_{iJ} = \sum_{j=r,\theta,\varphi}\tilde{\tilde{\epsilon}}_{ij}C_{jJ}. \tag{39}$$

If the basis used to represent the tensor elements differs from the set of unit vectors of the spherical coordinate system, then i and j stay for the basic vectors, for example, in the Cartesian coordinate system $i,j=x,y,z$. In contrast, the last subscript $J=1,2,3$ corresponds to the tangential or normal field components, which form the column F_ϵ, Eq. (29). Since they are scalars, they do not depend on the coordinate system. Using this convention, we can write Eq. (38) in a more compact form:

$$\sum_{p,\eta} D_{\eta,p}\mathbf{W}_p^{(\eta)} = \epsilon_0\sum_{J,p}(\tilde{\tilde{\epsilon}}\mathbf{C}_J)F_{\epsilon,J,p}Y_p. \tag{40}$$

The next step is to use the orthogonality of the vector spherical harmonics with respect to their argument:

$$\int_0^{4\pi} \mathrm{d}\Omega\,\mathbf{W}_p^{(\eta)}(\theta,\varphi)\cdot\mathbf{W}_q^{*(\tau)}(\theta,\varphi) = \delta_{pq}\delta_{\eta\tau}. \tag{41}$$

Multiplying Eq. (40) by $\mathbf{W}_q^{*(\tau)}$ and integrating over the entire solid angle, one obtains

$$D_{\tau,q}(r) = \epsilon_0\sum_{J,p}\langle\mathbf{W}_q^{(\tau)}|(\tilde{\tilde{\epsilon}}\mathbf{C}_J)Y_p\rangle F_{\epsilon,J,p}(r) = \epsilon_0\sum_{J,p}\{\tilde{\tilde{\epsilon}}C\}_{\tau,J,qp}F_{\epsilon,J,p}(r), \tag{42}$$

where

$$\{\tilde{\bar{\epsilon}}C\}_{\tau J,qp} = \langle \mathbf{W}_q^{(\tau)} | (\tilde{\bar{\epsilon}}\mathbf{C}_J) Y_p \rangle = \int_0^{4\pi} \mathrm{d}\Omega \mathbf{W}_q^{*(\tau)}(\theta,\varphi) \cdot (\tilde{\bar{\epsilon}}\mathbf{C}_J) Y_p(\theta,\varphi), \tag{43}$$

and the dot product here is reduced to the ordinary scalar product. This equation is written in a form independent of the coordinate system used, owing to the scalar product, which has to be explicitly calculated in each specific coordinate system.

Owing to Eq. (A22) of Part I,[9] the φ dependence of the integrand in Eq. (43) is exponential, $\exp\{i[m(p)-m(q)]\varphi\}$, so that the integration with respect to φ represents a Fourier transform of $(\tilde{\bar{\epsilon}}C)_{iJ}$. In addition, the facts that $\mathbf{Y}_p$ are parallel to $\hat{\mathbf{r}}$ and that $\mathbf{X}_p$ and $\mathbf{Z}_p$ are perpendicular to $\hat{\mathbf{r}}$ simplify the form of $\{\tilde{\bar{\epsilon}}C\}$ when it is represented in spherical coordinates:

$$\{\tilde{\bar{\epsilon}}C\}_{YJ,pq} = \langle Y_p | (\tilde{\bar{\epsilon}}C)_{rJ} Y_q \rangle,$$

$$\{\tilde{\bar{\epsilon}}C\}_{XJ,pq} = \sum_{i=\theta,\varphi} \langle X_{p,i} | (\tilde{\bar{\epsilon}}C)_{iJ} Y_q \rangle,$$

$$\{\tilde{\bar{\epsilon}}C\}_{ZJ,pq} = \sum_{i=\theta,\varphi} \langle Z_{p,i} | (\tilde{\bar{\epsilon}}C)_{iJ} Y_q \rangle. \tag{44}$$

The integration with respect to θ is significantly simplified when $(\tilde{\bar{\epsilon}}C)_{iJ}$ can be represented in the form of series of scalar spherical harmonics. This is the case of isotropic media, as discussed in detail in Ref. 1. Another situation is discussed in Section 5 and concerns the case of absence of discontinuity of the permittivity tensor inside the modulated region, for example, gradient-index anisotropy. Two more cases are described in detail in Appendix A.

Equations (42) and (43) establish the direct factorization rule.

B. Inverse Rule

As already discussed, all the components of the column F_ϵ are continuous across S. However, some of the components of $\mathbf{E}$ may be discontinuous there. Thus, it is necessary to apply the inverse rule to Eq. (30). This is simply done by applying the direct factorization rule as stated in Eqs. (42) and (43) to Eq. (36), taking into account that C is discontinuous, while F_ϵ is continuous. Thus, Eq. (36) can be written in components

$$E_{\tau,q}(r) = \sum_{J,p} C_{\tau J,qp} F_{\epsilon,J,p}(r), \tag{45}$$

where the elements

$$C_{\tau J,qp} = \langle \mathbf{W}_q^{(\tau)} | (\mathbf{C}_J) Y_p \rangle = \int_0^{4\pi} \mathrm{d}\Omega \mathbf{W}_q^{*(\tau)}(\theta,\varphi) \cdot (\mathbf{C}_J) Y_p(\theta,\varphi) \tag{46}$$

form a square matrix $\{C\}$ with nine blocks $C_{\tau J}$. Its numerical inversion makes it possible to express the components of F_ϵ as function of $[E_Y]$, $[E_X]$, and $[E_Z]$:

$$[F_\epsilon] = \{C\}^{-1}[\mathbf{E}]. \tag{47}$$

The remarks following Eq. (43) and concerning $\{\tilde{\bar{\epsilon}}C\}$ also hold for the matrix $\{C\}$ derived in Eq. (46). Equation (44) again apply by replacement of $\tilde{\bar{\epsilon}}C$ with C.

Equations (46) and (47) state the inverse factorization rule extended to anisotropic materials.

