Light diffraction by a three-dimensional object: differential theory

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The differential theory of diffraction of light by an arbitrary object described in spherical coordinates is developed. Expanding the fields on the basis of vector spherical harmonics, we reduce the Maxwell equations to an infinite first-order differential set. In view of the truncation required for numerical integration, correct factorization rules are derived to express the components of **D** in terms of the components of **E**, a process that extends the fast Fourier factorization to the basis of vector spherical harmonics. Numerical overflows and instabilities are avoided through the use of the S-matrix propagation algorithm for carrying out the numerical integration. The method can analyze any shape and/or material, dielectric or conducting. It is particularly simple when applied to rotationally symmetric objects.

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1. INTRODUCTION

Light scattering from arbitrarily shaped 3D objects comparable in size to the wavelength of the scattering radiation is an important problem with applications covering a vast range of fields of science and technology, including astrophysics, atmospheric physics, radiative transfer in optically thick media such as paints and papers, and remote detection. By "comparable in size with the wavelength," we are most often speaking of particles having a characteristic size D within an order of magnitude of the wavelength, $\lambda/10 \lesssim D \lesssim 10\lambda$. In this size regime, and for scatterers of sufficiently high dielectric contrast, popular approximations such as the Rayleigh–Gans[1,2] or geometric optics approximations[1,2] are invalid; one must resort to an essentially full solution of the Maxwell equations.

The first full solution to the electromagnetic scattering by a fully 3D object is that of Lorenz and Mie for the scattering by a single homogeneous isotropic spherical object embedded in a homogeneous isotropic external medium.[3–5] This renowned solution takes the form of an infinite (but rapidly converging) series of coefficients involving spherical Bessel functions. Being the only analytically manageable exact solution to the full electromagnetic scattering problem, the Mie solution has played a preponderate role in light-scattering calculations for nearly a century.

In view of the size range in which the Mie theory is most useful, it comes as no surprise that Mie theory is most frequently applied to media containing a large number of scattering inclusions. Since the Mie theory is a solution only to an isolated particle, it has frequently been coupled with the independent scattering approximation and applied to tenuous media systems containing only a week volume density of scatterers.[6]

The increasing interest in recent decades of light scattering by aggregates and light propagation in dense media such as composites, containing a high volume density of inclusions, has fueled considerable progress in the multiple-scattering problem of such dense media.[7–9] In view of the already considerable difficulty of the multiple-scattering equations, a majority of these studies have continued to use spheres as the fundamental scattering element. In reality, of course, it is extremely rare for scattering inclusions to be so obliging as to separate themselves into distinct compact spheres, even though an impressive number of mechanical and chemical processes in a number of industries have been developed with exactly this goal in mind (grinding, surfactants,…). Furthermore, it has long been clear that nonspherical inclusions can yield quantitatively different results on the macroscopic scale than spherical inclusions.

Many multiple-scattering codes and theories have employed with considerable success the notion of a transfer matrix (frequently called the T matrix in the multiple-scattering community; see the note[10]) that consists of a linear transformation between the excitation field incident on a scatterer and the scattered field emanating from it.[2,7–9,11] The transfer matrix is more than a single solution to the scattering problem corresponding to a given incident field; rather it can be viewed as a complete solution to the scattering problem for any possible incident field. In the multiple-scattering theories employing transfer matrices, the Mie solution to the sphere takes the form of a diagonal transfer matrix in a basis of the vector spherical wave functions. It has long been recognized by those working in this field that nonspherical scatterers can rather readily be integrated into existing multiple-scattering theories by simply replacing the diagonal Mie transfer matrices of spheres by the full transfer matrices of nonspherical objects.

There exist a number of techniques for treating scattering by nonspherical objects, but not all of these can readily provide the complete solution required to derive a transfer matrix, and the reliability and applicability of these various techniques is a recurring stumbling bock. One of the most popular techniques in the literature is the Waterman (or extended boundary condition) method, whose popularity is in large part due to the fact that one can readily obtain from it a full transfer matrix for a large variety of nonspherical shapes.[12] It has been shown, however, that the Waterman technique yields the same algorithm as one obtains from a Rayleigh hypothesis.[11] Both the Rayleigh hypothesis and the Waterman technique have been demonstrated to have considerable limitations in the theories of diffraction gratings,[13] and it is well established that both the Waterman technique and the Rayleigh hypothesis can break down for scatterers with high aspect ratios.[11]

The above remarks have in part provided our motivation to propose a new differential theory for deriving the transfer matrix of nonspherical scatterers. Although differential theories have been studied previously for 3D scatterers, we have developed our theory from first principles and made full use of recent breakthroughs in the differential theory of 1D, 2D, and 3D diffraction gratings that have greatly improved the reliability and convergence of differential theories. The new methods in question have been presented and elaborated in a number of articles[14–19] and a recent book,[20] but these works are not a prerequisite for understanding the present work, which has been conceived to be self-contained. The differential technique in diffraction gratings makes extensive use of Fourier series, and their extension to the 3D problem leads us to make considerable use of vector spherical harmonics (VSHs) in the derivation of our formulas. The VSHs, however, do not appear in the final computational method, and the finer details of the VSH manipulations are provided in Appendix C.

The work is organized as follows. We present the problem in Section 2. We introduce the VSHs in Section 3 and introduce their applications to field expansions in Section 4. The propagation equations are derived in Section 5, and the fast numerical factorization (FNF) required for convergence of the series is thoroughly discussed in Section 6. We study field developments outside the modulated region in Section 7 and present the prescription for resolving the boundary-value problem in Section 8. We conclude this work by briefly illustrating the necessary formula for extracting physically relevant quantities such as cross sections and scattering matrices.

2. PRESENTATION OF THE PROBLEM

Figure 1 shows a finite object, made of an isotropic material, with arbitrary shape limited by a surface (S). This surface is described in spherical coordinates (r,θ,ϕ), with $\theta\in[0,\pi]$ defined in the figure by the equation

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

or

$$r=g(\theta,\phi). \tag{2}$$

At a given point M on the surface, the external normal unit vector is $\hat{\mathbf{N}}$, and the unit vectors of spherical coordinates are denoted $\hat{\mathrm{r}}$, $\hat{\boldsymbol{\theta}}$, $\hat{\boldsymbol{\phi}}$. The surface (S) divides the space into two regions. The first region, contained within (S), is filled with a linear, homogeneous, and isotropic me-

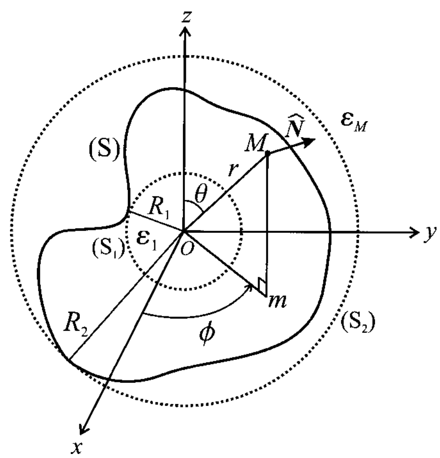

Fig. 1. Description of the diffracting object and notations.

dium, dielectric or conducting, described by complex permittivity ϵ_1. The second region lies outside (S) and has real permittivity ϵ_m. In view of developing the differential theory, we divide space into three regions by introducing the inscribed sphere (S_1) with radius R_1 and the circumscribed sphere (S_2) with radius R_2; the region between (S_1) and (S_2) is called the "modulated region," a denotation that recalls that for any constant value r_0 of r between R_1 and R_2, the permittivity, ϵ, is a function of θ and ϕ and, furthermore, is obviously periodic with respect to ϕ with a period of 2π and piecewise constant with respect to θ and ϕ.

The object is subject to an incident harmonic electromagnetic field described by its electric field, $\mathbf{E}_{\mathrm{i}}$, with an $\exp(-i\omega t)$ time dependence. As is well known in quantum mechanics and electromagnetism,[21–23] any function of angular variables θ and ϕ can be developed on the basis of scalar spherical harmonics $Y_{nm}(\theta,\phi)$. The dimensionless relative dielectric constant, $\varepsilon(r,\theta,\phi)$, defined such that $\epsilon_0\varepsilon(r,\theta,\phi)\equiv\epsilon(r,\theta,\phi)$ can therefore be expressed as

$$\varepsilon(r,\theta,\phi)=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\varepsilon_{nm}(r)Y_{nm}(\theta,\phi), \tag{3}$$

which implies that $\varepsilon_{nm}(r)$ can be obtained from the Hermitian product:

$$\varepsilon_{nm}(r)=\langle Y_{nm}|\varepsilon\rangle\equiv\int_0^{4\pi}Y_{nm}^*(\theta,\phi)\varepsilon(r,\theta,\phi)\mathrm{d}\Omega. \tag{4}$$

The reader should note that in Eq. (4) and throughout this work we have adopted the convention for scalar Hermitian products such that

$$\langle g|f\rangle\equiv\int g^*(x)f(x)\mathrm{d}x. \tag{5}$$

In Eq. (4), the asterisk denotes the complex conjugate, and Ω is the solid angle. Equation (4) can thus be rewritten as

$$\varepsilon_{nm}(r)=\int_0^{2\pi}\int_0^{\pi}\varepsilon(r,\theta,\phi)Y_{nm}^*(\theta,\phi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi. \tag{6}$$

A development of the vector electromagnetic field is a more complicated affair. One might first be tempted to expand each spherical coordinate component of the total field $(\mathbf{E},\mathbf{H})$ on the basis of the scalar spherical harmonics, similar to Eq. (3). But when such expansions are put into the Maxwell equations, derivatives of the Y_{nm} functions arise that are difficult to calculate and manipulate. Consequently, we choose another way to expand vector fields; i.e., we represent them on the basis of VSHs.

3. VECTOR SPHERICAL HARMONICS

VSHs are described in several reference books,[6,21–23] although their definitions and notations vary with the authors. They arise in vector solutions of the wave equation (Helmholtz equation) and when appropriately defined can form an orthogonal complete basis to represent the electromagnetic field. We choose to define and denote them by the following equations:

$$\mathbf{Y}_{nm}(\theta,\phi) \equiv \hat{\mathrm{r}} Y_{nm}(\theta,\phi), \tag{7}$$

$$\mathbf{X}_{nm}(\theta,\phi) \equiv \mathbf{Z}_{nm}(\theta,\phi) \times \hat{\mathrm{r}}, \tag{8}$$

where

$$\mathbf{Z}_{nm}(\theta,\phi) \equiv \frac{r\,\boldsymbol{\nabla}\, Y_{nm}(\theta,\phi)}{\sqrt{n(n+1)}}$$

$$\text{if } n \neq 0,\ \mathbf{Z}_{00}(\theta,\phi) \equiv 0. \tag{9}$$

Equation (8) implies that

$$\mathbf{Z}_{nm}(\theta,\phi) = \hat{\mathrm{r}} \times \mathbf{X}_{nm}(\theta,\phi). \tag{10}$$

All the VSHs are mutually orthonormal in the sense that if $\mathbf{W}_{nm}^{(i)}$ $(i=1, 2, 3)$ denotes the vector harmonics $\mathbf{Y}_{nm}$, $\mathbf{X}_{nm}$, or $\mathbf{Z}_{nm}$, we have

$$\langle \mathbf{W}_{nm}^{(i)} | \mathbf{W}_{\nu\mu}^{(j)} \rangle \equiv \int_0^{4\pi} \mathbf{W}_{nm}^{(i)*} \cdot \mathbf{W}_{\nu\mu}^{(j)} \mathrm{d}\Omega = \delta_{ij}\delta_{n\nu}\delta_{m\mu}, \tag{11}$$

where δ_{ij} is the Kronecker symbol and the Hermitian product of Eq. (4) has been extended to vector fields. We also remark from Eqs. (7)–(9) that if the $\mathbf{W}_{nm}^{(i)}(\theta,\phi)$ were real the trihedral $(\mathbf{Y}_{nm},\mathbf{X}_{nm},\mathbf{Z}_{nm})$ would be direct.

Let us recall that the scalar spherical harmonics $Y_{nm}(\theta,\phi)$ are expressed in terms of associated Legendre functions $P_n^m(\cos\theta)$ as[23]

$$Y_{nm}(\theta,\phi) = \left[\frac{2n+1}{4\pi} \frac{(n-m)!}{(n+m)!} \right]^{1/2} P_n^m(\cos\theta)\exp(im\phi) \tag{12}$$

or by including the square root in the definitions of normalized associated Legendre functions $\bar{P}_n^m$:

$$Y_{nm}(\theta,\phi) = \bar{P}_n^m(\cos\theta)\exp(im\phi). \tag{13}$$

Introducing functions $\bar{u}_n^m$ and $\bar{s}_n^m$ defined by

$$\bar{u}_n^m(\cos\theta) = \frac{1}{\sqrt{n(n+1)}} \frac{m}{\sin\theta} \bar{P}_n^m(\cos\theta), \tag{14}$$

$$\bar{s}_n^m(\cos\theta) = \frac{1}{\sqrt{n(n+1)}} \frac{\mathrm{d}}{\mathrm{d}\theta} \bar{P}_n^m(\cos\theta), \tag{15}$$

we can express the vector harmonics $\mathbf{X}_{nm}$ and $\mathbf{Z}_{nm}$ as

$$\mathbf{X}_{nm}(\theta,\phi) = i\bar{u}_n^m(\cos\theta)\exp(im\phi)\hat{\boldsymbol{\theta}} - \bar{s}_n^m(\cos\theta)\exp(im\phi)\hat{\boldsymbol{\phi}}, \tag{16}$$

$$\mathbf{Z}_{nm}(\theta,\phi) = \bar{s}_n^m(\cos\theta)\exp(im\phi)\hat{\boldsymbol{\theta}} + i\bar{u}_n^m(\cos\theta)\exp(im\phi)\hat{\boldsymbol{\phi}}. \tag{17}$$

Equations (16) and (17), combined with Eq. (7), clearly show that for a given n, m the $(\mathbf{Y}_{nm},\mathbf{X}_{nm},\mathbf{Z}_{nm})$ are mutually perpendicular in the sense that $\mathbf{W}_{nm}^{(i)} \cdot \mathbf{W}_{nm}^{(j)} = 0$ for $i \neq j$.

Other interesting relations are the curl of products of a radially dependent function $h(r)$ by a $\mathrm{W}_{nm}^{(i)}$. These relations will prove to be useful in the derivation of the propagation equations and are given by

$$\mathbf{curl}[h(r)\mathbf{Y}_{nm}] = [n(n+1)]^{1/2} \frac{h(r)}{r} \mathbf{X}_{nm}, \tag{18}$$

$$\mathbf{curl}[h(r)\mathbf{X}_{nm}] = \frac{h(r)}{r}[n(n+1)]^{1/2}\mathbf{Y}_{nm} + \left[\frac{h(r)}{r} + h'(r) \right] \mathbf{Z}_{nm}, \tag{19}$$

$$\mathbf{curl}[h(r)\mathbf{Z}_{nm}] = -\left[\frac{h(r)}{r} + h'(r) \right] \mathbf{X}_{nm}. \tag{20}$$

4. FIELD EXPANSIONS

An arbitrary vector field $\mathbf{U}(r,\theta,\phi)$ can be expressed in a development of the VSHs as stated by

$$\mathbf{U}(r,\theta,\phi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} [A_{Ynm}(r)\mathbf{Y}_{nm}(\theta,\phi) + A_{Xnm}(r)\mathbf{X}_{nm}(\theta,\phi) + A_{Znm}(r)\mathbf{Z}_{nm}(\theta,\phi)]. \tag{21}$$

Such a development will be subsequently applied to the total electric field $\mathbf{E}$, the total magnetic field $\mathbf{H}$, the displacement $\mathbf{D}$, the incident electric field $\mathbf{E}_{\mathrm{i}}$, and the unit normal vector $\hat{\mathbf{N}}$. However, in view of a numerical treatment, the summation in Eq. (21) will have to be limited to a value of n equal to $n_{\max}$. Also, the double subscript (n,m) will be replaced by a single subscript p, varying from 1 to N. It is then easy to establish that Eq. (21) takes the form

$$\mathbf{U}(r,\theta,\phi) = \sum_{p=1}^{N} [A_{Yp}(r)\mathbf{Y}_p(\theta,\phi) + A_{Xp}(r)\mathbf{X}_p(\theta,\phi) + A_{Zp}(r)\mathbf{Z}_p(\theta,\phi)], \tag{22}$$

where $N \equiv (n_{\max}+1)^2$ and

$$p = n(n+1) + m + 1. \tag{23}$$

On the other hand, if p is given, n and m can be derived from it through the equations

$$n = \mathrm{Int}\sqrt{p-1}, \quad m = p - 1 - n(n+1), \tag{24}$$

where the function Int(x) calculates the integer part of x.