C. Fast Numerical Factorization Equation

It is now straightforward to determine the relation between $[D_Y]$, $[D_X]$, and $[D_Z]$ on one side and $[E_Y]$, $[E_X]$, and $[E_Z]$ on the other side. Combining Eqs. (42) and (47), we obtain

$$[\mathbf{D}] = \epsilon_0 \{\tilde{\bar{\epsilon}}C\}\{C\}^{-1}[\mathbf{E}]. \tag{48}$$

Thus the matrix Q_ϵ takes the form

$$Q_\epsilon = \{\tilde{\bar{\epsilon}}C\}\{C\}^{-1}. \tag{49}$$

It is worth noticing that Eq. (49), together with Eqs. (43) and (46), generalize Eq. (114) of Ref. 1 to anisotropic media. When applied to isotropic medium, they lead to Eqs. (76), (82), (83), (88), and (89) of Ref. 1 with ϵ being a scalar. This can be easily observed by taking into account that for isotropic media the triad $(\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_3)$ simplifies into $(\hat{\mathbf{T}}_1, 1/\epsilon\hat{\mathbf{N}}, \hat{\mathbf{T}}_2)$. When projected onto the basis $(\mathbf{Y}_p, \mathbf{X}_p, \mathbf{Z}_p)$ as stated by Eq. (46), matrix $\{C\}$ becomes

$$\{C\} = \left(\{\hat{\mathbf{T}}_1\}, \left\{\frac{1}{\epsilon}\right\}\{\hat{\mathbf{N}}\}, \{\hat{\mathbf{T}}_2\} \right) \tag{50}$$

and can be inverted analytically:

$$\{C\}^{-1} = \begin{pmatrix} \{\hat{\mathbf{T}}_1\}^{\mathrm{T}} \\ \left\{\dfrac{1}{\epsilon}\right\}^{-1} \{\hat{\mathbf{N}}\}^{\mathrm{T}} \\ \{\hat{\mathbf{T}}_2\}^{\mathrm{T}} \end{pmatrix}. \tag{51}$$

On the other hand, Eq. (43) simplifies to the form

$$\{\tilde{\bar{\epsilon}}C\} = (\{\epsilon\}\{\hat{\mathbf{T}}_1\}, \{\hat{\mathbf{N}}\}, \{\epsilon\}\{\hat{\mathbf{T}}_2\}) \tag{52}$$

so that matrix Q_ϵ takes the form written in Eq. (116) of Ref. 1 when we take into account the relation $\hat{\mathbf{T}}_1\hat{\mathbf{T}}_1 + \hat{\mathbf{T}}_2\hat{\mathbf{T}}_2 + \hat{\mathbf{N}}\hat{\mathbf{N}} = \mathbb{I}$.

In contrast to the isotropic case, in the anisotropic case the elements of matrix Q_ϵ are determined numerically and cannot be explicitly written, as they were in Ref. 1. We also note that the matrix product in Eq. (49) cannot cancel matrix C and its inverse, because the matrix elements of $\{\tilde{\bar{\epsilon}}C\}$ are not represented as elements of the product of two matrices, $\{\tilde{\bar{\epsilon}}C\} \neq \{\tilde{\bar{\epsilon}}\}\{C\}$, owing to the integration in Eq. (43). $\{\tilde{\bar{\epsilon}}C\}$ would be the product of two matrices only if one worked in a nontruncated basis, which is impossible numerically.

5. INHOMOGENEOUS SPHERICAL BODY

If the permittivity tensor does not present any discontinuity inside the modulated region but presents only smooth inhomogeneity, it is not necessary to use the fast numerical factorization (FNF) rules. Such an example contains a spherical optically inhomogeneous anisotropic body with the elements of $\bar{\bar{\epsilon}}$ being continuously varying functions of (x,y,z), for example, a graded-permittivity anisotropic sphere. In that case both $\mathbf{D}$ and $\mathbf{E}$ are continuous and the first relation in Eq. (37) can be directly used: $\mathbf{D}=\epsilon_0\tilde{\tilde{\epsilon}}\mathbf{E}$. Both $\mathbf{D}$ and $\mathbf{E}$ are expressed in terms of vector spherical harmonics, Eq. (10), and the left-hand side of Eq. (38), so that

$$\mathbf{D}=\epsilon_0\tilde{\tilde{\epsilon}}\mathbf{E} \Rightarrow \sum_{\eta,p} D_{\eta p}(r)\mathbf{W}_p^{(\eta)}(\theta,\varphi) = \epsilon_0\tilde{\tilde{\epsilon}}(r,\theta,\varphi)\sum_{\tau,q} E_{\tau q}(r)\mathbf{W}_q^{(\tau)}(\theta,\varphi). \tag{53}$$

Multiplying by $\mathbf{W}_p^{*(\tau)}$ and integrating over the entire solid angle leads to a simplified form of matrix Q_ϵ in Eq. (18):

$$Q_\epsilon = \{\tilde{\tilde{\epsilon}}\}, \tag{54}$$

where the elements of the matrix $\{\tilde{\tilde{\epsilon}}\}$ are given by

$$\{\tilde{\tilde{\epsilon}}\}_{\tau\eta,pq}(r) = \langle \mathbf{W}_p^{(\tau)} | (\tilde{\tilde{\epsilon}}) \mathbf{W}_q^{(\eta)} \rangle = \int_0^{4\pi} \mathrm{d}\Omega \mathbf{W}_p^{*(\tau)}(\theta,\varphi)\cdot\tilde{\tilde{\epsilon}}(r,\theta,\varphi)\mathbf{W}_q^{(\eta)}(\theta,\varphi). \tag{55}$$

Each element $\{\tilde{\tilde{\epsilon}}\}_{\tau\eta,pq}$ is a scalar independent of the coordinate system and contains a product of the tensor $\tilde{\tilde{\epsilon}}$ with the vector $\mathbf{W}_p^{*(\tau)}$ on the left and $\mathbf{W}_q^{(\eta)}$ on the right. In a specific coordinate system it is represented as a summation over the tensorial indices i and j of $\tilde{\tilde{\epsilon}}$:

$$\mathbf{W}_p^{*(\tau)}\cdot\tilde{\tilde{\epsilon}}\mathbf{W}_q^{(\eta)} = \sum_{i,j} W_{p,i}^{*(\tau)}\tilde{\tilde{\epsilon}}_{ij}W_{q,j}^{(\eta)}, \tag{56}$$

where $W_{q,j}^{(\eta)}=\mathbf{W}_q^{(\eta)}\cdot\hat{\mathbf{j}}$ is the projection of $\mathbf{W}_q^{(\eta)}$ onto the coordinate unit vector $\hat{\mathbf{j}}$.