Throughout the rest of the work, the coefficients of the various field vectors will frequently be put in columns. As a result of Eq. (22), the total field **E**, for example, will be represented by a column $[E]$ composed of three blocks containing the functions E_{Yp}, E_{Xp}, and E_{Zp}. Since $p \in [1,(n_{\max}+1)^2]$, the vector **E** will have $3\times(n_{\max}+1)^2$ components $E_l : \mathrm{E} \leftrightarrow [E]$, i.e.,

$$\begin{bmatrix} \vdots \\ E_l \\ \vdots \end{bmatrix} \equiv \left.\begin{bmatrix} — \\ \vdots \\ E_{Y,p} \\ \vdots \\ — \\ \vdots \\ E_{X,p} \\ \vdots \\ — \\ \vdots \\ E_{Z,p} \\ \vdots \\ — \end{bmatrix}\right\} 3 \times (n_{\max}+1)^2. \tag{25}$$

The unit vector $\hat{\mathbf{N}}$ can be represented in such a column once the surface S is specified; i.e., the function $f(r,\theta,\phi)$ is known. Since $\hat{\mathbf{N}}$ is given by

$$\hat{\mathbf{N}}(\theta,\phi) = \left.\frac{\mathbf{grad}\, f}{\|\mathbf{grad}\, f\|}\right|_{f=0}, \tag{26}$$

we obtain in spherical coordinates

$$N_r = \left.\frac{\dfrac{\partial f}{\partial r}}{\|\mathbf{grad}\, f\|}\right|_{f=0}, \quad N_\theta = \left.\frac{\dfrac{1}{r}\dfrac{\partial f}{\partial \theta}}{\|\mathbf{grad}\, f\|}\right|_{f=0},$$

$$N_\phi = \left.\frac{\dfrac{1}{r\sin\theta}\dfrac{\partial f}{\partial \phi}}{\|\mathbf{grad}\, f\|}\right|_{f=0}. \tag{27}$$

With $\hat{\mathbf{N}}$ known, its components on the VSHs are derived from the scalar products

$$N_{Ynm} = \langle \mathbf{Y}_{nm} | \hat{\mathbf{N}} \rangle = \langle Y_{nm}\hat{\mathrm{r}} | \hat{\mathrm{r}} N_r \rangle = \int_0^{4\pi} Y^*_{nm}(\theta,\phi) N_r(\theta,\phi)\mathrm{d}\Omega$$
$$= \int_0^{2\pi}\int_0^{\pi} N_r \bar{P}_n^m(\cos\theta)\exp(-im\phi)\sin\theta \mathrm{d}\theta\mathrm{d}\phi, \tag{28}$$

$$N_{Xnm} = \int_0^{2\pi}\int_0^{\pi} [iN_\theta \bar{u}_n^m(\cos\theta) - N_\phi \bar{s}_n^m(\cos\theta)]$$
$$\times\exp(-im\phi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi, \tag{29}$$

$$N_{Znm} = \int_0^{2\pi}\int_0^{\pi} [N_\theta \bar{s}_n^m(\cos\theta) + iN_\phi \bar{u}_n^m(\cos\theta)]$$
$$\times\exp(-im\phi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi. \tag{30}$$

From Eqs. (28)–(30), the column associated with vector $\hat{\mathbf{N}}$, containing the three blocks N_{Yp}, N_{Xp}, and N_{Zp}, $p \in [1,(n_{\max}+1)^2]$, is fully determined. The case of a diffracted object with a revolution symmetry is especially simple. Then not only is N_ϕ null [which eliminates a term in Eqs. (29) and (30)] but more interesting is the fact that N_r and N_θ, are then ϕ independent. Then all terms with subscript m different from zero are null, and Eqs. (28)–(30) reduce to

$$N_{Yn0} = 2\pi\int_0^{\pi} N_r(\theta)\bar{P}_n^0(\cos\theta)\sin\theta\mathrm{d}\theta, \tag{31}$$

$$N_{Xn0} = 0, \tag{32}$$

$$N_{Zn0} = 2\pi\int_0^{\pi} N_\theta(\theta)\bar{s}_n^0(\cos\theta)\sin\theta\mathrm{d}\theta, \tag{33}$$

where we have used the fact that $\bar{u}_n^0(\cos\theta)=0$.

Of course, replacing double integrals by single ones, combined with the reduction of their number from $3\times(n_{\max}+1)^2$ to $2\times(n_{\max}+1)$ leads to great savings in computation time. The same remark also applies to $\varepsilon(r,\theta,\phi)$, whose components on the $Y_n^m(\theta,\phi)$ basis reduce to $\varepsilon_{n,0}$, given by

$$\varepsilon_{n,0} = 2\pi\int_0^{\pi} \varepsilon(r,\theta)\bar{P}_n^0(\cos\theta)\sin\theta\mathrm{d}\theta. \tag{34}$$

Details concerning an analytical calculation of $\varepsilon_{n,0}$ are given in Appendix A.

5. PROPAGATION EQUATIONS

The main advantage of the field representation over the basis of VSHs lies in the simplicity of the propagation equations resulting from Maxwell equations. Writing $\mathbf{curl}\,\mathbf{E} = i\omega\mu\mu_0\mathbf{H}$, with μ as the dimensionless relative magnetic permeability, and representing **E** and **H** by expansions of the form given by Eq. (22), we find

$$\sum_{p=1}^{N}\{\mathbf{curl}[E_{Yp}(r)\mathbf{Y}_p] + \mathbf{curl}[E_{Xp}(r)\mathbf{X}_p] + \mathbf{curl}[E_{Zp}(r)\mathbf{Z}_p]\}$$
$$= i\omega\mu\mu_0\sum_{p=1}^{N}(H_{Yp}\mathbf{Y}_p + H_{Xp}\mathbf{X}_p + H_{Zp}\mathbf{Z}_p). \tag{35}$$

Using Eqs. (18)–(20) and equating the p components on both sides in Eq. (35), we also have

$$\sqrt{n(n+1)}\frac{E_{Yp}(r)}{r}\mathbf{X}_p+\sqrt{n(n+1)}\frac{E_{Xp}(r)}{r}\mathbf{Y}_p+\left[\frac{E_{Xp}(r)}{r}+\frac{\mathrm{d}E_{Xp}(r)}{\mathrm{d}r}\right]\mathbf{Z}_p-\left[\frac{E_{Zp}(r)}{r}+\frac{\mathrm{d}E_{Zp}(r)}{\mathrm{d}r}\right]\mathbf{X}_p$$
$$=i\omega\mu\mu_0(H_{Yp}\mathbf{Y}_p+H_{Xp}\mathbf{X}_p+H_{Zp}\mathbf{Z}_p). \quad (36)$$

Introducing $a_p=\sqrt{n(n+1)}$, where $n=\mathrm{Int}\sqrt{p-1}$, and projecting both members of Eq. (36) on vectors $\mathbf{Y}_p$, $\mathbf{X}_p$, and $\mathbf{Z}_p$, we obtain

$$a_p\frac{E_{Xp}}{r} = i\omega\mu\mu_0 H_{Yp}, \quad (37)$$

$$a_p\frac{E_{Yp}}{r}-\frac{E_{Zp}}{r}-\frac{\mathrm{d}E_{Zp}}{\mathrm{d}r} = i\omega\mu\mu_0 H_{Xp}, \quad (38)$$

$$\frac{E_{Xp}}{r}+\frac{\mathrm{d}E_{Xp}}{\mathrm{d}r} = i\omega\mu\mu_0 H_{Zp}. \quad (39)$$

Similarly, the Maxwell equation, **curl H**$=-i\omega\mathbf{D}$ leads to

$$a_p\frac{H_{Xp}}{r} = -i\omega D_{Yp}, \quad (40)$$

$$a_p\frac{H_{Yp}}{r}-\frac{H_{Zp}}{r}-\frac{\mathrm{d}H_{Zp}}{\mathrm{d}r} = -i\omega D_{Xp}, \quad (41)$$

$$\frac{H_{Xp}}{r}+\frac{\mathrm{d}H_{Xp}}{\mathrm{d}r} = -i\omega D_{Zp}. \quad (42)$$

Since we work in linear optics ($\mathbf{D}=\epsilon_0\varepsilon\mathbf{E}$), and since $\mathbf{E}$ and $\mathbf{D}$ are represented on the same basis, there exists a square matrix Q_ε that links the column $[E]$ to the column $[D]$ such that

$$[D]=\epsilon_0 Q_\varepsilon[E]. \quad (43)$$

This Q_ε matrix is made of nine square blocks, each block having dimension $(n_{\max}+1)^2$, which depend on the components of ε defined in Eq. (6), and will be calculated in Subsection 6.C. We represent Q_ε by the following block structure:

$$Q_\varepsilon=\begin{pmatrix} Q_{\varepsilon YY} & Q_{\varepsilon YX} & Q_{\varepsilon YZ} \\ Q_{\varepsilon XY} & Q_{\varepsilon XX} & Q_{\varepsilon XZ} \\ Q_{\varepsilon ZY} & Q_{\varepsilon ZX} & Q_{\varepsilon ZZ}\end{pmatrix}. \quad (44)$$

From Eqs. (43) and (44), we thus obtain

$$\frac{1}{\epsilon_0}[D_Y]=Q_{\varepsilon YY}[E_Y]+Q_{\varepsilon YX}[E_X]+Q_{\varepsilon YZ}[E_Z], \quad (45)$$

which gives

$$[E_Y]=(Q_{\varepsilon YY})^{-1}\left(\frac{1}{\epsilon_0}[D_Y]-Q_{\varepsilon YX}[E_X]-Q_{\varepsilon YZ}[E_Z]\right). \quad (46)$$

Moreover,

$$\frac{1}{\epsilon_0}[D_X]=Q_{\varepsilon XY}[E_Y]+Q_{\varepsilon XX}[E_X]+Q_{\varepsilon XZ}[E_Z], \quad (47)$$

$$\frac{1}{\epsilon_0}[D_Z]=Q_{\varepsilon ZY}[E_Y]+Q_{\varepsilon ZX}[E_X]+Q_{\varepsilon ZZ}[E_Z]. \quad (48)$$

We first insert Eq. (40) into Eq. (46). We then insert Eq. (46) into Eqs. (47) and (48) in order to express $[D_X]$ and $[D_Z]$ in terms of $[E_X]$, $[E_Z]$, and $[H_X]$, expressions that are then inserted into Eqs. (41) and (42). In Eq. (41) $[H_{Yp}]$ is eliminated thanks to Eq. (37). In Eq. (38) $[E_Y]$ is eliminated thanks to Eqs. (40) and (46). Introducing a diagonal matrix a with elements $a_p\delta_{p,q}$, we finally reduce the set of six equations, Eqs. (37)–(42), to four equations with unknowns E_{Xp}, E_{Zp}, H_{Xp}, and H_{Zp} only:

$$\frac{E_{Xp}}{r}+\frac{\mathrm{d}E_{Xp}}{\mathrm{d}r}=i\omega\mu\mu_0 H_{Zp} \quad (49)$$

$$\frac{a_p}{r}\left((Q_{\varepsilon YY})^{-1}\left[\frac{ia}{\omega\epsilon_0 r}[H_X]-Q_{\varepsilon YX}[E_X]-Q_{\varepsilon YZ}[E_Z]\right]\right)_p-\frac{E_{Z_p}}{r}-\frac{\mathrm{d}E_{Zp}}{\mathrm{d}r}=i\omega\mu\mu_0 H_{Xp}, \quad (50)$$

$$\frac{H_{Xp}}{r}+\frac{\mathrm{d}H_{Xp}}{\mathrm{d}r}=-i\omega\epsilon_0(Q_{\varepsilon ZX}[E_X])_p-i\omega\epsilon_0(Q_{\varepsilon ZZ}[E_Z])_p-i\omega\epsilon_0\left(Q_{\varepsilon ZY}Q_{\varepsilon YY}^{-1}\left(\frac{ia}{\omega\epsilon_0 r}[H_X]-Q_{\varepsilon YX}[E_X]-Q_{\varepsilon YZ}[E_Z]\right)\right)_p, \quad (51)$$

$$i\frac{a_p^2}{\omega\mu\mu_0}\frac{E_{Xp}}{r^2}+\frac{H_{Zp}}{r}+\frac{\mathrm{d}H_{Zp}}{\mathrm{d}r}=i\omega\epsilon_0(Q_{\varepsilon XX}[E_X])_p+i\omega\epsilon_0(Q_{\varepsilon XZ}[E_Z])_p+i\omega\epsilon_0\left(Q_{\varepsilon XY}Q_{\varepsilon YY}^{-1}\left(\frac{ia}{\omega\epsilon_0 r}[H_X]-Q_{\varepsilon YX}[E_X]-Q_{\varepsilon YZ}[E_Z]\right)\right)_p. \quad (52)$$

It is now useful to construct a column $[F]$ containing the unknowns of the problem, made with four blocks, each block having $(n_{\max}+1)^2$ components:

$$[F]=\begin{bmatrix}[E_X]\\ [E_Z]\\ [\tilde{H}_X]\\ [\tilde{H}_Z]\end{bmatrix}, \quad (53)$$

where the tilde means that the magnetic field is multiplied by the vacuum impedance Z_0 so that it has the same dimension as an electric field:

$$\tilde{\mathbf{H}} \equiv Z_0 \mathbf{H} = \sqrt{\frac{\mu_0}{\epsilon_0}} \mathbf{H} = \frac{1}{c\epsilon_0} \mathbf{H}. \quad (54)$$

The propagation equations, Eqs. (49)–(52), can then be written in matrix form:

$$\frac{\mathrm{d}[F]}{\mathrm{d}r} = M(r)[F], \quad (55)$$

where $M(r)$ is a square matrix made with 16 square blocks, each of them having dimension $(n_{\max}+1)^2$, which can be explicitly written as

$$M_{11} = -\frac{\mathbb{1}}{r}, \quad M_{12} = M_{13} = 0, \quad M_{14} = i\mu\frac{\omega}{c}\mathbb{1},$$

$$M_{21} = -\frac{a}{r} Q_{\varepsilon YY}^{-1} Q_{\varepsilon YX}, \quad M_{22} = -\frac{\mathbb{1}}{r} - \frac{a}{r} Q_{\varepsilon YY}^{-1} Q_{\varepsilon YZ},$$

$$M_{23} = i\frac{\omega}{c}\left(\left(\frac{c}{r\omega}\right)^2 a Q_{\varepsilon YY}^{-1} a - \mu\mathbb{1}\right), \quad M_{24} = 0,$$

$$M_{31} = i\frac{\omega}{c}(Q_{\varepsilon ZY} Q_{\varepsilon YY}^{-1} Q_{\varepsilon YX} - Q_{\varepsilon ZX}),$$

$$M_{32} = i\frac{\omega}{c}(Q_{\varepsilon ZY} Q_{\varepsilon YY}^{-1} Q_{\varepsilon YZ} - Q_{\varepsilon ZZ}),$$

$$M_{33} = \frac{1}{r}(Q_{\varepsilon ZY} Q_{\varepsilon YY}^{-1} a - \mathbb{1}), \quad M_{34} = 0,$$

$$M_{41} = i\frac{\omega}{c}\left(Q_{\varepsilon XX} - Q_{\varepsilon XY} Q_{\varepsilon YY}^{-1} Q_{\varepsilon YX} - \frac{\mathbb{1}}{\mu}\left(\frac{ac}{\omega r}\right)^2\right),$$

$$M_{42} = i\frac{\omega}{c}(Q_{\varepsilon XZ} - Q_{\varepsilon XY} Q_{\varepsilon YY}^{-1} Q_{\varepsilon YZ}),$$

$$M_{43} = -Q_{\varepsilon XY} Q_{\varepsilon YY}^{-1} \frac{a}{r}, \quad M_{44} = -\frac{\mathbb{1}}{r}, \quad (56)$$

where $\mathbb{1}$ is the unit matrix.

Equations (55) and (56) are the propagation equations. They will have to be numerically integrated across the modulated region, and the numerical solution will have to be matched with analytical expressions of the field in each homogeneous region ($r<R_1$ and $r>R_2$). It is known that such a process will determine the field everywhere. However, two difficulties are common in the process.[20] The first difficulty is the exponential growth of the numerical solutions during the integration process. This will have to be avoided by using the S-matrix propagation algorithm.[14,20] The second difficulty comes with the slow convergence of the field expansions, which requires integrating overly large sets of equations, which aggravates the exponential growth. In the case of grating theory, the difficulty has been resolved[15,16,20] by developing a technique called fast Fourier factorization (FFF), which is based on factorization rules developed by Li.[17] Such a technique has been recently extended to basis functions different from the Fourier basis[18] and is then called fast numerical factorization (FNF). It has been applied with success to the Bessel–Fourier basis used to analyze objects in cylindrical coordinates.[19] Its extension to spherical harmonics is not trivial and is described in Section 6.

6. FAST NUMERICAL FACTORIZATION APPLIED TO A SPHERICAL HARMONIC BASIS

The difficulty of slow convergence of field expansion is linked to the necessity of truncating the set of propagation equations. From a mathematical point of view, field expansions are infinite series, as stated by Eq. (21). Thus the set of Eqs. (37)–(42) should be infinite, as should be the set in Eq. (55). The truncation of Eq. (21) performed in Eq. (22) limits the range of p in Eqs. (37)–(42) to $(n_{\max+1})^2$, and the question that arises is how can D_{Yp}, D_{Xp}, and D_{Zp} in Eqs. (40)–(42) be correctly expressed in terms of E_{Yp}, E_{Xp}, and E_{Zp}.

It has been known for a long time that reconstructing a discontinuous function from its Fourier series leads to the Gibbs phenomenon, which means that, at the discontinuity points, the sum of the truncated series does not converge to the value of the function. Such a phenomenon does not exist for continuous functions, which results in the fact that continuous functions are better reconstructed by summing their truncated Fourier series than discontinuous ones. This remark was used by Li to propose factorization rules[17] that allowed a breakthrough in grating theory.[15,16,20] Extending the previous hypothesis to arbitrary basis functions, namely, that continuous functions are better reconstructed than discontinuous functions by summing their truncated expansion on an arbitrary continuous function basis, we were able to establish factorization rules valid for an arbitrary basis. We briefly recall the basic ideas here.

A. Factorization Rules

Let us consider three functions f, g, and h of a common variable x with $h=gf$ and assume that the truncation expansion of f over a continuous function basis φ_m is known: $f(x)=\Sigma_{m=1}^{N} f_m \varphi_m(x)$. The function $g(x)$ may be known explicitly or from an expansion over a different or identical function basis. The question is how to determine with the best accuracy the coefficients h_m of the development of $h=gf$ over the φ_m basis: $h(x)=\Sigma_{m=1}^{N} h_m \varphi_m(x)$. The answer depends on whether f and g are discontinuous at a same value of x or not.

1. Direct Rule

If f is a continuous function while g is discontinuous, which implies that h is discontinuous, we have

$$h_m = \langle \varphi_m | h \rangle = \langle \varphi_m | gf \rangle = \left\langle \varphi_m \middle| g \sum_p f_p \varphi_p \right\rangle. \quad (57)$$

In Eq. (57), the summation is a rapidly converging series, since f is continuous. From the linearity of the scalar product we find

$$h_m = \sum_p \langle \varphi_m | g f_p \varphi_p \rangle = \sum_p \langle \varphi_m | g \varphi_p \rangle f_p. \tag{58}$$

Defining

$$g_{mp} \equiv \langle \varphi_m | g \varphi_p \rangle, \tag{59}$$

we obtain the direct rule

$$h_m = \sum_p g_{mp} f_p. \tag{60}$$

Since the sum in Eq. (57) is rapidly converging, so is the sum in Eq. (60), which means that the h_m components are well calculated with p limited to small values. It is worth noticing that the components g_n of the function g are not involved in the direct rule. It is the g_{mp} coefficients given by Eq. (59) that are required.

2. Inverse rule

Let us now assume that f and g are functions that are discontinuous at the same point, with a continuous product h. In order to find the same situation as in Subsection 6.A.1, we then consider $f=(1/g)h$, where h is continuous and $1/g$ and f are discontinuous. We thus find

$$f_m = \langle \varphi_m | f \rangle = \left\langle \varphi_m \left| \frac{1}{g} h \right. \right\rangle = \left\langle \varphi_m \left| \frac{1}{g} \sum_p h_p \varphi_p \right. \right\rangle = \sum_p \left\langle \varphi_m \left| \frac{1}{g} \varphi_p \right. \right\rangle h_p, \tag{61}$$

which will be a rapidly converging summation. Defining

$$g_{\text{inv},mp} \equiv \left\langle \varphi_m \left| \frac{1}{g} \varphi_p \right. \right\rangle, \tag{62}$$

we obtain

$$f_m = \sum_p g_{\text{inv},mp} h_p. \tag{63}$$

Again, the fast convergence of the summation in Eq. (61) due to the continuity of h ensures that the coefficients f_m are well calculated. Inverting the relation in Eq. (63), we have

$$h_m = \sum_p [(g_{\text{inv}})^{-1}]_{mp} f_p, \tag{64}$$

which is the inverse rule.

B. Factorization Rules for Spherical Harmonic Expansions

In electromagnetism, the tangential component $\mathbf{D}_{\text{T}}$ of the displacement is the product of a discontinuous function ε by a continuous vector $\mathbf{E}_{\text{T}}$. The calculation of its component on any basis will thus require using the direct rule. On the other hand, the components of $\mathbf{D}_{\text{N}}=\hat{\mathbf{N}}(\hat{\mathbf{N}}\cdot\mathbf{D})$ will have to be obtained using the inverse rule.

1. Direct Rule

Representing both $\mathbf{D}_{\text{T}}$ and $\mathbf{E}_{\text{T}}$ by truncated expansions (21), we have

$$\mathbf{E}_{\text{T}} = \sum_{n,m} (E_{\text{T}Ynm}\mathbf{Y}_{nm} + E_{\text{T}Xnm}\mathbf{X}_{nm} + E_{\text{T}Znm}\mathbf{Z}_{nm}), \tag{65}$$

$$\mathbf{D}_{\text{T}} = \sum_{n,m} (D_{\text{T}Ynm}\mathbf{Y}_{nm} + D_{\text{T}Xnm}\mathbf{X}_{nm} + D_{\text{T}Znm}\mathbf{Z}_{nm}). \tag{66}$$

The $\mathbf{D}_{\text{T}}$ and $\mathbf{E}_{\text{T}}$ vectors are linked through the relation

$$\mathbf{D}_{\text{T}} = \epsilon_0 \varepsilon \mathbf{E}_{\text{T}}, \tag{67}$$

and we want to express this in terms of a matrix relation among their components on the spherical harmonic basis:

$$[\mathbf{D}_{\text{T}}] = \epsilon_0 \{\varepsilon^{(\text{T})}\}[\mathbf{E}_{\text{T}}], \tag{68}$$

where

$$\{\varepsilon^{(\text{T})}\} = \begin{pmatrix} \{\varepsilon_{YY}\} & \{\varepsilon_{YX}\} & \{\varepsilon_{YZ}\} \\ \{\varepsilon_{XY}\} & \{\varepsilon_{XX}\} & \{\varepsilon_{XZ}\} \\ \{\varepsilon_{ZY}\} & \{\varepsilon_{ZX}\} & \{\varepsilon_{ZZ}\} \end{pmatrix} \tag{69}$$

and each square block has dimension $(n_{\max}+1)^2$. Our aim in what follows is to explicitly determine these blocks.

As established in Appendix B, since a given $\mathbf{Y}_{nm}$ is perpendicular to all $\mathbf{X}_{\nu\mu}$ and $\mathbf{Z}_{\nu\mu}$ vectors, we have $\{\varepsilon_{YX}\}=\{\varepsilon_{XY}\}=\{\varepsilon_{YZ}\}=\{\varepsilon_{ZY}\}=0$, and $\varepsilon^{(\text{T})}$ takes the form

$$\{\varepsilon^{(\text{T})}\} = \begin{pmatrix} \{\varepsilon_{YY}\} & 0 & 0 \\ 0 & \{\varepsilon_{XX}\} & \{\varepsilon_{XZ}\} \\ 0 & \{\varepsilon_{ZX}\} & \{\varepsilon_{ZZ}\} \end{pmatrix}. \tag{70}$$

Putting Eqs. (65) and (66) in Eq. (67) above, we have

$$\sum_{n',m'} (D_{\text{T}Yn'm'}\mathbf{Y}_{n'm'} + D_{\text{T}Xn'm'}\mathbf{X}_{n'm'} + D_{\text{T}Zn'm'}\mathbf{Z}_{n'm'}) = \epsilon_0 \varepsilon(r,\theta,\phi) \sum_{\nu,\mu} (E_{\text{T}Y\nu\mu}\mathbf{Y}_{\nu\mu} + E_{\text{T}X\nu\mu}\mathbf{X}_{\nu\mu} + E_{\text{T}Z\nu\mu}\mathbf{Z}_{\nu\mu}). \tag{71}$$

If we perform an ordinary scalar product of both sides of Eq. (71) by $\mathbf{Y}^*_{nm}$, we obtain

$$\mathbf{Y}^*_{nm} \cdot \sum_{n',m'} (D_{\text{T}Yn'm'}\mathbf{Y}_{n'm'} + D_{\text{T}Xn'm'}\mathbf{X}_{n'm'} + D_{\text{T}Zn'm'}\mathbf{Z}_{n'm'}) = \epsilon_0 \varepsilon(r,\theta,\phi) \mathbf{Y}^*_{nm} \cdot \sum_{\nu,\mu} (E_{\text{T}Y\nu\mu}\mathbf{Y}_{\nu\mu} + E_{\text{T}X\nu\mu}\mathbf{X}_{\nu\mu} + E_{\text{T}Z\nu\mu}\mathbf{Z}_{\nu\mu}), \tag{72}$$

and, using the fact that

$$\mathbf{Y}^*_{nm} \cdot \mathbf{X}_{n'm'} = \mathbf{Y}^*_{nm} \cdot \mathbf{Z}_{n'm'} = \mathbf{Y}^*_{nm} \cdot \mathbf{X}_{\nu\mu} = \mathbf{Y}^*_{nm} \cdot \mathbf{Z}_{\nu\mu} = 0,$$

we find

$$\sum_{n',m'} D_{\text{T}Yn'm'} \mathbf{Y}^*_{nm} \cdot \mathbf{Y}_{n'm'} = \epsilon_0 \varepsilon(r,\theta,\phi) \sum_{\nu,\mu} E_{\text{T}Y\nu\mu} \mathbf{Y}^*_{nm} \cdot \mathbf{Y}_{\nu\mu}. \tag{73}$$

Integrating both sides of this equation over the solid angles,

$$\sum_{n',m'} D_{\mathrm{T}Yn'm'} \int_0^{4\pi} \mathrm{d}\Omega \mathbf{Y}^*_{nm} \cdot \mathbf{Y}_{n'm'}$$
$$= \epsilon_0 \sum_{\nu,\mu} E_{\mathrm{TY}_{\nu\mu}} \int_0^{4\pi} \mathrm{d}\Omega \varepsilon(r,\theta,\phi) \mathbf{Y}^*_{nm} \cdot \mathbf{Y}_{\nu\mu}, \quad (74)$$

and using the functional orthonormality of the VSHs, we then obtain

$$D_{\mathrm{TY}nm} = \epsilon_0 \sum_{\nu,\mu} E_{\mathrm{TY}\nu\mu} \int_0^{4\pi} \mathrm{d}\Omega \varepsilon(r,\theta,\phi) \mathbf{Y}^*_{nm} \cdot \mathbf{Y}_{\nu\mu}. \quad (75)$$

Defining

$$\varepsilon_{YYnm,\nu\mu} \equiv \int_0^{4\pi} \mathrm{d}\Omega \varepsilon(r,\theta,\phi) \mathbf{Y}^*_{nm} \cdot \mathbf{Y}_{\nu\mu} \equiv \langle \mathbf{Y}_{nm} | \varepsilon \mathbf{Y}_{\nu\mu} \rangle, \quad (76)$$

we find the linear relation between $D_{\mathrm{TY}nm}$ and $E_{\mathrm{TY}\nu\mu}$ reads as

$$D_{\mathrm{TY}nm} = \epsilon_0 \sum_{\nu,\mu} \varepsilon_{YYnm,\nu\mu} E_{\mathrm{TY}\nu\mu}. \quad (77)$$

Of course, the double subscripts (n,m) and (ν,μ) can, respectively, be replaced by single subscripts, p and q, using Eq. (23). Then Eq. (77) takes a compact form:

$$D_{\mathrm{TY}p} = \epsilon_0 \sum_q \varepsilon_{YYp,q} E_{\mathrm{TY}q}, \quad (78)$$

which defines the elements of the block $\{\varepsilon_{YY}\}$ and where we recall that $\{\varepsilon_{YY}\}$ is a square block with dimensions $(n_{\max}+1)^2$.

We derive the expressions of the other blocks in a similar way. Multiplying both sides of Eq. (71) now by $\mathbf{X}^*_{nm}$, we obtain

$$\mathbf{X}^*_{nm} \cdot \sum_{n',m'} (D_{\mathrm{TY}n'm'} \mathbf{Y}_{n'm'} + D_{\mathrm{TX}n'm'} \mathbf{X}_{n'm'} + D_{\mathrm{TZ}n'm'} \mathbf{Z}_{n'm'})$$
$$= \epsilon_0 \varepsilon(r,\theta,\phi) \mathbf{X}^*_{nm} \cdot \sum_{\nu,\mu} (E_{\mathrm{TY}\nu\mu} \mathbf{Y}_{\nu\mu} + E_{\mathrm{TX}\nu\mu} \mathbf{X}_{\nu\mu} + E_{\mathrm{TZ}\nu\mu} \mathbf{Z}_{\nu\mu}). \quad (79)$$

Using the fact that $\mathbf{X}^*_{nm} \cdot \mathbf{Y}_{n'm'} = \mathbf{X}^*_{nm} \cdot \mathbf{Y}_{\nu\mu} = 0$, we obtain

$$\sum_{n',m'} (D_{\mathrm{TX}n'm'} \mathbf{X}^*_{nm} \cdot \mathbf{X}_{n'm'} + D_{\mathrm{TZ}n'm'} \mathbf{X}^*_{nm} \cdot \mathbf{Z}_{n'm'})$$
$$= \epsilon_0 \varepsilon(r,\theta,\phi) \mathbf{X}^*_{nm} \cdot \sum_{\nu,\mu} (E_{\mathrm{TX}\nu\mu} \mathbf{X}_{\nu\mu} + E_{\mathrm{TZ}\nu\mu} \mathbf{Z}_{\nu\mu}). \quad (80)$$

Integrating over the solid angle Ω, we obtain

$$D_{\mathrm{TX}nm} = \epsilon_0 \sum_{\nu,\mu} \int_0^{4\pi} \mathrm{d}\Omega \varepsilon(r,\theta,\phi) \mathbf{X}^*_{nm} \cdot (E_{\mathrm{TX}\nu\mu} \mathbf{X}_{\nu\mu} + E_{\mathrm{TZ}\nu\mu} \mathbf{Z}_{\nu\mu}). \quad (81)$$

We then define

$$\varepsilon_{XXnm,\nu\mu} \equiv \int_0^{4\pi} \mathrm{d}\Omega \varepsilon(r,\theta,\phi) \mathbf{X}^*_{nm} \cdot \mathbf{X}_{\nu\mu} \equiv \langle \mathbf{X}_{nm} | \varepsilon \mathbf{X}_{\nu\mu} \rangle, \quad (82)$$

$$\varepsilon_{XZnm,\nu\mu} \equiv \int_0^{4\pi} \mathrm{d}\Omega \varepsilon(r,\theta,\phi) \mathbf{X}^*_{nm} \cdot \mathbf{Z}_{\nu\mu} \equiv \langle \mathbf{X}_{nm} | \varepsilon \mathbf{Z}_{\nu\mu} \rangle, \quad (83)$$

so that, after the single-subscript notation is introduced, Eq. (81) reduces to

$$\frac{1}{\epsilon_0} D_{\mathrm{TX}p} = \sum_q \varepsilon_{XXp,q} E_{\mathrm{TX}q} + \sum_q \varepsilon_{XZp,q} E_{\mathrm{TZ}q}, \quad (84)$$

which gives the $\{\varepsilon_{XX}\}$ and $\{\varepsilon_{XZ}\}$ blocks.