Unfortunately, Eq. (55) requires a numerical integration of the products of spherical harmonics. However, in some cases, it is possible to avoid this by using Eq. (5). If the inhomogeneity of $\tilde{\tilde{\epsilon}}$ is such that its elements can be represented with only a few terms in the expansion on scalar spherical harmonics, Eq. (5), these terms can be used to rapidly calculate the integrals that appear in Eq. (55). In Cartesian or cylindrical coordinates, the projection $\mathbf{W}_p^{(\eta)}(\theta,\varphi)\cdot\hat{\mathbf{j}}$ of $\mathbf{W}_p^{(\eta)}(\theta,\varphi)$ on the axis $\hat{\mathbf{j}}$ takes a simple form (see Appendix B) proportional to the scalar spherical harmonics $Y_{nm}(\theta,\varphi)$:

$$\mathbf{W}_{nm}^{(\eta)}(\theta,\varphi)\cdot\hat{\mathbf{j}} = \sum_{\nu=-1}^{+1} b_{nm,\mu\nu j}^{(\eta)} Y_{n+\nu,m+\mu}(\theta,\varphi). \tag{57}$$

with coefficients $b_{nm,\mu\nu j}^{(\eta)}$ proportional to the projections of the vector spherical harmonics on the basis $(\hat{\mathbf{j}})$, as given in Appendix B. With the use of Eq. (57), the integrand in Eq. (55) becomes a triple product of scalar spherical harmonics. As discussed in Appendix D of Ref. 1, the integrals of triple products represent the normalized Gaunt coefficients $\bar{a}$[12]:

$$\bar{a}(\{\nu',\mu'\},\{\nu,\mu\},\{n,m\}) = \int_0^{2\pi}\mathrm{d}\varphi\int_0^{\pi}\sin\theta\mathrm{d}\theta Y_{\nu',\mu'}(\theta,\varphi) \times Y_{\nu,\mu}(\theta,\varphi)Y_{nm}(\theta,\varphi), \tag{58}$$

which can be calculated rapidly through recursion relations.[13] Then each element $\{\tilde{\tilde{\epsilon}}\}_{\tau\eta,qp}$ is given as a linear combination of the products of Gaunt coefficients $\bar{a}$ and the coefficients $b_{nm,\mu\nu j}^{(\eta)}$ seen in Eq. (57), which depend on the coordinate system used to represent the permittivity tensor.

6. RESOLUTION OF THE BOUNDARY-VALUE PROBLEM

The integration of Eq. (20) can be done numerically between R_1 and R_2. However, this requires starting values of the components of the unknown column $[F(r)]$. In addition, as long as this column contains electromagnetic field components that are continuous across S_1 and S_2, it is necessary to match the results of the integration with the corresponding field components outside S_2 and inside S_1.

Using the expansion of a plane wave on the vector spherical harmonic basis in an anisotropic material, Eqs. (50) and (55) of Part I,[9] the column $[F]$ at the innermost sphere S_1 takes the form

$$[F(R_j)] = \Psi_{\text{aniso}}(R_1)[\tilde{A}] \tag{59}$$

with a column $[\tilde{A}]$ containing the unknown amplitudes inside S_1,

$$[\tilde{A}] = \begin{pmatrix}[\tilde{A}_1]\\ [\tilde{A}_2]\end{pmatrix} = \begin{pmatrix}\vdots\\ \tilde{A}_{1,\nu}\\ \vdots\\ \tilde{A}_{2,\nu}\\ \vdots\end{pmatrix}, \tag{60}$$

and the matrix Ψ_{aniso} having a block form,

$$\Psi_{\text{aniso}} = (\Psi_{1,\text{aniso}}\ \Psi_{2,\text{aniso}}), \tag{61}$$

in which each block consists of four subblocks with rank $p_{\text{Max}}-1$:

$$\Psi_{j,\text{aniso}}(r) = \begin{pmatrix} \left[\dfrac{1}{k_{j,\nu}r}a_{h,p,j,\nu}\psi_n(k_{j,\nu}r)\right] \\ \left[\dfrac{1}{k_{j,\nu}r}[a_{e,p,j,\nu}\psi_n'(k_{j,\nu}r)+a_p a_{o,p,j,\nu}j_n(k_{j,\nu}r)]\right] \\ \left[\dfrac{1}{ik_0r}a_{e,p,j,\nu}\psi_n(k_{j,\nu}r)\right] \\ \left[\dfrac{1}{ik_0r}a_{h,p,j,\nu}\psi_n'(k_{j,\nu}r)\right] \end{pmatrix}. \tag{62}$$