In a third step, multiplying both sides of Eq. (71) by $\mathbf{Z}^*_{nm}$, we find

$$\mathbf{Z}^*_{nm} \cdot \sum_{n',m'} (D_{\mathrm{TY}n'm'} \mathbf{Y}_{n'm'} + D_{\mathrm{TX}n'm'} \mathbf{X}_{n'm'} + D_{\mathrm{TZ}n'm'} \mathbf{Z}_{n'm'})$$
$$= \epsilon_0 \varepsilon(r,\theta,\phi) \mathbf{Z}^*_{nm} \cdot \sum_{\nu,\mu} (E_{\mathrm{TY}\nu\mu} \mathbf{Y}_{\nu\mu} + E_{\mathrm{TX}\nu\mu} \mathbf{X}_{\nu\mu} + E_{\mathrm{TZ}\nu\mu} \mathbf{Z}_{\nu\mu}), \quad (85)$$

and, using the fact that $\mathbf{Z}^*_{nm} \cdot \mathbf{Y}_{n'm'} = \mathbf{Z}^*_{nm} \cdot \mathbf{Y}_{\nu\mu} = 0$, we obtain

$$\sum_{n',m'} (D_{\mathrm{TX}n'm'} \mathbf{Z}^*_{nm} \cdot \mathbf{X}_{n'm'} + D_{\mathrm{TZ}n'm'} \mathbf{Z}^*_{nm} \cdot \mathbf{Z}_{n'm'})$$
$$= \epsilon_0 \varepsilon(r,\theta,\phi) \mathbf{Z}^*_{nm} \cdot \sum_{\nu,\mu} (E_{\mathrm{TX}\nu\mu} \mathbf{X}_{\nu\mu} + E_{\mathrm{TZ}\nu\mu} \mathbf{Z}_{\nu\mu}). \quad (86)$$

Integrating over the solid angle Ω, we obtain

$$D_{\mathrm{TZ}nm} = \epsilon_0 \sum_{\nu,\mu} \int_0^{4\pi} \mathrm{d}\Omega \varepsilon(r,\theta,\phi) \mathbf{Z}^*_{nm} \cdot (E_{\mathrm{TX}\nu\mu} \mathbf{X}_{\nu\mu} + E_{\mathrm{TZ}\nu\mu} \mathbf{Z}_{\nu\mu}). \quad (87)$$

We then define

$$\varepsilon_{ZXnm,\nu\mu} \equiv \int_0^{4\pi} \mathrm{d}\Omega \varepsilon(r,\theta,\phi) \mathbf{Z}^*_{nm} \cdot \mathbf{X}_{\nu\mu} \equiv \langle \mathbf{Z}_{nm} | \varepsilon \mathbf{X}_{\nu\mu} \rangle, \quad (88)$$

$$\varepsilon_{ZZnm,\nu\mu} \equiv \int_0^{4\pi} \mathrm{d}\Omega \varepsilon(r,\theta,\phi) \mathbf{Z}^*_{nm} \cdot \mathbf{Z}_{\nu\mu} \equiv \langle \mathbf{Z}_{nm} | \varepsilon \mathbf{Z}_{\nu\mu} \rangle. \quad (89)$$

After introducing the simplified subscript notation, we find that Eq. (87) reduces to

$$\frac{1}{\epsilon_0} D_{\mathrm{TZ}P} = \sum_q \varepsilon_{ZXp,q} E_{\mathrm{TX}q} + \sum_q \varepsilon_{ZZp,q} Z_{\mathrm{TX}q}, \quad (90)$$

which gives the elements of the $\{\varepsilon_{ZX}\}$ and $\{\varepsilon_{ZZ}\}$ blocks. It is worth noticing a simplification that comes from the expression of $\mathbf{X}_{nm}$ and $\mathbf{Z}_{nm}$ established in Eqs. (16) and (17). It is straightforward to verify that $\mathbf{X}^*_{nm} \cdot \mathbf{X}_{\nu\mu} = \mathbf{Z}^*_{nm} \cdot \mathbf{Z}_{\nu\mu}$ and that $\mathbf{X}^*_{nm} \cdot \mathbf{Z}_{\nu\mu} = -\mathbf{Z}^*_{nm} \cdot \mathbf{X}_{\nu\mu}$. From Eqs. (82), (83), (88), and (89), we then obtain

$$\{\varepsilon_{XX}\} = \{\varepsilon_{ZZ}\}, \quad \{\varepsilon_{XZ}\} = -\{\varepsilon_{ZX}\}. \quad (91)$$

In summary, the matrix $\{\varepsilon^{(\mathrm{T})}\}$ in Eq. (70) will include the following blocks:

$$\{\varepsilon^{(\mathrm{T})}\} = \begin{pmatrix} \{\varepsilon_{YY}\} & 0 & 0 \\ 0 & \{\varepsilon_{XX}\} & \{\varepsilon_{XZ}\} \\ 0 & -\{\varepsilon_{XZ}\} & \{\varepsilon_{XX}\} \end{pmatrix}. \tag{92}$$

Considering Eqs. (76), (82), (83), (88), and (89), we remark that the blocks of the matrix in Eqs. (68) and (69) can be expressed in the concise form $\varepsilon_{ij,nm,\nu\mu} = \langle \mathbf{W}_{nm}^{(i)} | \varepsilon \mathbf{W}_{\nu\mu}^{(j)} \rangle$, with $i, j = 1, 2, 3$ and $\varepsilon_{11} \equiv \varepsilon_{YY}$, $\varepsilon_{23} \equiv \varepsilon_{XZ}$, etc. Furthermore, Eqs. (91) and (92) can be seen as specifying certain interesting properties of these matrix elements.

2. Inverse Rule

Concerning the normal components $\mathbf{D}_\mathrm{N}$ and $\mathbf{E}_\mathrm{N}$ of $\mathbf{D}$ and $\mathbf{E}$, which are related by

$$\mathbf{D}_\mathrm{N} = \epsilon_0 \varepsilon \mathbf{E}_\mathrm{N}, \tag{93}$$

we want to find the matrix relation that links their components in the form

$$[\boldsymbol{D}_\mathrm{N}] = \epsilon_0 \{\varepsilon^{(\mathrm{N})}\} [\boldsymbol{E}_\mathrm{N}], \tag{94}$$

where, for the same reasons as pointed out for $\{\varepsilon^{(\mathrm{T})}\}$, $\{\varepsilon^{(\mathrm{N})}\}$ will have the following block structure:

$$\{\varepsilon^{(\mathrm{N})}\} = \begin{pmatrix} \{\varepsilon_{YY}^{(\mathrm{N})}\} & 0 & 0 \\ 0 & \{\varepsilon_{XX}^{(\mathrm{N})}\} & \{\varepsilon_{XZ}^{(\mathrm{N})}\} \\ 0 & -\{\varepsilon_{XZ}^{(\mathrm{N})}\} & \{\varepsilon_{XX}^{(\mathrm{N})}\} \end{pmatrix}. \tag{95}$$

From Eq. (93), we have $\mathbf{E}_\mathrm{N} = (1/\epsilon_0 \varepsilon) \mathbf{D}_\mathrm{N}$ where $1/\varepsilon$ is discontinuous while $\mathbf{D}_\mathrm{N}$ is continuous. Thus the direct rule has to be used to calculate the components of $\mathbf{E}_\mathrm{N}$ from those of $1/\varepsilon$ and $\mathbf{D}_\mathrm{N}$. Following the line stated in Subsection 6.A.2 and similar to Eq. (71), we write

$$\sum_{n',m'} (E_{\mathrm{NY}n'm'} \mathbf{Y}_{n'm'} + E_{\mathrm{NX}n'm'} \mathbf{X}_{n'm'} + E_{\mathrm{NZ}n'm'} \mathbf{Z}_{n'm'}) = \frac{1}{\epsilon_0 \varepsilon(r,\theta,\phi)} \sum_{\nu,\mu} (D_{\mathrm{NY}\nu\mu} \mathbf{Y}_{\nu\mu} + D_{\mathrm{NX}\nu\mu} \mathbf{X}_{\nu\mu} + D_{\mathrm{NZ}\nu\mu} \mathbf{Z}_{\nu\mu}). \tag{96}$$

We continue the process as we did for obtaining Eqs. (76) and (77); defining

$$\left(\frac{1}{\varepsilon}\right)_{YYnm;\nu\mu} \equiv \int_0^{4\pi} \mathrm{d}\Omega \frac{1}{\varepsilon(r,\theta,\phi)} \mathbf{Y}_{nm}^* \cdot \mathbf{Y}_{\nu\mu} \equiv \left\langle \mathbf{Y}_{nm} \middle| \frac{1}{\varepsilon} \mathbf{Y}_{\nu\mu} \right\rangle, \tag{97}$$

we obtain

$$\epsilon_0 E_{\mathrm{NY}nm} = \sum_{\nu\mu} \left(\frac{1}{\varepsilon}\right)_{YYnm,\nu\mu} D_{\mathrm{NY}\nu\mu} \tag{98}$$

or, with the single subscript,

$$\epsilon_0 E_{\mathrm{NY}p} = \sum_q \left(\frac{1}{\varepsilon}\right)_{YYp,q} D_{\mathrm{NY}q}. \tag{99}$$

Inversing this relation, we obtain an equation identical to the inverse rule in Eq. (64) that we established for scalar functions:

$$D_{\mathrm{NY}p} = \epsilon_0 \sum_q \left[\left(\frac{1}{\varepsilon}\right)_{YY}^{-1} \right]_{p,q} E_{\mathrm{NY}q}, \tag{100}$$

which is to be expected, since $D_{\mathrm{NY}q}$ depend only on $E_{\mathrm{NY}q}$ and thus behave like scalars. Equation (100) provides the first block in $\{\varepsilon^{(\mathrm{N})}\}$:

$$\{\varepsilon_{YY}^{(\mathrm{N})}\} = \left(\left(\frac{1}{\varepsilon}\right)_{YY} \right)^{-1}. \tag{101}$$

Things are a bit more complicated for the other blocks, since both $[D_\mathrm{NX}]$ and $[D_\mathrm{NZ}]$ depend on $[E_\mathrm{NX}]$ and $[E_\mathrm{NZ}]$. But, following the same lines, we obtain

$$\epsilon_0 E_{\mathrm{NX}nm} = \sum_{\nu,\mu} \left(\frac{1}{\varepsilon}\right)_{XXnm,\nu\mu} D_{\mathrm{NX}\nu\mu} + \sum_{\nu,\mu} \left(\frac{1}{\varepsilon}\right)_{XZnm,\nu\mu} D_{\mathrm{NZ}\nu\mu}, \tag{102}$$

where

$$\left(\frac{1}{\varepsilon}\right)_{XXnm,\nu\mu} \equiv \left\langle \mathbf{X}_{nm} \middle| \frac{1}{\varepsilon} \mathbf{X}_{\nu\mu} \right\rangle, \tag{103}$$

$$\left(\frac{1}{\varepsilon}\right)_{XZnm,\nu\mu} \equiv \left\langle \mathbf{X}_{nm} \middle| \frac{1}{\varepsilon} \mathbf{Z}_{\nu\mu} \right\rangle. \tag{104}$$

Put in matrix form, Eq. (102) reads as

$$\epsilon_0 [E_\mathrm{NX}] = \left(\frac{1}{\varepsilon}\right)_{XX} [D_\mathrm{NX}] + \left(\frac{1}{\varepsilon}\right)_{XZ} [D_\mathrm{NZ}], \tag{105}$$

which, with the help of Eq. (95), gives

$$\epsilon_0 [E_\mathrm{NZ}] = -\left(\frac{1}{\varepsilon}\right)_{XZ} [D_\mathrm{NX}] + \left(\frac{1}{\varepsilon}\right)_{XX} [D_\mathrm{NZ}]. \tag{106}$$

Inverting Eqs. (105) and (106) leads to

$$\begin{bmatrix} [D_\mathrm{NX}] \\ [D_\mathrm{NZ}] \end{bmatrix} = \epsilon_0 \begin{pmatrix} \left(\frac{1}{\varepsilon}\right)_{XX} & \left(\frac{1}{\varepsilon}\right)_{XZ} \\ -\left(\frac{1}{\varepsilon}\right)_{XZ} & \left(\frac{1}{\varepsilon}\right)_{XX} \end{pmatrix}^{-1} \begin{bmatrix} [E_\mathrm{NX}] \\ [E_\mathrm{NZ}] \end{bmatrix}, \tag{107}$$

and Eq. (95) reads as

$$\{\varepsilon^{(\mathrm{N})}\} = \begin{pmatrix} \{\varepsilon_{YY}^{(\mathrm{N})}\} & 0 & 0 \\ 0 & \{\varepsilon_{XX}^{(\mathrm{N})}\} & \{\varepsilon_{XZ}^{(\mathrm{N})}\} \\ 0 & -\{\varepsilon_{XZ}^{(\mathrm{N})}\} & \{\varepsilon_{XX}^{(\mathrm{N})}\} \end{pmatrix} = \begin{pmatrix} \left(\left(\frac{1}{\varepsilon}\right)_{YY}\right)^{-1} & 0 & 0 \\ 0 & \multicolumn{2}{c}{\begin{pmatrix} \left(\frac{1}{\varepsilon}\right)_{XX} & \left(\frac{1}{\varepsilon}\right)_{XZ} \\ -\left(\frac{1}{\varepsilon}\right)_{XZ} & \left(\frac{1}{\varepsilon}\right)_{XX} \end{pmatrix}^{-1}} \\ 0 & & \end{pmatrix}. \tag{108}$$

Equations (94) and (108), together with Eqs. (97), (103), and (104), state the inverse rule that applies to the vectorial functions **D** and **E** represented on the basis of VSHs.

The determination of the various blocks of $\{\varepsilon^{(\mathrm{T})}\}$ and $\{\varepsilon^{(\mathrm{N})}\}$ requires computing integrals involving scalar products of two VSHs, as shown in Eqs. (82) and (83), for example. The introduction of the Gaunt coefficients[23] developed by theoreticians working in quantum mechanics gives analytic expressions for these integrals. This is explained in Appendix D.

C. Total Field Representation: Fast Numerical Factorization Applied to Spherical Harmonic Basis

The concept of normal and tangential components of **E** or **D** is defined only on a surface S, whereas the direct and inverse rules have to be applied into the entire modulated region in order to calculate the **D** components on the VSHs. The basic idea of what was first called the fast Fourier factorization (FFF) in grating theory[16,20] consisted of extending the definition of $\hat{\mathbf{N}}$ stated by Eq. (26) toward the entire modulated area by simply stating that

$$\forall r \in [R_1, R_2], \quad \hat{\mathbf{N}}(r,\theta,\phi) = \left.\frac{\mathbf{grad}\, f}{\|\mathbf{grad}\, f\|}\right|_{f=0}. \tag{109}$$

Equation (109) allows one to derive a normal component $\mathbf{E}_{\mathrm{N}}$ of the field E via

$$\mathbf{E}_{\mathrm{N}} = \hat{\mathbf{N}}(\hat{\mathbf{N}}\cdot\mathbf{E}), \tag{110}$$

and its tangential component, $\mathbf{E}_{\mathrm{T}}$, is given by

$$\mathbf{E}_{\mathrm{T}} = \mathbf{E} - \mathbf{E}_{\mathrm{N}} = \mathbf{E} - \hat{\mathbf{N}}(\hat{\mathbf{N}}\cdot\mathbf{E}); \tag{111}$$

these definitions hold in the entire modulated area. Dealing with an isotropic medium then leads to

$$\mathbf{D} = \epsilon_0\varepsilon\mathbf{E} = \epsilon_0\varepsilon(\mathbf{E}_{\mathrm{T}} + \mathbf{E}_{\mathrm{N}}) = \epsilon_0\varepsilon(\mathbf{E} - \hat{\mathbf{N}}(\hat{\mathbf{N}}\cdot\mathbf{E})) + \epsilon_0\varepsilon\hat{\mathbf{N}}(\hat{\mathbf{N}}\cdot\mathbf{E}). \tag{112}$$

Expressing the components of $\mathbf{D}_{\mathrm{T}} = \epsilon_0\varepsilon(\mathbf{E} - \hat{\mathbf{N}}(\hat{\mathbf{N}}\cdot\mathbf{E}))$ implies the direct rule that requires $\{\varepsilon^{(\mathrm{T})}\}$, whereas the components of $\mathbf{D}_{\mathrm{N}} = \epsilon_0\varepsilon\hat{\mathbf{N}}(\hat{\mathbf{N}}\cdot\mathbf{E})$ requires the inverse rule and thus requires $\{\varepsilon^{(\mathrm{N})}\}$. Introducing the matrix $\{\hat{\mathbf{N}}\hat{\mathbf{N}}\}$, with nine blocks $\{N_iN_j\}$, with i and j equal to Y, X, and Z, which relates $[E]$ to $[E_{\mathrm{N}}]$, we thus have

$$\begin{aligned}\frac{1}{\epsilon_0}[D] &= \{\varepsilon^{(\mathrm{T})}\}[E_{\mathrm{T}}] + \{\varepsilon^{(\mathrm{N})}\}[E_{\mathrm{N}}] \\ &= (\{\varepsilon^{(\mathrm{T})}\}(\mathbb{1} - \{\hat{\mathbf{N}}\hat{\mathbf{N}}\}) + \{\varepsilon^{(\mathrm{N})}\}\{\hat{\mathbf{N}}\hat{\mathbf{N}}\})[E].\end{aligned} \tag{113}$$

As a result, matrix Q_ε defined in Eq. (44) reads

$$Q_\varepsilon = \{\varepsilon^{(\mathrm{T})}\} + (\{\varepsilon^{(\mathrm{N})}\} - \{\varepsilon^{(\mathrm{T})}\})\{\hat{\mathbf{N}}\hat{\mathbf{N}}\},$$

an equation that has to be interpreted in block form as

$$Q_{\varepsilon ij} = \{\varepsilon^{(\mathrm{T})}_{ij}\} + \sum_k (\{\varepsilon^{(\mathrm{N})}_{ik}\} - \{\varepsilon^{(\mathrm{T})}_{ik}\})\{\hat{\mathbf{N}}_k\hat{\mathbf{N}}_j\}. \tag{114}$$

In order to state explicitly the various blocks, we first introduce the matrix $\Delta \equiv \{\varepsilon^{(\mathrm{N})}\} - \{\varepsilon^{(\mathrm{T})}\}$, with blocks $\Delta_{ij} = \{\varepsilon^{(\mathrm{N})}_{ij}\} - \{\varepsilon^{(\mathrm{T})}_{ij}\}$, which reads

$$\Delta = \begin{pmatrix} \Delta_{YY} & 0 & 0 \\ 0 & \Delta_{XX} & \Delta_{XZ} \\ 0 & -\Delta_{XZ} & \Delta_{XX} \end{pmatrix}. \tag{115}$$

Thus, finally, Q_ε has the following blocks:

$$\begin{aligned}
&Q_{\varepsilon YY} = \Delta_{YY}\{N_YN_Y\} + \{\varepsilon_{YY}\}, \quad Q_{\varepsilon YX} = \Delta_{YY}\{N_YN_X\}, \\
&Q_{\varepsilon YZ} = \Delta_{YY}\{N_YN_Z\}, \\
&Q_{\varepsilon XY} = \Delta_{XX}\{N_XN_Y\} + \Delta_{XZ}\{N_ZN_Y\}, \\
&Q_{\varepsilon XX} = \Delta_{XX}\{N_XN_X\} + \Delta_{XZ}\{N_ZN_X\} + \{\varepsilon_{XX}\}, \\
&Q_{\varepsilon XZ} = \Delta_{XX}\{N_XN_Z\} + \Delta_{XZ}\{N_ZN_Z\} + \{\varepsilon_{XZ}\}, \\
&Q_{\varepsilon ZY} = \Delta_{XX}\{N_ZN_Y\} - \Delta_{XZ}\{N_XN_Y\}, \\
&Q_{\varepsilon ZX} = \Delta_{XX}\{N_ZN_X\} - \Delta_{XZ}\{N_XN_X\} - \{\varepsilon_{XZ}\}, \\
&Q_{\varepsilon ZZ} = \Delta_{XX}\{N_ZN_Z\} - \Delta_{XZ}\{N_XN_Z\} + \{\varepsilon_{XX}\}.
\end{aligned} \tag{116}$$

The differential set written in Eqs. (55) and (56) with matrix Q_ε given by Eqs. (116) is the fast converging formulation of the Maxwell equations projected onto a truncated spherical harmonic basis, and the way of deriving them is the fast numerical factorization (FNF) in spherical coordinates.

7. FIELD EXPANSIONS OUTSIDE THE MODULATED REGION

Inside a homogeneous isotropic medium characterized by the relative electric and magnetic permitivities, ε_j and μ_j, the two Maxwell curl equations result in a second-order propagation equation involving the electric field:

$$\mathbf{curl}(\mathbf{curl}\,\mathbf{E}) - (\omega/c)^2\varepsilon_j\mu_j\mathbf{E} = \mathbf{0}. \tag{117}$$

In a source-free medium, div $\mathbf{E} = \mathbf{0}$, and Eq. (117) leads to the vector Helmholtz equation:

$$\mathbf{\Delta E} + k_j^2\mathbf{E} = \mathbf{0}, \tag{118}$$

where

$$k_j^2 = (\omega/c)^2\varepsilon_j\mu_j. \tag{119}$$

Classical textbooks[1] explain how to construct the general solution of Eq. (117). Searching for a general vectorial solution of the form $\mathbf{M} \propto \mathbf{curl}(\mathrm{r}\psi)$ and expressing the Laplacian operator in spherical coordinates, we find that ψ is a solution of the scalar Helmholtz equation:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + k_j^2\psi = 0. \tag{120}$$

Expressing ψ on the basis of scalar spherical harmonics,

$$\psi(r,\theta,\phi) = \sum_{n,m} R(r)Y_{nm}(\theta,\phi), \tag{121}$$

we find that $R(r)$ verifies

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right)+[k_j^2r^2-n(n+1)]R(r)=0. \quad (122)$$

Introducing the dimensionless variable $\rho \equiv k_j r$ and the function $\check{R}\equiv R\sqrt{\rho}$ we find that Eq. (122) leads to

$$\frac{\mathrm{d}^2\check{R}}{\mathrm{d}^2\rho}+\frac{1}{\rho}\frac{\mathrm{d}\check{R}}{\mathrm{d}\rho}+\left[1-\frac{\left(n+\frac{1}{2}\right)^2}{\rho^2}\right]\check{R}(\rho)=0. \quad (123)$$

Equation (123) is the Bessel equation with half-integer order $n+1/2$; its independent solutions are thus the half-integer Bessel functions $\check{R}=J_{n+1/2}(\rho)$ and $Y_{n+1/2}(\rho)$ or Hankel functions $\check{R}=H^+_{n+1/2}(\rho)$ and $H^-_{n+1/2}(\rho)$. Consequently, linearly independent solutions of Eq. (122) are called spherical Bessel functions and are defined by

$$R(r)=j_n(k_jr)\equiv\sqrt{\frac{\pi}{2k_jr}}J_{n+1/2}(k_jr),$$
$$R(r)=y_n(k_jr)\equiv\sqrt{\frac{\pi}{2k_jr}}Y_{n+1/2}(k_jr), \quad (124)$$

where the factor $\sqrt{\pi/2}$ is introduced for convenience.

Any combination of $j_n(\rho)$ and $y_n(\rho)$ is also a solution to Eq. (122). Two such combinations deserve special attention, which are called spherical Bessel functions of the third and fourth kind, or spherical Hankel functions:

$$h_n^+(\rho)=j_n(\rho)+iy_n(\rho),$$
$$h_n^-(\rho)=j_n(\rho)-iy_n(\rho). \quad (125)$$

It will be useful to designate one of the four spherical Bessel functions by the generic notation $z_n(k_jr)$. Following Eqs. (121)–(125), ψ can be expressed as a series of elementary functions ψ_{nm}, with

$$\psi_{nm}(r,\theta,\varphi)=z_n(k_jr)Y_{nm}(\theta,\phi). \quad (126)$$

Each ψ_{nm} can be used to generate a solution to Eq. (117) (frequently called a vector spherical wave function):

$$\mathbf{M}_{nm}\equiv\frac{\mathbf{curl}(\mathrm{r}\psi_{nm})}{\sqrt{n(n+1)}}. \quad (127)$$

From $\mathbf{M}_{nm}$, a second solution to Eq. (117) can be constructed[1] by taking $\mathbf{N}_{nm}\equiv\mathbf{curl}\,\mathbf{M}_{nm}/k_j$. Classical textbooks[1] then establish that one can write

$$\mathbf{M}_{nm}(\rho,\theta,\phi)=z_n(\rho)\mathbf{X}_{nm}(\theta,\phi), \quad (128)$$

$$\mathbf{N}_{nm}(\rho,\theta,\phi)=\frac{1}{\rho}\{\sqrt{n(n+1)}z_n(\rho)\mathbf{Y}_{nm}(\theta,\phi)+[\rho z_n(\rho)]'\mathbf{Z}_{nm}(\theta,\phi)\}, \quad (129)$$

where the prime here, and from here on, is a shorthand for expressing derivatives with respect to the argument of the Bessel function; i.e., explicitly we have

$$f'(x_0)\equiv\left.\frac{\mathrm{d}}{\mathrm{d}x}f(x)\right|_{x=x_0}. \quad (130)$$

From Eq. (128) and (129), it is established that $\mathbf{N}_{nm}(\rho)$ are orthogonal to $\mathbf{M}_{nm}(\rho)$ and are thus linearly independent. As a result, the general solution of the propagation equation inside a homogeneous medium, Eq. (117), can be written as

$$\mathbf{E}(\mathrm{r})=\sum_{n,m}\left\{A^{(j)}_{h,nm}j_n(k_jr)\mathbf{X}_{nm}+\frac{A^{(j)}_{e,nm}}{k_jr}\times[\sqrt{n(n+1)}j_n(k_jr)\mathbf{Y}_{nm}+(k_jrj_n(k_jr))'\mathbf{Z}_{nm}]\right\}+\sum_{n,m}\left\{B^{(j)}_{h,nm}h_n^+(k_jr)\mathbf{X}_{nm}+\frac{B^{(j)}_{e,nm}}{k_jr}\times[\sqrt{n(n+1)}h_n^+(k_jr)\mathbf{Y}_{nm}+(k_jrh_n^+(k_jr))'\mathbf{Z}_{nm}]\right\}. \quad (131)$$

The coefficients $A^{(j)}_{h,nm}$, $A^{(j)}_{e,nm}$, and $B^{(j)}_{h,nm}$, $B^{(j)}_{e,nm}$, play in the 3D scattering problem the same role as Rayleigh coefficients in grating theory.[20] The choice made among the $z_n(k_jr)$ functions allows one to distinguish the terms that remain bounded at the coordinate origin (corresponding to $A^{(j)}_{h,nm}$, $A^{(j)}_{e,nm}$,) from terms that correspond to outgoing waves or waves decaying at infinity (corresponding to $B^{(j)}_{h,nm}$, $B^{(j)}_{e,nm}$,).

The general expression for **E** in Eq. (131) is applicable to the inner region ($r\leqslant R_1$) and the outer region ($r>R_2$). For $r\leqslant R_1$, in order to obtain a solution that remains bounded, we impose

$$B^{(1)}_{e,nm}=0=B^{(1)}_{h,nm}\quad\forall\, n,m. \quad (132)$$

Let us introduce the Ricatti–Bessel functions, $\psi_n(z)$ and $\xi_n(z)$, defined in Appendix E, so that Eq. (131) for $r\leqslant R_1$ reduces to

$$\mathbf{E}=\sum_{n,m}\left\{A^{(1)}_{h,nm}j_n(k_1r)\mathbf{X}_{nm}+\frac{A^{(1)}_{e,nm}}{k_1r}\times[\sqrt{n(n+1)}j_n(k_1r)\mathbf{Y}_{nm}+\psi_n'(k_1r)\mathbf{Z}_{nm}]\right\}. \quad (133)$$

On the other hand, if $r>R_2$, the field must be the sum of the diffracted field, expressed by the second summation in Eq. (131), and the incident field. This means that the first summation in Eq. (131) must here reduce to the incident field, with coefficients denoted $A^{\mathrm{i}}_{h,nm}$, and $A^{\mathrm{i}}_{e,nm}$. Expressed in terms of the polarization vector, $\hat{\mathrm{e}}_{\mathrm{i}}$, these coefficients for an incident plane wave $\mathbf{E}_{\mathrm{i}}=\exp(i\mathbf{k}_M\cdot\mathbf{r})\hat{\mathbf{e}}_{\mathrm{i}}$ have analytic expressions[2,6,24]:

$$A^{\mathrm{i}}_{h,nm}=4\pi i^n\mathbf{X}^*_{nm}(\theta_{\mathrm{i}},\phi_{\mathrm{i}})\cdot\hat{\mathbf{e}}_{\mathrm{i}}, \quad (134)$$

$$A^{\mathrm{i}}_{e,nm}=4\pi i^{n-1}\mathbf{Z}^*_{nm}(\theta_{\mathrm{i}},\phi_{\mathrm{i}})\cdot\hat{\mathbf{e}}_{\mathrm{i}}, \quad (135)$$

where θ_{i} and ϕ_{i} specify the direction of the incident wave, $\theta_{\mathrm{i}}=|(\hat{\mathbf{z}},\mathbf{k}_M)|$, with $\theta_{\mathrm{i}}\in[0,\pi]$, and $\phi_{\mathrm{i}}=(\hat{\mathbf{x}},\mathbf{k}_{Mt})$, where $\mathbf{k}_{Mt}$ is the projection of $\mathbf{k}_M$ on the xOy plane while $\hat{\mathbf{z}}$ and $\hat{\mathbf{x}}$ are the unit vectors of the z and x axes. It could be useful to notice that in order to be able to analyze a circularly polarized incident plane wave, we allow $\hat{\mathbf{e}}_{\mathrm{i}}$ to be a complex unit vector. Defining $k_M=(\omega/c)\sqrt{\varepsilon_M\mu_M}$, we find that the field for $r\geqslant R_2$ reads as

$$\mathbf{E}=\sum_{n,m}\left\{A^{\mathrm{i}}_{h,nm}j_n(k_Mr)\mathbf{X}_{nm}+\frac{A^{\mathrm{i}}_{e,nm}}{k_Mr}\times[\sqrt{n(n+1)}j_n(k_Mr)\mathbf{Y}_{nm}+\psi_n'(k_Mr)\mathbf{Z}_{nm}]\right\}+\sum_{n,m}\left\{B^{(M)}_{h,nm}h^+_n(k_Mr)\mathbf{X}_{nm}+\frac{B^{(M)}_{e,nm}}{k_Mr}\times[\sqrt{n(n+1)}h^+_n(k_Mr)\mathbf{Y}_{nm}+\xi_n'(k_Mr)\mathbf{Z}_{nm}]\right\}. \quad (136)$$

8. RESOLUTION OF THE BOUNDARY-VALUE PROBLEM

The problem is now reduced to the numerical integration on the $[R_1,R_2]$ interval of the first-order differential set stated by Eqs. (55), (56), and (114)–(116) in such a way that the numerical solution matches the boundary conditions stated by Eqs. (133) and (136), concerning both the unknown functions and their derivatives. When dealing with objects far different from a sphere, the distance R_2-R_1 can be large enough so that numerical overflows and instabilities may appear. It is then safer to make a partition of the modulated region and to use the S-matrix propagation algorithm.

A. Partition of the Modulated Area and *S*-Matrix Propagation Algorithm

We follow a process similar to that performed in grating theory.[20] As illustrated in Fig. 2 for an example with $M=6$, the modulated region with thickness R_2-R_1 is cut into $M-1$ slices with equal thicknesses at radial distances $r_j=R_1+[(R_2-R_1)/(M-2)](j-1)$, so that $r_1=R_1$ and $r_{M-1}=R_2$. With this partition, a region labeled by the subscript j lies between r_{j-1} and r_j, region 1 lying between 0 and R_1, while region M extends from $r_{M-1}(\equiv R_2)$ toward infinity. At each distance $r_j(j>1)$, we introduce infinitely thin slices of a medium with electric and magnetic permittivity ε_M and μ_M. In each of these infinitely thin homogeneous regions, the general expansion in Eq. (131) fully defines the field, provided that k_j is taken equal to k_M, that

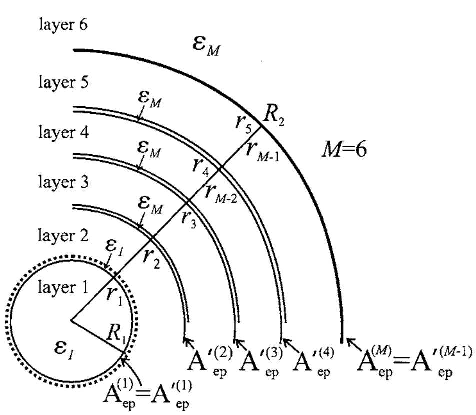

Fig. 2. Example of the partition of the modulated region in which $M=6$, and an illustration of the notation for the coefficients appearing in Eq. (131) used inside the various homogeneous regions.