As usual, j_n and h_n^+ are the spherical Bessel functions and ψ_n and ξ_n are the Ricatti–Bessel functions:

$$\psi_n(z) = zj_n(z), \qquad \xi_n(z) = zh_n^+(z). \tag{63}$$

The matrix Ψ_{aniso} can be used as a starting matrix at $r=R_1$ in the process of numerical integration of Eq. (20). At the end of the integration, the integrated matrix $[F_{\text{integ}}]$ represents the transmission matrix of the system:

$$T(R_2,R_1) = [F_{\text{integ}}], \tag{64}$$

which links the field on S_2 to the unknown amplitudes $[\tilde{A}]$ inside S_1:

$$[F(R_2)] = T(R_2,R_1)[\tilde{A}]. \tag{65}$$

On the other hand, the field components $[F(R_2)]$ are continuous across S_2 and can be expressed through the incident and diffracted field amplitudes in the outermost homogeneous and isotropic medium, discussed in detail in Part I[9]:

$$E_{X,p}(r=R_2) = [A^{(i)}_{h,p} j_n(n_{\text{out}}k_0R_2) + B_{h,p}h^{+}_n(n_{\text{out}}k_0R_2)],$$

$$E_{Z,p}(r=R_2) = \frac{1}{n_{\text{out}}k_0R_2}[A^{(i)}_{e,p}\psi'_n(n_{\text{out}}k_0R_2) + B_{e,p}\xi'_n(n_{\text{out}}k_0R_2)], \tag{66}$$

$$\tilde{H}_{X,p}(r=R_2) = \frac{1}{ik_0R_2}[A^{(i)}_{e,p}\psi_n(n_{\text{out}}k_0R_2) + B_{e,p}\xi_n(n_{\text{out}}k_0R_2)],$$

$$\tilde{H}_{Z,p}(r=R_2) = \frac{1}{ik_0R_2}[A^{(i)}_{h,p}\psi'_n(n_{\text{out}}k_0R_2) + B_{h,p}\xi'_n(n_{\text{out}}k_0R_2)], \tag{67}$$

where $A^{(i)}_{h,p}$ and $A^{(i)}_{e,p}$ are the incident (known) field amplitudes and $B_{h,p}$ and $B_{e,p}$ are the diffracted (unknown) field amplitudes in the outermost region. With these expressions, the column $[F]$ in the outermost region takes the form

$$[F(R_2)] = \Psi_{\text{iso}}(n_{\text{out}}k_0R_2)\begin{pmatrix} \vdots \\ A^{(i)}_{e,p}\psi'_n(n_{\text{out}}k_0R_2)/n_{\text{out}}k_0R_2 \\ \vdots \\ A^{(i)}_{h,p}\psi_n(n_{\text{out}}k_0R_2)/n_{\text{out}}k_0R_2 \\ \vdots \\ B_{e,p}\xi'_n(n_{\text{out}}k_0R_2)/n_{\text{out}}k_0R_2 \\ \vdots \\ B_{h,p}\xi_n(n_{\text{out}}k_0R_2)/n_{\text{out}}k_0R_2 \\ \vdots \end{pmatrix}, \tag{68}$$

where

$$\Psi_{\text{iso}} = \begin{pmatrix} 0 & \mathbb{I} & 0 & \mathbb{I} \\ \mathbb{I} & 0 & \mathbb{I} & 0 \\ \dfrac{-in_{\text{out}}}{p(n_{\text{out}}k_0R_2)} & 0 & \dfrac{-in_{\text{out}}}{q(n_{\text{out}}k_0R_2)} & 0 \\ 0 & -in_{\text{out}}p(n_{\text{out}}k_0R_2) & 0 & -in_{\text{out}}q(n_{\text{out}}k_0R_2) \end{pmatrix} \tag{69}$$

and

$$p_{p,q}(z) = \delta_{p,q}\frac{\psi'_n(z)}{\psi_n(z)}, \quad q_{p,q}(z) = \delta_{p,q}\frac{\xi'_n(z)}{\xi_n(z)}. \tag{70}$$

Equations (65) and (68) represent the same column $[F(R_2)]$, and thus they form a set of $4(N_\nu - 1) = 4(p_{\text{Max}} - 1)$ linear algebraic equations for the unknown field amplitudes $[\tilde{A}_1]$, $[\tilde{A}_2]$, $[B_e]$, and $[B_h]$. The set can be solved numerically when the incident field amplitudes $A^{(i)}_{h,p}$ and $A^{(i)}_{e,p}$ are known.

During the integration process, one can expect the appearance of numerical problems, and it is necessary to divide the integration region into subregions so that inside each subregion the integration remains possible. Instead of obtaining the transmission matrix T, it is possible to directly determine the scattering matrix S, which links the diffracted to the incident amplitudes. This procedure is well known in the diffraction theories in Cartesian and cylindrical coordinates and is explained in detail in Ref. 1. The equations in the case of anisotropic media do not differ from the formulas developed in the isotropic case; the interested reader can find them in Ref. 1. The first difference is the start of the integration, which uses as a shooting matrix the matrix Ψ_{aniso}, defined by Eqs. (61) and (62), which requires $2(p_{\text{Max}} - 1)$ independent starting vectors. The second difference is the form of the Q_ϵ matrix, discussed in detail in Section 4.

7. CONCLUSION

This work extends the differential theory of diffraction to an arbitrary-shaped 3D body made of arbitrary anisotropic lossless or lossy material. The theory extends the fast numerical factorization (FNF) of products of continuous and discontinuous vector functions to anisotropic media described in vector spherical harmonic basis. It is able to analyze uniaxial, biaxial or chiral materials. Moreover, the theory can be applied to ferromagnetic materials, described by a tensorial magnetic permeability.

Some particular cases permit significant simplifications that avoid numerical integration of the products of spherical harmonics. Certain examples are the optically uniaxial finite-length cylinder and arbitrary-anisotropic parallelepiped, described in detail in Appendix A. In addition, the theory can be directly applied to graded-permittivity materials by using only the direct rule of factorization.

APPENDIX A: TWO PARTICULAR GEOMETRIES

Let us consider two particular cases, which permit significant simplifications in calculating the matrix elements of $\{C\}$ and $\{\tilde{\tilde{\epsilon}}C\}$.

1. Finite-Length Circular Cylinder with Uniaxial Anisotropy

Let us consider a finite-length circular cylinder with height H and radius R with axis coinciding with the z axis and the origin of the coordinate system located in the center of the body, Fig. 2. The numerical integration of Eq. (20) has to be performed from $r=R_1=\min(R,H/2)$ to $R_2=[R^2+(H/2)^2]^{1/2}$, and it is necessary to extend the definition of the normal vectors defined at the surface to the entire region of integration. This can be done, for example, as represented in Fig. 2. If the cylinder material has uniaxial anisotropy with the optic axis coinciding with the axis of symmetry, the permittivity tensor has the same form in a Cartesian and in a cylindrical coordinate system:

$$\tilde{\tilde{\epsilon}} = \begin{pmatrix} \epsilon_x & 0 & 0 \\ 0 & \epsilon_x & 0 \\ 0 & 0 & \epsilon_z \end{pmatrix}. \tag{A1}$$

Since the normal and the tangential vectors can be simply expressed in cylindrical coordinates, we represent the matrices C and $(\tilde{\tilde{\epsilon}}C)$ in cylindrical basis $(\hat{\boldsymbol{\rho}},\hat{\boldsymbol{\varphi}},\hat{\mathbf{z}})$. We distinguish two cases:

(1) $\theta \in (\theta_c, \pi-\theta_c)$. In this interval, we can write

$$\hat{\mathbf{N}} = \hat{\boldsymbol{\rho}}, \qquad \hat{\mathbf{T}}_1 = \hat{\mathbf{z}}, \qquad \hat{\mathbf{T}}_2 = \hat{\boldsymbol{\varphi}}, \tag{A2}$$

so that $\xi_0=\epsilon_x$ in Eq. (35) and matrices C and $(\tilde{\tilde{\epsilon}}C)$ become

$$C = \begin{pmatrix} 0 & 1/\epsilon_x & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \qquad (\tilde{\tilde{\epsilon}}C) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \epsilon_x \\ \epsilon_z & 0 & 0 \end{pmatrix}. \tag{A3}$$

(2) $\theta \notin (\theta_c, \pi-\theta_c)$. Equations (A2) and (A3) become, respectively,

$$\hat{\mathbf{N}} = \hat{\mathbf{z}}, \qquad \hat{\mathbf{T}}_1 = -\hat{\boldsymbol{\rho}}, \qquad \hat{\mathbf{T}}_2 = \hat{\boldsymbol{\varphi}}, \tag{A4}$$

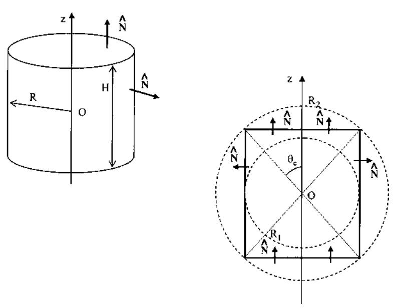

Fig. 2. Finite-length cylinder and notation.

$$C = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1/\epsilon_z & 0 \end{pmatrix}, \qquad (\tilde{\tilde{\epsilon}}C) = \begin{pmatrix} -\epsilon_x & 0 & 0 \\ 0 & 0 & \epsilon_x \\ 0 & 1 & 0 \end{pmatrix}. \tag{A5}$$

As can be observed, both C and $(\tilde{\tilde{\epsilon}}C)$ are piecewise-constant functions of θ and do not depend on φ. Moreover, the components of $\hat{\mathbf{T}}_2$ are constant in θ as well. It is straightforward to represent the elements of (C) and $(\tilde{\tilde{\epsilon}}C)$ in the basis of scalar spherical functions, Eq. (5):

$$(C)_{ij}(\theta) = \sum_{n=0}^{\infty} (C)_{ij,n} Y_{n0}(\theta,\varphi) \equiv \sum_{n=0}^{\infty} (C)_{ij,n} \bar{P}_n^0(\cos\theta),$$

$$(\tilde{\tilde{\epsilon}}C)_{ij}(\theta) = \sum_{n=0}^{\infty} (\tilde{\tilde{\epsilon}}C)_{ij,n} Y_{n0}(\theta,\varphi) \equiv \sum_{n=0}^{\infty} (\tilde{\tilde{\epsilon}}C)_{ij,n} \bar{P}_n^0(\cos\theta). \tag{A6}$$

Their components $(C)_{ij,n}$ and $(\tilde{\tilde{\epsilon}}C)_{ij,n}$ do not depend on r and can be evaluated analytically, taking into account the relations (see Appendix A of Ref. 1):

$$\bar{P}_n^0 = \sqrt{\frac{2n+1}{4\pi}} P_n^0,$$

$$\int_{\theta_1}^{\theta_2} P_n^0(\cos\theta)\sin\theta \mathrm{d}\theta = \frac{1}{n}[\cos\theta P_n^0(\cos\theta) - P_{n+1}^0(\cos\theta)]\Big|_{\theta_1}^{\theta_2}. \tag{A7}$$

To obtain the components of $\{C\}$ and $(\tilde{\tilde{\epsilon}}C)$, Eqs. (46) and (43), it is necessary to project the vector spherical harmonics onto the same basis of coordinate vectors $(\hat{\boldsymbol{\rho}},\hat{\boldsymbol{\varphi}},\hat{\mathbf{z}})$. This can be done using the form of $\mathbf{W}_p^{(\eta)}$ in the basis of Cartesian spherical vectors $\hat{\boldsymbol{\chi}}_\mu$, presented in Appendix B. The transformation matrix $\mathfrak{R}$ is obtained by calculating the scalar products of the basic vectors:

$$\mathfrak{R} = \begin{pmatrix} \hat{\boldsymbol{\chi}}_{-1}\cdot\hat{\boldsymbol{\rho}} & \hat{\boldsymbol{\chi}}_{-1}\cdot\hat{\boldsymbol{\varphi}} & \hat{\boldsymbol{\chi}}_{-1}\cdot\hat{\mathbf{z}} \\ \hat{\boldsymbol{\chi}}_{0}\cdot\hat{\boldsymbol{\rho}} & \hat{\boldsymbol{\chi}}_{0}\cdot\hat{\boldsymbol{\varphi}} & \hat{\boldsymbol{\chi}}_{0}\cdot\hat{\mathbf{z}} \\ \hat{\boldsymbol{\chi}}_{+1}\cdot\hat{\boldsymbol{\rho}} & \hat{\boldsymbol{\chi}}_{+1}\cdot\hat{\boldsymbol{\varphi}} & \hat{\boldsymbol{\chi}}_{+1}\cdot\hat{\mathbf{z}} \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{1}{\sqrt{2}}\exp(-i\varphi) & \dfrac{-i}{\sqrt{2}}\exp(-i\varphi) & 0 \\ 0 & 0 & 1 \\ \dfrac{-1}{\sqrt{2}}\exp(i\varphi) & \dfrac{-i}{\sqrt{2}}\exp(i\varphi) & 0 \end{pmatrix}. \tag{A8}$$