$r=r_j$, and that we use primed coefficients (see Ref. 20 and the following paragraph for a discussion of the primed coefficients). We thus consider a column matrix $V^{(j)}$ constructed with the Z and X components of the impinging and outgoing waves, defined by

$$[V^{(j)}]=\begin{bmatrix}\vdots\\ A'^{(j)}_{e,p}\psi_n'(k_Mr_j)/(k_Mr_j)\\ \vdots\\ A'^{(j)}_{h,p}j_n(k_Mr_j)\\ \vdots\\ B'^{(j)}_{e,p}\xi_n'(k_Mr_j)/(k_Mr_j)\\ \vdots\\ B'^{(j)}_{h,p}h^+_n(k_Mr_j)\\ \vdots\end{bmatrix}, \quad (137)$$

where p is related to (n,m) through Eq. (23). One should note that the prime on the coefficients serves as a reminder that the field is developed inside one of the infinitesimal homogeneous slices within the modulated region (the prime on the coefficients does not stand for the derivative). Inside the circumscribed sphere, the field is developed in a truly homogeneous region and

$$A'^{(1)}_{e,p}=A^{(1)}_{e,p};\quad A'^{(1)}_{h,p}=A^{(1)}_{h,p};\quad B'^{(1)}_{e,p}=B^{(1)}_{e,p};\quad B'^{(1)}_{h,p}=B^{(1)}_{h,p}, \quad (138)$$

while

$$A'^{(M-1)}_{e,p}=A^{(M)}_{e,p};\quad A'^{(M-1)}_{h,p}=A^{(M)}_{h,p};\quad B'^{(M-1)}_{e,p}=B^{(M)}_{e,p}; \quad (139)$$

$$B'^{(M-1)}_{h,p}=B^{(M)}_{h,p}.$$

Since we are working in linear optics, there exists a linear relation between the field at ordinate r_{j-1} and the field at ordinate r_j. We thus have

$$[V^{(j)}]=T^{(j)}[V^{(j-1)}], \quad (140)$$

a relation that defines the transmission matrix, $T^{(j)}$, of the region (j) (not to be confused with the transfer matrix of the object).

When the four-block S matrix of the stack including j regions (not to be confused with the S matrix of the jth region nor with the S matrix of scattering theory!) is defined by

$$\begin{bmatrix} \vdots \\ B'^{(j)}_{e,p}\xi'_n(k_M r_j)/(k_M r_j) \\ \vdots \\ B'^{(j)}_{h,p}h^+_n(k_M r_j) \\ \vdots \\ \text{—} \\ \vdots \\ A^{(1)}_{e,p}\psi'_n(k_1 r_1)/(k_1 r_1) \\ \vdots \\ A^{(1)}_{h,p}j_n(k_1 r_1) \\ \vdots \end{bmatrix} = \begin{pmatrix} S^{(j)}_{11} & S^{(j)}_{12} \\ \text{—} & \text{—} \\ S^{(j)}_{21} & S^{(j)}_{22} \end{pmatrix} \times \begin{bmatrix} \vdots \\ B^{(1)}_{e,q}\xi'_n(k_1 r_1)/(k_1 r_1) \\ \vdots \\ B^{(1)}_{h,q}h^+_n(k_1 r_1) \\ \vdots \\ \text{—} \\ \vdots \\ A'^{(j)}_{e,q}\psi'_n(k_M r_j)/(k_M r_j) \\ \vdots \\ A'^{(j)}_{h,q}j_n(k_M r_j) \\ \vdots \end{bmatrix}, \tag{141}$$

the S-matrix propagation algorithm[14,20] reads as

$$S^{(j)}_{12} = (T^{(j)}_{21} + T^{(j)}_{22}S^{(j-1)}_{12})Z^{(j-1)}, \tag{142}$$

$$S^{(j)}_{22} = S^{(j-1)}_{22}Z^{(j-1)}, \tag{143}$$

where

$$Z^{(j-1)} = (T^{(j)}_{11} + T^{(j)}_{12}S^{(j-1)}_{12})^{-1}. \tag{144}$$

The recursive evaluation for the $S^{(j)}$ matrices is started[20] by taking $S^{(1)}_{12}=0$ and $S^{(1)}_{22}=\mathbb{1}$, which means that when there is no boundary, no reflection occurs, and the transmission is unity. Each recursive step requires the corresponding $T^{(j)}$ matrix, which is determined through the following shooting method.

B. Shooting Method: Determination of the $T^{(j)}$ Matrices

Considering the jth region, we have to integrate numerically, from r_{j-1} to r_j, the differential set stated by Eqs. (55), (56), and (116) in order to construct the matrix $T^{(j)}$. However, Eq. (55) deals with the column $[F]$, while $T^{(j)}$ links columns $[V^{(j)}]$. The first step is to express the link between these two columns via a matrix $\Psi(r)$.

Indeed, at any value of $r_j (j \neq 1)$, from Eq. (131) we have

$$[E_X]_p = A'^{(j)}_{h,p}j_n(k_M r_j) + B'^{(j)}_{h,p}h^+_n(k_M r_j), \tag{145}$$

$$[E_Z]_p = \frac{1}{k_M r_j}\{A'^{(j)}_{e,p}\psi'_n(k_M r_j) + B'^{(j)}_{e,p}\xi'_n(k_M r_j)\}. \tag{146}$$

Equations (38), (54), and (131) yield

$$\begin{aligned}[\tilde{H}_X]_p = \frac{1}{i\omega\mu_M\sqrt{\epsilon_0\mu_0}}\Bigg\{ & \frac{n(n+1)}{k_M r_j^2}[A'^{(j)}_{e,p}j_n(k_M r_j) + B'^{(j)}_{e,p}h^+_n(k_M r_j)] \\ & - \frac{1}{k_M r_j^2}[A'^{(j)}_{e,p}\psi'_n(k_M r_j) + B'^{(j)}_{e,p}\xi'_n(k_M r_j)] \\ & - \frac{\mathrm{d}}{\mathrm{d}r}\left[A'^{(j)}_{e,p}\frac{\psi'_n(k_M r_j)}{k_M r_j} + B'^{(j)}_{e,p}\frac{\xi'_n(k_M r_j)}{k_M r_j}\right]\Bigg\} \\ = \frac{1}{i\omega\mu_M\sqrt{\epsilon_0\mu_0}}\frac{1}{k_M r_j^2}\Big\{ & n(n+1)[A'^{(j)}_{e,p}j_n(k_M r_j) \\ & + B'^{(j)}_{e,p}h^+_n(k_M r_j)] - [A'^{(j)}_{e,p}(k_M r_j)^2 j'_n(k_M r_j) \\ & + B'^{(j)}_{e,p}(k_M r_j)^2 (h^+_n)'(k_M r_j)]'\Big\}, \end{aligned} \tag{147}$$

where we have used the relation

$$\rho^2\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\frac{1}{\rho}(\rho z_n(\rho))'\right) + (\rho z_n(\rho))' = \frac{\mathrm{d}}{\mathrm{d}\rho}(\rho^2 z'_n(\rho)). \tag{148}$$

Using now the fact that the spherical Bessel functions satisfy Eq. (122) shows us that

$$n(n+1)z_n(\rho) - \frac{\mathrm{d}}{\mathrm{d}\rho}(\rho^2 z'_n(\rho)) = \rho^2 z_n(\rho).$$

One obtains finally the compact result:

$$[\tilde{H}_X]_p = -i\sqrt{\frac{\varepsilon_M}{\mu_M}}[A'^{(j)}_{e,p}j_n(k_M r_j) + B'^{(j)}_{e,p}h^+_n(k_M r_j)]. \tag{149}$$

Moreover, with Eqs. (39), (54), and (131) one finds

$$[\tilde{H}_Z]_p = -i\sqrt{\frac{\varepsilon_M}{\mu_M}}\frac{1}{k_M r_j}\{A'^{(j)}_{h,p}\psi'_n(k_M r_j) + B'^{(j)}_{h,p}\xi'_n(k_M r_j)\}. \tag{150}$$

As a result, we obtain

$$[F^{(j)}] \equiv \begin{bmatrix} [E^{(j)}_X] \\ [E^{(j)}_Z] \\ [\tilde{H}^{(j)}_X] \\ [\tilde{H}^{(j)}_Z] \end{bmatrix} \equiv \Psi^{(j)} \begin{bmatrix} \vdots \\ A'^{(j)}_{e,p}\psi'_n(k_M r_j)/(k_M r_j) \\ \vdots \\ A'^{(j)}_{h,p}j_n(k_M r_j) \\ \vdots \\ B'^{(j)}_{e,p}\xi'_n(k_M r_j)/(k_M r_j) \\ \vdots \\ B'^{(j)}_{h,p}h^+_n(k_M r_j) \\ \vdots \end{bmatrix} = \Psi^{(j)}[V^{(j)}], \tag{151}$$

which entails

$$\Psi^{(j)} = \begin{pmatrix} 0 & \mathbb{1} & 0 & \mathbb{1} \\ \mathbb{1} & 0 & \mathbb{1} & 0 \\ -i\sqrt{\frac{\varepsilon_M}{\mu_M}}/p^{(j)} & 0 & -i\sqrt{\frac{\varepsilon_M}{\mu_M}}/q^{(j)} & 0 \\ 0 & -i\sqrt{\frac{\varepsilon_M}{\mu_M}}p^{(j)} & 0 & -i\sqrt{\frac{\varepsilon_M}{\mu_M}}q^{(j)} \end{pmatrix}, \tag{152}$$

with

$$p_{p,q}^{(j)} \equiv \delta_{p,q} \left.\frac{\psi_n'(z)}{\psi_n(z)}\right|_{z=k_M r_j}, \quad q_{p,q}^{(j)} \equiv \delta_{p,q} \left.\frac{\xi_n'(z)}{\xi_n(z)}\right|_{z=k_M r_j}. \tag{153}$$

The calculation of the $p_{p,q}^{(j)}$ and $q_{p,q}^{(j)}$ matrix elements is simplified by invoking the recurrence relations of the Ricatti–Bessel functions as shown in Appendix E.

The matrix $\Psi^{(j-1)}$ (at r_{j-1}) links the column $[V^{(j-1)}]$ to the field $[F]$, noted $[F^{(j-1)}]$, and, since the columns $[V^{(j)}]$ have $4\times(n_{\max}+1)^2$ components, we perform successively $4\times(n_{\max}+1)^2$ numerical integrations with linearly independent columns $[V^{(j-1)}]_i$, $i\in[1,4(n_{\max}+1)^2]$, by taking their elements as $V_{p,i}^{(j-1)}=\delta_{pi}$. As a result, these vectors form a square matrix $[\hat{V}^{(j-1)}]$ with

$$[\hat{V}^{(j-1)}] = \mathbb{1}. \tag{154}$$

We thus take, for initiating the integration, columns $[F^{(j-1)}(r_{j-1})]_i=\Psi^{(j-1)}[V^{(j-1)}]_i$, which form a square matrix $[\hat{F}(r_{j-1})]=\Psi^{(j-1)}\mathbb{1}=\Psi^{(j-1)}$. Performing the numerical integration with a standard subroutine leads to numerical values at $r=r_j$, which form a matrix named $[\hat{F}_{\text{int}}(r_j)]$. Inverting the matrix relation of Eq. (151), $[F^{(j)}]=\Psi^{(j)}[V^{(j)}]$, we then deduce

$$[\hat{V}_{\text{int}}^{(j)}] = [\Psi^{(j)}(r_j)]^{-1}[\hat{F}_{\text{int}}(r_j)], \tag{155}$$

which, thanks to Eq. (154), results in

$$[\hat{V}_{\text{int}}^{(j)}] = [\Psi^{(j)}(r_j)]^{-1}[\hat{F}_{\text{int}}(r_j)][\hat{V}^{(j-1)}]. \tag{156}$$

Comparison with Eq. (140) shows that

$$T^{(j)} = [\Psi^{(j)}(r_j)]^{-1}[\hat{F}_{\text{int}}(r_j)]. \tag{157}$$

Thus the shooting method provides the transmission matrix at the end of the integration process.

C. Determination of the Diffracted Field

Once the $T^{(j)}$ matrices for each region have been calculated, the S-matrix propagation algorithm given by Eqs. (142)–(144) is performed in order to find the S matrix of the total modulated area $S^{(M-1)}$. Using a block notation that includes the various Bessel and Ricatti functions, we thus obtain

$$\begin{bmatrix} [B_e'^{(M-1)}] \\ [B_h'^{(M-1)}] \\ [A_e^{(1)}] \\ [A_h^{(1)}] \end{bmatrix} = S^{(M-1)} \begin{bmatrix} [B_e^{(1)}] \\ [B_h^{(1)}] \\ [A_e'^{(M-1)}] \\ [A_h'^{(M-1)}] \end{bmatrix}, \tag{158}$$

and, from Eq. (139), we obtain

$$\begin{bmatrix} [B_e^{(M)}] \\ [B_h^{(M)}] \\ [A_e^{(1)}] \\ [A_h^{(1)}] \end{bmatrix} = \left(\begin{array}{c|c} S_{11} & S_{12} \\ \hline S_{21} & S_{22} \end{array}\right)^{(M-1)} \begin{bmatrix} [B_e^{(1)}] \\ [B_h^{(1)}] \\ [A_e^{(M)}] \\ [A_h^{(M)}] \end{bmatrix}. \tag{159}$$

Recalling that inside the sphere S_1 the field must remain bounded, especially at $r=0$, we must state $B_{eq}^{(1)}=0=B_{hq}^{(1)}\forall q$. Thus Eq. (159) gives the diffracted field through

$$\begin{bmatrix} [B_e^{(M)}] \\ [B_h^{(M)}] \end{bmatrix} = S_{12}^{(M-1)} \begin{bmatrix} [A_e^{(M)}] \\ [A_h^{(M)}] \end{bmatrix}, \tag{160}$$

where $B_{eq}^{(M)}$, $B_{hq}^{(M)}$ will be called the scattering coefficients and the union of the two $(n_{\max}+1)^2$ column matrices $[B_e^{(M)}]$, $[B_h^{(M)}]$ will henceforth simply be denoted $[B^{(M)}]$.

The $A_{e,p}^{(M)}$, $A_{e,p}^{(M)}$ are provided by the incident field:

$$A_{e,p}^{(M)} = A_{e,p}^{\text{i}}, \quad A_{h,p}^{(M)} = A_{h,p}^{\text{i}}, \tag{161}$$

which for an incident plane wave are given by Eqs. (134) and (135). It may be useful in some problems to determine the field inside sphere S_1. Equation (159) indeed leads to

$$\begin{bmatrix} [A_e^{(1)}] \\ [A_h^{(1)}] \end{bmatrix} = S_{22}^{(M-1)} \begin{bmatrix} [A_e^{(M)}] \\ [A_h^{(M)}] \end{bmatrix}. \tag{162}$$

From the coefficients $A_{e,p}^{(1)}$ and $A_{h,p}^{(1)}$, the field everywhere inside the modulated area could be computed if necessary.

9. EXTRACTION OF PHYSICAL QUANTITIES

One should remark that the $S_{22}^{(M-1)}$ and $S_{12}^{(M-1)}$ block matrices obtained by our method are rather complicated objects owing to the fact they contain a great deal of physical information in both near and far fields. This detailed information is essential if we wish to use these matrices as the basic building blocks for multiple-scattering codes.[2,25] For a given single-scattering situation, however, one is typically interested in studying more limited, but more physical accessible, quantities such as cross sections. This extraction of physical quantities has been extensively studied elsewhere,[24–27] and we content ourselves here with a few illustrative formulas.