Let us first consider Eq. (46). The projections of $\mathbf{W}^{*(\tau)}_{n'm'}$ onto $(\hat{\boldsymbol{\rho}},\hat{\boldsymbol{\varphi}},\hat{\mathbf{z}})$ are represented as a product of $\mathbf{W}^{*(\tau)}_{p}\cdot\hat{\boldsymbol{\chi}}_{\mu}$ and the transformation matrix in Eq. (A8) and are expressed through the coefficients $b^{(\eta)}_{nm,\mu\nu,j}$, $j=\rho,\varphi,z$, obtained using Eqs. (B6)–(B9). They are used together with expansion (A6) to give for the integrand in Eq. (46) the form

$$\mathbf{W}^{*(\tau)}_{n'm'}(\theta,\varphi)\cdot(\mathbf{C}_J)Y_{nm}(\theta,\varphi)=\sum_{\mu,\nu=-1}^{+1}\sum_{j=\rho,\varphi,z}\sum_{n''=0}^{\infty}b^{*(\tau)}_{n'm',\mu\nu,j}\times Y^{*}_{n'+\nu,m'+\mu}(C)_{jJ,n''}Y_{n''0}Y_{nm}. \tag{A9}$$

Thus the integrand is represented as a triple product of scalar spherical harmonics. The only other dependence is the φ dependence of some of the elements of $\mathfrak{R}$ stated in Eq. (A8). Given the simple form of this dependence, the integration in φ can easily be performed, while the θ integration can be avoided by using Gaunt coefficients, Eq. (58). Thus, the elements of $\{C\}$ can be obtained without numerical integration.

The same reasoning applies for $(\tilde{\tilde{\epsilon}}C)$.

2. Optically Anisotropic Brick

Let us consider a parallelepiped consisting of anisotropic material (see Fig. 3). The parallelepiped is divided into six pyramids each of which contains a wall of the parallelepiped and has an apex at the origin of coordinates. The prolongation of the vectors normal and tangential to each wall is made inside the pyramidal regions. Let us denote each region as $V_j^{\pm}$, $j=x,y,z$, so that, for example, V_x^{+} is the pyramid containing the wall perpendicular to the x axis and crossing it at $x>0$, V_x^{-} is the opposite wall, etc. The three vectors have the following form in V_x^{+}:

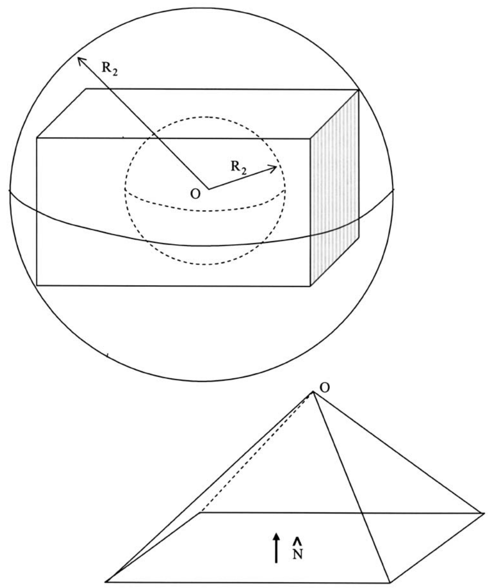

Fig. 3. Anisotropic brick and notation.

$$\hat{\mathbf{T}}_1=\hat{\mathbf{z}},\qquad \hat{\mathbf{N}}=\hat{\mathbf{x}},\qquad \hat{\mathbf{T}}_2=\hat{\mathbf{y}}, \tag{A10}$$

and thus

$$\xi_0=\epsilon_{xx},\qquad \xi_1=\epsilon_{xz},\qquad \xi_2=\epsilon_{xy}. \tag{A11}$$

Matrix C is written in $V_x^{\pm}$ as

$$C\equiv(\mathbf{C}_1,\mathbf{C}_2,\mathbf{C}_3)=\begin{cases}\left(\hat{\mathbf{z}}-\dfrac{\epsilon_{xz}}{\epsilon_{xx}}\hat{\mathbf{x}},\dfrac{1}{\epsilon_{xx}}\hat{\mathbf{x}},\hat{\mathbf{y}}-\dfrac{\epsilon_{xy}}{\epsilon_{xx}}\hat{\mathbf{x}}\right), & \text{inside the parallelepiped}\\[2ex] \left(\hat{\mathbf{z}},\ \dfrac{1}{\epsilon_{\text{out}}}\hat{\mathbf{x}},\ \hat{\mathbf{y}}\right), & \text{outside the parallelepiped}\end{cases}. \tag{A12}$$

Similar expressions are obtained in $V_y^{\pm}$ and $V_z^{\pm}$. As can be observed, matrix C is a piecewise-constant function of θ and φ. The same is valid for $(\tilde{\tilde{\epsilon}}C)$, as the permittivity tensor is independent of (x,y,z) inside each medium. Thus, the two matrices can be represented in the form of Eq. (5). The main difference from the matrices for the finite-length cylinder is that now they depend on φ and thus will contain spherical harmonics Y_{nm} with $m\neq 0$, in addition to Y_{n0}. These supplementary components cannot be evaluated analytically, unlike in the case of Eq. (A7), so that it is necessary to numerically integrate the integrals in θ.