Physical quantities of interest can usually be obtained directly from analytical formulas of the coefficients of the incident and scattered fields. We recall that for a given incident field, with expansion coefficients placed in a $[A^{\mathrm{i}}]$ column vector and multiplied by suitable Bessel and Ricatti functions to obtain the vector $[A^{(M)}]$, Eq. (160) allows us to obtain the scattering vector $[B^{(M)}]$ via

$$[B^{(M)}] = S_{12}^{(M-1)}[A^{(M)}], \tag{163}$$

from which a vector $[B_{\mathrm{c}}^{(M)}]$ containing only the scattering coefficients can be derived. We shall define the Hermitian conjugate or adjoint vector $[B_{\mathrm{c}}]^{\dagger}$, which takes the form of a row matrix of the complex conjugates of the $[B_{\mathrm{c}}^{(M)}]$ elements:

$$[B_{\mathrm{c}}^{(M)}]^{\dagger} \equiv [\ldots, B_{eq}^{(M),*}, \ldots | \ldots, B_{hq}^{(M),*}, \ldots]. \tag{164}$$

The T-matrix, denoted here by t, familiar to the 3D scattering community is defined by the equation

$$[B_{\mathrm{c}}^{(M)}] \equiv t[A^{\mathrm{i}}], \tag{165}$$

and a comparison with Eqs. (141), (160), and (163) shows that the elements of t can be obtained from the elements of $S_{12}^{(M-1)}$ through the multiplication by appropriate ratios of Ricatti–Bessel functions.

With $[B_{\mathrm{c}}^{(M)}]$, one can readily express the total scattering, extinction, and absorption cross sections, respectively, given by[24,26]

$$\sigma_s = \frac{1}{k_M^2}[B_{\mathrm{c}}]^{\dagger}[B_{\mathrm{c}}],$$

$$\sigma_{\mathrm{e}} = \mathrm{Re}\left\{\frac{1}{k_M^2}[B_{\mathrm{c}}]^{\dagger}[A^{\mathrm{i}}]\right\},$$

$$\sigma_{\mathrm{a}} = \sigma_{\mathrm{e}} - \sigma_{\mathrm{s}}. \tag{166}$$

For a number of applications, however, total cross sections provide too-crude information, and one is interested in the angular distribution of the scattered radiation in the far field. For such situations, it is frequently useful to define an amplitude scattering matrix,[2,6] F [not to be confused with the F column used in propagation equations (53) and (55) nor with the S matrix of Eqs. (141) and (159)]. The scattering matrix is defined in the context of an incident plane wave, which we express as $\mathbf{E}_{\mathrm{i}} = E \exp(i\mathbf{k}_M \cdot \mathbf{r})(e_\theta \hat{\boldsymbol{\theta}}_{\mathrm{i}} + e_\phi \hat{\boldsymbol{\phi}}_{\mathrm{i}})$, where $\hat{\boldsymbol{\theta}}_{\mathrm{i}}$ and $\hat{\boldsymbol{\phi}}_{\mathrm{i}}$ are the spherical unit vectors associated with the incident wave vector, $\mathbf{k}_M$. The scalar E has the dimensions of an electric field. We are in the habit of normalizing the polarization factors e_θ and e_ϕ such that $|e_\theta|^2 + |e_\phi|^2 = 1$, in which case E is simply the electric field amplitude $\|E_{\mathrm{i}}\| = E$. In the far-field limit, the scattered field at $r \to \infty$ will have the form

$$\lim_{r\to\infty} \mathbf{E}_{\mathrm{s}}(\mathbf{r}) = E\frac{\exp(ikr)}{ikr}(E_{\mathrm{s},\theta}\hat{\boldsymbol{\theta}} + E_{\mathrm{s},\phi}\hat{\boldsymbol{\phi}}), \tag{167}$$

where $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ are the spherical unit vectors associated with the vector $\mathbf{r}$. The scattered field factors $E_{\mathrm{s},\theta}$ and $E_{\mathrm{s},\phi}$ can be calculated in terms of the 2×2 scattering matrix F:

$$\begin{pmatrix} E_{\mathrm{s},\theta} \\ E_{\mathrm{s},\phi} \end{pmatrix} = E\frac{\exp(ikr)}{ikr}\begin{pmatrix} F_{\theta\theta} & F_{\theta\phi} \\ F_{\phi\theta} & F_{\phi\phi} \end{pmatrix}\begin{pmatrix} e_\theta \\ e_\phi \end{pmatrix}, \tag{168}$$

where each of the F elements is a function of the incident field direction θ_{i}, ϕ_{i} and the observation angle of the scattered field θ, ϕ. They can be calculated by defining the scattering dyadic $\bar{\bar{F}}$:

$$\bar{\bar{F}} \equiv 4\pi[\boldsymbol{\mathcal{X}}^*(\hat{\mathbf{r}}), \boldsymbol{\mathcal{Z}}^*(\hat{\mathbf{r}})]t\begin{bmatrix} \boldsymbol{\mathcal{X}}(\hat{\mathbf{k}}_{\mathrm{i}}) \\ \boldsymbol{\mathcal{Z}}(\hat{\mathbf{k}}_{\mathrm{i}}) \end{bmatrix}, \tag{169}$$

where we call $\boldsymbol{\mathcal{X}}$ and $\boldsymbol{\mathcal{Z}}$ the phase-modified VSH[24]:

$$\boldsymbol{\mathcal{X}}_{nm}(\hat{\mathbf{r}}) \equiv i^n \mathbf{X}_{nm}^*(\hat{\mathbf{r}}), \quad \boldsymbol{\mathcal{Z}}_{nm}(\hat{\mathbf{r}}) \equiv i^{n-1}\mathbf{Z}_{nm}^*(\hat{\mathbf{r}}). \tag{170}$$

The F elements of Eq. (168) can then be readily expressed as

$$F_{\theta\theta} \equiv \hat{\boldsymbol{\theta}} \cdot \bar{\bar{F}} \cdot \hat{\boldsymbol{\theta}}_{\mathrm{i}}, \quad F_{\theta\phi} \equiv \hat{\boldsymbol{\theta}} \cdot \bar{\bar{F}} \cdot \hat{\boldsymbol{\phi}}_{\mathrm{i}}, \quad F_{\phi\theta} \equiv \hat{\boldsymbol{\phi}} \cdot \bar{\bar{F}} \cdot \hat{\boldsymbol{\theta}}_{\mathrm{i}},$$

$$F_{\phi\phi} \equiv \hat{\boldsymbol{\phi}} \cdot \bar{\bar{F}} \cdot \hat{\boldsymbol{\phi}}_{\mathrm{i}}. \tag{171}$$

The scattering matrix can subsequently be invoked to derive other angularly dependent physical quantities such as the Stokes matrix.[6,24,27] Here we simply remark that a quantity of frequent interest is the differential cross section $\mathrm{d}\sigma/\mathrm{d}\Omega$, which in our notation can be computed from[6,24,27]

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(\theta,\phi;\theta_{\mathrm{i}},\phi_{\mathrm{i}}) = \lim_{r\to\infty} r^2\frac{\|\mathbf{E}_{\mathrm{s}}(\mathbf{r})\|^2}{E^2} = \frac{|E_{\mathrm{s},\theta}|^2 + |E_{\mathrm{s},\phi}|^2}{k^2}$$

$$= \frac{|F_{\theta\theta}\, e_\theta + F_{\theta\phi}\, e_\phi|^2 + |F_{\phi\theta}\, e_\theta + F_{\phi\phi} e_\phi|^2}{k^2}. \tag{172}$$

10. CONCLUSION

This achieves the detailed presentation of the differential theory of light diffraction by a 3D object. Although the theory makes use of the basis of vector spherical harmonics, which is much more complicated to manipulate than the Fourier basis used in Cartesian coordinates, the final result looks quite simple in the sense that it is not more complicated than analyzing crossed gratings,[20] for which the propagation equations are quite similar.

The current theory can also be extended to treat the diffraction from anisotropic materials. A forthcoming paper will present numerical results concerning prolate and oblate spheroids and will include comparisons with results given by approximate methods in view of studying their domain of validity.

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APPENDIX A: CALCULATION OF $\varepsilon_{N,0}$

In the case of an axisymmetric object, in the modulated region the permittivity $\varepsilon(r,\theta)$ is a piecewise constant function with step discontinuities. With $c=\cos\theta$, $\varepsilon(r,\theta)$ is transformed into $\tilde{\varepsilon}(r,c)$, and Eq. (34) reads as $\varepsilon_{n,0}=2\pi\int_{-1}^{1}\tilde{\varepsilon}(r,c)\bar{P}_n^0(c)\mathrm{d}c$, where $\bar{P}_n^0$ are the normalized Legendre polynomials:

$$\bar{P}_n^0(\cos\theta)=\left(\frac{2n+1}{4\pi}\right)^{1/2}P_n^0(\cos\theta). \quad \text{(A1)}$$

We can evaluate this integral by invoking the recurrence relation

$$(n+1)P_n^0(c)=\frac{\mathrm{d}}{\mathrm{d}c}P_{n+1}^0(c)-c\frac{\mathrm{d}}{\mathrm{d}c}P_n^0(c). \quad \text{(A2)}$$

Using the relation

$$\frac{\mathrm{d}}{\mathrm{d}c}(cP_n^0(c))=c\frac{\mathrm{d}}{\mathrm{d}c}P_n^0(c)+P_n^0(c), \quad \text{(A3)}$$

we find

$$c\frac{\mathrm{d}}{\mathrm{d}c}P_n^0(c)=\frac{\mathrm{d}}{\mathrm{d}c}(cP_n^0(c))-P_n^0(c), \quad \text{(A4)}$$

and the recurrence relation becomes

$$P_n^0(c)=\frac{1}{n}\frac{\mathrm{d}}{\mathrm{d}c}P_{n+1}^0(c)-\frac{1}{n}\frac{\mathrm{d}}{\mathrm{d}c}(cP_n^0(c)). \quad \text{(A5)}$$

We have then

$$\int_{c_2}^{c_1}P_n^0(c)\mathrm{d}c=\frac{1}{n}\int_{c_2}^{c_1}\frac{\mathrm{d}}{\mathrm{d}c}P_{n+1}^0(c)\mathrm{d}c-\frac{1}{n}\int_{c_2}^{c_1}\frac{\mathrm{d}}{\mathrm{d}c}(cP_n^0(c))\mathrm{d}c, \quad \text{(A6)}$$

and the piecewise integral is then

$$\int_{c_2}^{c_1}P_n^0(c)\mathrm{d}c=\frac{1}{n}[P_{n+1}^0(c_1)-P_{n+1}^0(c_2)]+\frac{1}{n}[c_2P_n^0(c_2)-c_1P_n^0(c_1)]. \quad \text{(A7)}$$

An example of the determination of the $\varepsilon_{n,0}$ coefficients is illustrated on a spheroid with half large and small axes a and b, respectively; Oz is the symmetry axis, and, in the yOz plane, its Cartesian equation is

$$\frac{z^2}{a^2}+\frac{y^2}{b^2}=1. \quad \text{(A8)}$$

Since $z=r\cos\theta$ and $y=r\sin\theta$, this equation in spherical coordinates reads as

$$r(\theta)=\frac{ab}{\sqrt{a^2+(b^2-a^2)\cos^2\theta}}. \quad \text{(A9)}$$

Inversing this relation leads to

$$\theta(r)=\arccos\left(\frac{a}{r}\sqrt{\frac{r^2-b^2}{a^2-b^2}}\right) \quad \text{(A10)}$$

$\forall r\in[b,a]$; Eq. (A10) defines a value $\theta_1(r)$, with $\theta_1(r)\in[0,\pi/2]$. Defining $\theta_2(r)=\pi-\theta_1(r)$, we have

$$\varepsilon(r,\theta)=\varepsilon_1 \quad \text{if } \theta\in[0,\theta_1(r)]\cup[\theta_2(r),\pi],$$

$$\varepsilon(r,\theta)=\varepsilon_M \quad \text{if } \theta\in[\theta_1(r),\theta_2(r)]. \quad \text{(A11)}$$

The limits c_1 and c_2 that appear in Eq. (A7) are $\cos\theta_1(r)$ and $\cos\theta_2(r)$.

APPENDIX B: VANISHING OF SOME ELEMENTS OF THE Q_ε MATRIX

Expanding $\mathbf{D}$ and $\mathbf{E}$ on the basis of VSH, the equation $\mathbf{D}=\epsilon_0\varepsilon\mathbf{E}$ gives

$$\sum_{n',m'}(D_{Yn'm'}\mathbf{Y}_{n'm'}+D_{Xn'm'}\mathbf{X}_{n'm'}+D_{Zn'm'}\mathbf{Z}_{n'm'})=\epsilon_0\varepsilon(r,\theta,\phi)\sum_{\nu,\mu}(E_{Y\nu\mu}\mathbf{Y}_{\nu\mu}+E_{X\nu\mu}\mathbf{X}_{\nu\mu}+E_{Z\nu\mu}\mathbf{Z}_{\nu\mu}). \quad \text{(B1)}$$

Performing an ordinary scalar product of both sides of Eq. (B1) with $\mathbf{Y}_{nm}^*$, we obtain

$$\mathbf{Y}_{nm}^*\cdot\sum_{n',m'}(D_{Yn'm'}\mathbf{Y}_{n'm'}+D_{Xn'm'}\mathbf{X}_{n'm'}+D_{Zn'm'}\mathbf{Z}_{n'm'})=\epsilon_0\varepsilon(r,\theta,\phi)\mathbf{Y}_{nm}^*\cdot\sum_{\nu,\mu}(E_{Y\nu\mu}\mathbf{Y}_{\nu\mu}+E_{X\nu\mu}\mathbf{X}_{\nu\mu}+E_{Z\nu\mu}\mathbf{Z}_{\nu\mu}). \quad \text{(B2)}$$

Using the fact as one can see from Eqs. (7), (16), and (17) that $\mathbf{Y}_{nm}^*\cdot\mathbf{X}_{n'm'}=\mathbf{Y}_{nm}^*\cdot\mathbf{Z}_{n'm'}=\mathbf{Y}_{nm}^*\cdot\mathbf{X}_{\nu\mu}=\mathbf{Y}_{nm}^*\cdot\mathbf{Z}_{\nu\mu}=0$, we find

$$\sum_{n',m'}D_{Ynm}\mathbf{Y}_{nm}^*\cdot\mathbf{Y}_{n'm'}=\epsilon_0\varepsilon(r,\theta,\phi)\sum_{\nu,\mu}E_{Y\nu\mu}\mathbf{Y}_{nm}^*\cdot\mathbf{Y}_{\nu\mu}. \quad \text{(B3)}$$

This equation establishes a linear relation between D_{Ynm} and $E_{Y\nu\mu}$ only; thus $Q_{\varepsilon YX}$ and $Q_{\varepsilon YZ}$ must be null.

Now, performing a scalar product on both sides of Eq. (B1) with $\mathbf{X}_{nm}^*$, we find that

$$\mathbf{X}_{nm}^*\cdot\sum_{n',m'}(D_{Yn'm'}\mathbf{Y}_{n'm'}+D_{Xn'm'}\mathbf{X}_{n'm'}+D_{Zn'm'}\mathbf{Z}_{n'm'})=\epsilon_0\varepsilon(r,\theta,\phi)\mathbf{X}_{nm}^*\cdot\sum_{\nu,\mu}(E_{Y\nu\mu}\mathbf{Y}_{\nu\mu}+E_{X\nu\mu}\mathbf{X}_{\nu\mu}+E_{Z\nu\mu}\mathbf{Z}_{\nu\mu}). \quad \text{(B4)}$$

Using the fact that $\mathbf{X}_{nm}^*\cdot\mathbf{Y}_{n'm'}=\mathbf{X}_{nm}^*\cdot\mathbf{Y}_{\nu\mu}=0$, we obtain

$$\frac{1}{\epsilon_0}\sum_{n',m'}(D_{Xn'm'}\mathbf{X}^*_{nm}\cdot\mathbf{X}_{n'm'}+D_{Zn'm'}\mathbf{X}^*_{nm}\cdot\mathbf{Z}_{n'm'})$$
$$=\varepsilon(r,\theta,\phi)\mathbf{X}^*_{nm}\cdot\sum_{\nu,\mu}(E_{X\nu\mu}\mathbf{X}_{\nu\mu}+E_{Z\nu\mu}\mathbf{Z}_{\nu\mu}). \quad (B5)$$

Integrating over the solid angles Ω, we obtain, taking into account Eq. (11),

$$D_{Xnm}=\epsilon_0\sum_{\nu,\mu}\int_0^{4\pi}\mathrm{d}\Omega\,\varepsilon(r,\theta,\phi)\mathbf{X}^*_{nm}\cdot(E_{X\nu\mu}\mathbf{X}_{\nu\mu}+E_{Z\nu\mu}\mathbf{Z}_{\nu\mu}). \quad (B6)$$

Since D_{Xnm} does not depend on $E_{Y\nu\mu}$, we deduce that $Q_{\varepsilon XY}=0$.