The second difference from the cylindrical structure comes from the transformation matrix $\mathfrak{R}$, which here has a simpler form and has constant components:

$$\mathfrak{R}=\begin{pmatrix}\hat{\boldsymbol{\chi}}_{-1}\cdot\hat{\mathbf{x}} & \hat{\boldsymbol{\chi}}_{-1}\cdot\hat{\mathbf{y}} & \hat{\boldsymbol{\chi}}_{-1}\cdot\hat{\mathbf{z}}\\ \hat{\boldsymbol{\chi}}_{0}\cdot\hat{\mathbf{x}} & \hat{\boldsymbol{\chi}}_{0}\cdot\hat{\mathbf{y}} & \hat{\boldsymbol{\chi}}_{0}\cdot\hat{\mathbf{z}}\\ \hat{\boldsymbol{\chi}}_{+1}\cdot\hat{\mathbf{x}} & \hat{\boldsymbol{\chi}}_{+1}\cdot\hat{\mathbf{y}} & \hat{\boldsymbol{\chi}}_{+1}\cdot\hat{\mathbf{z}}\end{pmatrix}=\begin{pmatrix}\dfrac{1}{\sqrt{2}} & \dfrac{-i}{\sqrt{2}} & 0\\ 0 & 0 & 1\\ \dfrac{-1}{\sqrt{2}} & \dfrac{-i}{\sqrt{2}} & 0\end{pmatrix}. \tag{A13}$$

The coefficients $b^{(\eta)}_{nm,\mu,\nu,j}$, $j=x,y,z$ are obtained from Eq. (B12), they are independent of θ and φ because $\mathfrak{R}=\text{const}$. The integrand in Eq. (46) has the same form as that in Eq. (A9), adding a summation over the second index m'' of $Y_{n''m''}$:

$$\mathbf{W}^{*(\tau)}_{n'm'} \cdot (\mathbf{C}_J) Y_{nm} = \sum_{\mu,\nu=-1}^{+1} \sum_{j=xy,z} \sum_{n''=0}^{\infty} \sum_{m''=-n''}^{n''} b^{*(\tau)}_{n'm',\mu\nu,j} \times Y^{*}_{n'+\nu,m'+\mu} (\tilde{\tilde{\epsilon}} C)_{jJ,n''m''} Y_{n''m''} Y_{nm}. \tag{A14}$$

APPENDIX B: PROJECTION OF VECTOR SPHERICAL HARMONICS ONTO DIFFERENT BASIS

Let us recall the definition of Cartesian spherical unit vectors:

$$\hat{\boldsymbol{\chi}}_{-1} = \frac{1}{\sqrt{2}}(\hat{\mathbf{x}} - i\hat{\mathbf{y}}),$$

$$\hat{\boldsymbol{\chi}}_{0} = \hat{\mathbf{z}},$$

$$\hat{\boldsymbol{\chi}}_{+1} = -\frac{1}{\sqrt{2}}(\hat{\mathbf{x}} + i\hat{\mathbf{y}}). \tag{B1}$$

The vector spherical harmonics can be defined as a linear combination of these vectors, as discussed in Appendix A of Part I.[9] This fact makes them extremely suitable for projecting $\mathbf{W}_p^{(\eta)}$ onto a basis, independent of the observation point. Using the formulas in Appendix A of Part I, one obtains

$$\mathbf{Y}_{nm} \cdot \hat{\boldsymbol{\chi}}_\mu = \left(\sqrt{\frac{n}{2n+1}} \mathbf{Y}^m_{n,n-1} - \sqrt{\frac{n+1}{2n+1}} \mathbf{Y}^m_{n,n+1} \right) \cdot \boldsymbol{\chi}_\mu$$
$$= \sqrt{\frac{n}{2n+1}} \sum_{\mu'=-1}^{1} (n-1, m-\mu'; 1, \mu' | n, m) \times Y_{n-1,m-\mu'} \hat{\boldsymbol{\chi}}_{\mu'} \cdot \hat{\boldsymbol{\chi}}_\mu$$
$$- \sqrt{\frac{n+1}{2n+1}} \sum_{\mu'=-1}^{1} (n+1, m-\mu'; 1, \mu' | n, m) \times Y_{n+1,m-\mu'} \hat{\boldsymbol{\chi}}_{\mu'} \cdot \hat{\boldsymbol{\chi}}_\mu, \tag{B2}$$

$$\mathbf{X}_{nm} \cdot \hat{\boldsymbol{\chi}}_\mu = \frac{1}{i} \mathbf{Y}^m_{n,n} \cdot \hat{\boldsymbol{\chi}}_\mu = -i \sum_{\mu'=-1}^{1} (n, m-\mu'; 1, \mu' | n, m) Y_{n,m-\mu'} \hat{\boldsymbol{\chi}}_{\mu'} \cdot \hat{\boldsymbol{\chi}}_\mu. \tag{B3}$$

$$\mathbf{Z}_{nm} \cdot \hat{\boldsymbol{\chi}}_\mu = \left(\sqrt{\frac{n+1}{2n+1}} \mathbf{Y}^m_{n,n-1} + \sqrt{\frac{n}{2n+1}} \mathbf{Y}^m_{n,n+1} \right) \cdot \hat{\boldsymbol{\chi}}_\mu$$
$$= \sqrt{\frac{n+1}{2n+1}} \sum_{\mu'=-1}^{1} (n-1, m-\mu'; 1, \mu' | n, m) \times Y_{n-1,m-\mu'} \hat{\boldsymbol{\chi}}_{\mu'} \cdot \hat{\boldsymbol{\chi}}_\mu$$
$$+ \sqrt{\frac{n}{2n+1}} \sum_{\mu'=-1}^{1} (n+1, m-\mu'; 1, \mu' | n, m) \times Y_{n+1,m-\mu'} \hat{\boldsymbol{\chi}}_{\mu'} \cdot \hat{\boldsymbol{\chi}}_\mu. \tag{B4}$$

On the other hand, the scalar products of the Cartesian spherical vectors give, by use of Eq. (B1),

$$\hat{\boldsymbol{\chi}}_\mu \cdot \hat{\boldsymbol{\chi}}^*_\nu = \delta_{\mu\nu},$$

$$\hat{\boldsymbol{\chi}}_{-1} \cdot \hat{\boldsymbol{\chi}}_{-1} = 0, \qquad \hat{\boldsymbol{\chi}}_{-1} \cdot \hat{\boldsymbol{\chi}}_{0} = 0,$$

$$\hat{\boldsymbol{\chi}}_{-1} \cdot \hat{\boldsymbol{\chi}}_{+1} = -1,$$

$$\hat{\boldsymbol{\chi}}_{0} \cdot \hat{\boldsymbol{\chi}}_{0} = 1, \qquad \hat{\boldsymbol{\chi}}_{1} \cdot \hat{\boldsymbol{\chi}}_{0} = 0,$$

$$\hat{\boldsymbol{\chi}}_{+1} \cdot \hat{\boldsymbol{\chi}}_{+1} = 0. \tag{B5}$$

These relations finally produce

$$\mathbf{Y}_{nm} \cdot \hat{\boldsymbol{\chi}}_{-1} = -\sqrt{\frac{n}{2n+1}} (n-1, m-1; 1, 1 | n, m) Y_{n-1,m-1} + \sqrt{\frac{n+1}{2n+1}} (n+1, m-1; 1, 1 | n, m) Y_{n+1,m-1},$$

$$\mathbf{Y}_{nm} \cdot \hat{\boldsymbol{\chi}}_{0} = \sqrt{\frac{n}{2n+1}} (n-1, m; 1, 0 | n, m) Y_{n-1,m} - \sqrt{\frac{n+1}{2n+1}} (n+1, m; 1, 0 | n, m) Y_{n+1,m},$$

$$\mathbf{Y}_{nm} \cdot \hat{\boldsymbol{\chi}}_{1} = -\sqrt{\frac{n}{2n+1}} (n-1, m+1; 1, -1 | n, m) Y_{n-1,m+1} + \sqrt{\frac{n+1}{2n+1}} (n+1, m+1; 1, -1 | n, m) Y_{n+1,m+1}. \tag{B6}$$

$$\mathbf{X}_{nm} \cdot \hat{\boldsymbol{\chi}}_{-1} = i(n, m-1; 1, 1 | n, m) Y_{n,m-1},$$

$$\mathbf{X}_{nm} \cdot \hat{\boldsymbol{\chi}}_{0} = -i(n, m; 1, 0 | n, m) Y_{n,m},$$

$$\mathbf{X}_{nm} \cdot \hat{\boldsymbol{\chi}}_{1} = i(n, m+1; 1, -1 | n, m) Y_{n,m+1}. \tag{B7}$$

$$\mathbf{Z}_{nm} \cdot \hat{\boldsymbol{\chi}}_{-1} = -\sqrt{\frac{n+1}{2n+1}}(n-1,m-1;1,1|n,m)Y_{n-1,m-1} - \sqrt{\frac{n}{2n+1}}(n+1,m-1;1,1|n,m)Y_{n+1,m-1},$$

$$\mathbf{Z}_{nm} \cdot \hat{\boldsymbol{\chi}}_{0} = \sqrt{\frac{n+1}{2n+1}}(n-1,m;1,0|n,m)Y_{n-1,m} + \sqrt{\frac{n}{2n+1}}(n+1,m;1,0|n,m)Y_{n+1,m},$$

$$\mathbf{Z}_{nm} \cdot \hat{\boldsymbol{\chi}}_{1} = -\sqrt{\frac{n+1}{2n+1}}(n-1,m+1;1,-1|n,m)Y_{n-1,m+1} - \sqrt{\frac{n}{2n+1}}(n+1,m+1;1,-1|n,m)Y_{n+1,m+1}. \quad \text{(B8)}$$

The coefficients in front of $Y_{n,m}$ in Eqs. (B6)–(B8) represent the coefficients $b^{(\eta)}_{nm,\mu\nu,\chi}$, which express the projections of the vector spherical harmonics $\mathbf{W}^{(\eta)}_{nm}$ on $\hat{\boldsymbol{\chi}}_{\mu}$ in terms of scalar spherical harmonics $Y_{n,m}$:

$$\mathbf{W}^{(\eta)}_{nm} \cdot \hat{\boldsymbol{\chi}}_{\mu} = \sum_{\nu=-1}^{1} b^{(\eta)}_{nm,\mu,\nu,\chi} Y_{n+\nu,m+\mu}. \quad \text{(B9)}$$

A similar expression applies in an arbitrary basis $(\hat{\mathbf{j}}_{\mu})$:

$$\mathbf{W}^{(\eta)}_{nm} \cdot \hat{\mathbf{j}}_{\mu} = \sum_{\nu=-1}^{1} b^{(\eta)}_{nm,\mu\nu,j} Y_{n+\nu,m+\mu}. \quad \text{(B10)}$$

The transfer from the basis $(\hat{\boldsymbol{\chi}}_{\mu})$ to the basis $(\hat{\mathbf{j}}_{\mu})$ is made through the corresponding transformation matrix $\mathfrak{R} = (\hat{\mathbf{j}} \cdot \hat{\boldsymbol{\chi}}^{*})$, so that $(\hat{\mathbf{j}}_{\mu}) = \mathfrak{R}(\hat{\boldsymbol{\chi}}_{\nu})$. The components of vector spherical harmonics in different basis sets are related through the same transformation matrix:

$$\mathbf{W}^{(\eta)}_{nm} \cdot \hat{\mathbf{j}}_{\mu} \equiv \hat{\mathbf{j}}_{\mu} \cdot \mathbf{W}^{(\eta)}_{nm} = \sum_{\mu'} \mathfrak{R}_{\mu\mu'} \hat{\boldsymbol{\chi}}_{\mu'} \cdot \mathbf{W}^{(\eta)}_{nm}. \quad \text{(B11)}$$

This relation ensures the transfer between the two sets of b coefficients:

$$b^{(\eta)}_{nm,\mu,\nu,j} = \sum_{\mu'} \mathfrak{R}_{\mu\mu'} b^{(\eta)}_{nm,\mu',\nu,\chi}. \quad \text{(B12)}$$

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