A similar calculation starting from multiplying both sides of Eq. (B1) by $\mathbf{Z}^*_{nm}$ leads to $Q_{\varepsilon ZY}=0$.

APPENDIX C: TWO RELATIONS BETWEEN VECTOR SPHERICAL HARMONICS

In order to derive two relations between VSHs that are necessary to construct the theory, it is useful to invoke another set of VSHs, denoted $\mathbf{Y}^m_{n,n+1}$, $\mathbf{Y}^m_{n,n}$, and $\mathbf{Y}^m_{n,n-1}$, as introduced by quantum-mechanic theoreticians who worked on the angular-momentum coupling formalism.[23] We first recall the definition of the Cartesian spherical unit vectors[23]:

$$\boldsymbol{\mathcal{X}}_1=-\frac{1}{\sqrt{2}}(\hat{\mathbf{x}}+i\hat{\mathbf{y}}),\quad \boldsymbol{\mathcal{X}}_0=\hat{\mathbf{z}},\quad \boldsymbol{\mathcal{X}}_{-1}=\frac{1}{\sqrt{2}}(\hat{\mathbf{x}}-i\hat{\mathbf{y}}), \quad (C1)$$

where $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$ are the unit vectors of the Cartesian coordinate system. Making use of the Clebsch–Gordan coefficients,[23] we then define the new set of VSHs as

$$\mathbf{Y}^m_{n,l}=\sum_{\mu=-1}^{1}(l,m-\mu;1,\mu|n,m)Y_{l,m-\mu}\boldsymbol{\mathcal{X}}_\mu, \quad (C2)$$

with $l=n-1$, n, $n+1$.

Using the conversion from spherical to Cartesian coordinates and the expressions of our $\mathbf{Y}_{nm}$, $\mathbf{X}_{nm}$, $\mathbf{Z}_{nm}$ VSHs in a spherical coordinate system of Eqs. (7), (16), and (17), we can painstakingly verify that our $\mathbf{Y}_{nm}$, $\mathbf{X}_{nm}$, and $\mathbf{Z}_{nm}$ VSHs can be expressed in terms of the $\mathbf{Y}^m_{n,n+1}$, $\mathbf{Y}^m_{n,n+1}$, $\mathbf{Y}^m_{n,n+1}$ spherical harmonics via the relations

$$\mathbf{X}_{nm}=\frac{\mathbf{Y}^m_{n,n}}{i}, \quad (C3)$$

$$\mathbf{Z}_{nm}=\left(\frac{n+1}{2n+1}\right)^{1/2}\mathbf{Y}^m_{n,n-1}+\left(\frac{n}{2n+1}\right)^{1/2}\mathbf{Y}^m_{n,n+1}, \quad (C4)$$

$$\mathbf{Y}_{nm}=\left(\frac{n}{2n+1}\right)^{1/2}\mathbf{Y}^m_{n,n-1}-\left(\frac{n+1}{2n+1}\right)^{1/2}\mathbf{Y}^m_{n,n+1}. \quad (C5)$$

With the above equations in place, we first calculate the following two products.

1. $\mathbf{X}_{\nu\mu}\cdot\mathbf{X}^*_{nm}$

Using Eq. (C3), we find

$$\mathbf{X}_{\nu\mu}\cdot\mathbf{X}^*_{nm}=\mathbf{Y}^\mu_{\nu,\nu}\cdot(\mathbf{Y}^m_{n,n})^*. \quad (C6)$$

Putting Eq. (C2) in Eq. (C6) and calculating the Clebsch–Gordan coefficients lead us to

$$\mathbf{X}_{\nu\mu}\cdot\mathbf{X}^*_{nm}=\left[\frac{1}{n(n+1)\nu(\nu+1)}\right]^{1/2}\times\left\{\frac{1}{2}[(n+m+1)(n-m)(\nu+\mu+1)(\nu-\mu)]^{1/2}\times Y_{\nu,\mu+1}Y^*_{n,m+1}+m\mu Y_{\nu\mu}Y^*_{nm}+\frac{1}{2}[(n+m)(n-m+1)\times(\nu+\mu)(\nu-\mu+1)]^{1/2}Y_{\nu,\mu-1}Y^*_{n,m-1}\right\}. \quad (C7)$$

2. $\mathbf{X}_{\nu\mu}\cdot\mathbf{Z}^*_{nm}$

In order to calculate this scalar product, we use the fact that $\mathbf{X}_{\nu\mu}\cdot\mathbf{Y}^*_{nm}=0$. Thus Eq. (C5) gives

$$\left(\frac{n+1}{2n+1}\right)^{1/2}\mathbf{X}_{\nu\mu}\cdot\mathbf{Y}^{m,*}_{n,n+1}=\left(\frac{n}{2n+1}\right)^{1/2}\mathbf{X}_{\nu\mu}\cdot\mathbf{Y}^{m,*}_{n,n-1}, \quad (C8)$$

i.e.,

$$\mathbf{X}_{\nu\mu}\cdot\mathbf{Y}^{m,*}_{n,n+1}=\left(\frac{n}{n+1}\right)^{1/2}\mathbf{X}_{\nu\mu}\cdot\mathbf{Y}^{m,*}_{n,n-1}. \quad (C9)$$

Using Eq. (C4), we then obtain

$$\mathbf{X}_{\nu\mu}\cdot\mathbf{Z}^*_{nm}=\left(\frac{n+1}{2n+1}\right)^{1/2}\mathbf{X}_{\nu\mu}\cdot\mathbf{Y}^{m,*}_{n,n-1}+\left(\frac{n}{2n+1}\right)^{1/2}\mathbf{X}_{\nu\mu}\cdot\mathbf{Y}^{m,*}_{n,n+1}=\left(\frac{2n+1}{n+1}\right)^{1/2}\mathbf{X}_{\nu\mu}\cdot\mathbf{Y}^{m,*}_{n,n-1}=-i\left(\frac{2n+1}{n+1}\right)^{1/2}\mathbf{Y}^\mu_{\nu,\nu}\cdot\mathbf{Y}^{m,*}_{n,n-1}. \quad (C10)$$

Inserting Eq. (C2) and the expression of the Clebsch–Gordan coefficients into Eq. (C10) leads to

$$\mathbf{X}_{\nu\mu}\cdot\mathbf{Z}^*_{nm}=i\left(\frac{1}{n(n+1)\nu(\nu+1)}\frac{2n+1}{2n-1}\right)^{1/2}\times\left\{-\frac{Y_{\nu,\mu-1}Y^*_{n-1,m-1}}{2}\times[(n+m)(n+m-1)(\nu+\mu)(\nu-\mu+1)]^{1/2}\right.$$

$$+ \mu[(n^2 - m^2)]^{1/2} Y_{\nu,\mu} Y^*_{n-1,m} + \frac{Y_{\nu,\mu+1} Y^*_{n-1,m+1}}{2} \times [(n-m)(n-m-1)(\nu-\mu)(\nu+\mu+1)]^{1/2} \Big\}. \quad \text{(C11)}$$

APPENDIX D: USE OF THE GAUNT COEFFICIENTS

Theoreticians working on the coupling of angular momentum in quantum mechanics have introduced the concepts of Gaunt coefficients and Wigner $3J$ coefficients.[23,28] With our definitions, the normalized Gaunt coefficients, $\bar{a}$, arise from solid-angle integration of the product of three scalar spherical harmonics[23]:

$$\bar{a}(\{\nu',\mu'\},\{\nu,\mu\},\{n,m\}) \equiv \int_0^{2\pi}\int_0^{\pi} Y_{\nu'\mu'}(\theta,\phi) Y_{\nu\mu}(\theta,\phi) \times Y_{nm}(\theta,\phi) \sin\theta \mathrm{d}\theta \mathrm{d}\phi. \quad \text{(D1)}$$

These coefficients can be rapidly calculated through recursion relations.[29] They naturally appear if, starting from Eq. (71), we expand in it the $\varepsilon(r,\theta,\phi)$ function as stated in Eq. (3):

$$\sum_{n'm'} (D_{\mathrm{TY}n'm'} \mathbf{Y}_{n'm'} + D_{\mathrm{TX}n'm'} \mathbf{X}_{n'm'} + D_{\mathrm{TZ}n'm'} \mathbf{Z}_{n'm'}) = \epsilon_0 \sum_{\nu',\mu'} \sum_{\nu,\mu} \varepsilon_{\nu'\mu'} Y_{\nu'\mu'} (E_{\mathrm{TY}\nu\mu} \mathbf{Y}_{\nu\mu} + E_{\mathrm{TX}\nu\mu} \mathbf{X}_{\nu\mu} + E_{\mathrm{TZ}\nu\mu} \mathbf{Z}_{\nu\mu}). \quad \text{(D2)}$$

Multiplying both sides by $\mathbf{Y}^*_{nm}(\theta,\phi)$ and integrating over the angular variables θ, ϕ, we obtain

$$\begin{aligned}
\frac{1}{\epsilon_0} D_{\mathrm{TY}nm} &= \sum_{\nu',\mu'} \sum_{\nu,\mu} \varepsilon_{\nu'\mu'} E_{\mathrm{TY}\nu\mu} \iint Y_{\nu'\mu'}(\theta,\phi) Y_{\nu\mu}(\theta,\phi) \cdot Y^*_{nm}(\theta,\phi) \sin\theta \mathrm{d}\theta \mathrm{d}\phi \\
&= \sum_{\nu',\mu'} \sum_{\nu,\mu} \varepsilon_{\nu'\mu'} E_{\mathrm{TY}\nu\mu} (-1)^m \iint Y_{\nu'\mu'}(\theta,\phi) Y_{\nu\mu}(\theta,\phi) \cdot Y_{n,-m}(\theta,\phi) \sin\theta \mathrm{d}\theta \mathrm{d}\phi \\
&= \sum_{\nu',\mu'} \sum_{\nu,\mu} \varepsilon_{\nu'\mu'} E_{\mathrm{TY}\nu\mu} (-1)^m \iint Y_{\nu'\mu'}(\theta,\phi) Y_{\nu\mu}(\theta,\phi) Y_{n,-m}(\theta,\phi) \sin\theta \mathrm{d}\theta \mathrm{d}\phi \\
&= \sum_{\nu',\mu'} \sum_{\nu,\mu} \varepsilon_{\nu'\mu'} E_{\mathrm{TY}\nu\mu} (-1)^m \bar{a}(\{\nu',\mu'\},\{\nu,\mu\},\{n,-m\}).
\end{aligned} \quad \text{(D3)}$$

A useful property of Gaunt coefficients defined in Eq. (D1) is that they are null except if $\mu' = m - \mu$ and $\nu' \in [|n-\nu|, n+\nu]$. Thus the summation over μ' is eliminated, and Eq. (D3) reduces to

$$D_{\mathrm{TY}nm} = \epsilon_0 \sum_{\nu'=|n-\nu|}^{n+\nu} \sum_{\nu=0}^{N} \sum_{\mu=-\nu}^{\nu} (-1)^m \bar{a}(\{\nu', m-\mu\}, \{\nu,\mu\},\{n,-m\}) \varepsilon_{\nu',m-\mu} E_{\mathrm{TY}\nu\mu}. \quad \text{(D4)}$$

A comparison with Eq. (77) shows that

$$\varepsilon_{YYnm,\nu\mu} = (-1)^m \sum_{\nu'=|n-\nu|}^{n+\nu} \bar{a}(\{\nu', m-\mu\},\{\nu,\mu\},\{n, -m\}) \varepsilon_{\nu',m-\mu}(r), \quad \text{(D5)}$$

in which the calculation of $\varepsilon_{\nu',m-\mu}(r)$ involves computing the integrals stated in Eq. (6), which implies integrating single spherical harmonics multiplied by piecewise constant functions, a task that can readily be performed analytically as described in Appendix A.

We now can derive similar expressions for the other blocks. Multiplying both sides of Eq. (71) by $\mathbf{X}^*_{nm}(\theta,\phi)$, integrating over the angular variables θ, ϕ, and expanding ε as stated by Eq. (3), we obtain

$$\begin{aligned}
D_{\mathrm{TX}nm} &= \epsilon_0 \sum_{\nu',\mu'} \sum_{\nu,\mu} \varepsilon_{\nu'\mu'} E_{\mathrm{TX}\nu\mu} \int Y_{\nu'\mu'}(\theta,\phi) \mathbf{X}_{\nu\mu}(\theta,\phi) \cdot \mathbf{X}^*_{nm}(\theta,\phi) \sin\theta \mathrm{d}\theta \mathrm{d}\phi \\
&+ \sum_{\nu',\mu'} \sum_{\nu,\mu} \varepsilon_{\nu'\mu'} E_{\mathrm{TZ}\nu\mu} \int Y_{\nu'\mu'}(\theta,\phi) \mathbf{Z}_{\nu\mu}(\theta,\phi) \cdot \mathbf{X}^*_{nm}(\theta,\phi) \sin\theta \mathrm{d}\theta \mathrm{d}\phi.
\end{aligned} \quad \text{(D6)}$$

From Eq. (C7) in Appendix C we thus obtain

$$\varepsilon_{XXnm,\nu\mu}=\left[\frac{1}{n(n+1)\nu(\nu+1)}\right]^{1/2}(-1)^{-m}\sum_{\nu'=|n-\nu|}^{n+\nu}\varepsilon_{\nu',m-\mu}\times\Big\{-\frac{1}{2}[(n+m+1)(n-m)(\nu+\mu+1)(\nu-\mu)]^{1/2}\bar{a}(\{\nu',m-\mu\},\{\nu,\mu+1\},\{n,-m-1\})+\bar{a}(\{\nu',m-\mu\},\{\nu,\mu\},\{n,-m\})-\frac{1}{2}[(n+m)(n-m+1)(\nu+\mu)(\nu-\mu+1)]^{1/2}\bar{a}(\{\nu',m-\mu\},\{\nu,\mu-1\},\{n,-m+1\})\Big\}. \quad \text{(D7)}$$

From Eq. (C11) in Appendix C, we obtain

$$\varepsilon_{XZnm,\nu\mu}=\frac{i}{2}\left(\frac{1}{n(n+1)\nu(\nu+1)}\frac{2n+1}{2n-1}\right)^{1/2}(-1)^{m}\sum_{\nu'=|n-1-\nu|}^{n+\nu-1}\varepsilon_{\nu',m-\mu}\times\{-[(n+m)(n+m-1)(\nu+\mu)(\nu-\mu+1)]^{1/2}\bar{a}(\{\nu',m-\mu\},\{\nu,\mu\},\{n-1,-m+1\})+2\mu[(n^2-m^2)]^{1/2}\bar{a}(\{\nu',m-\mu\},\{\nu,\mu\},\{n-1,-m\})+[(n-m)(n-m-1)(\nu-\mu)(\nu+\mu+1)]^{1/2}\bar{a}(\{\nu',m-\mu\},\{\nu,\mu+1\},\{n-1,-m-1\})\}. \quad \text{(D8)}$$

An alternative exists to determine the Gaunt coefficients. Introducing the Wigner $3J$ coefficients

$$\begin{pmatrix} n_1 & n_2 & n_3 \\ m_1 & m_2 & m_3 \end{pmatrix},$$

which are given by standard subroutines, we can calculate the normalized Gaunt coefficients from

$$\bar{a}(\{\nu',\mu'\},\{\nu,\mu\},\{n,m\})=\left[\frac{(2\nu'+1)(2\nu+1)(2n+1)}{4\pi}\right]^{1/2}\times\begin{pmatrix} \nu' & \nu & n \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \nu' & \nu & n \\ \mu' & \mu & m \end{pmatrix}.$$

APPENDIX E: RICATTI–BESSEL FUNCTIONS

We recall the definition of the Ricatti–Bessel functions $\psi_n(z)$ and $\xi_n(z)$:

$$\psi_n(z)\equiv zj_n(z), \quad \xi_n(z)\equiv zh_n^{+}(z). \quad \text{(E1)}$$

Their derivatives $\psi_n'(z)$ and $\xi_n'(z)$ can be readily calculated using the Bessel function recursion relations:

$$\psi_n'(z)=\frac{(n+1)}{z}\psi_n(z)-\psi_{n+1}(z),$$

$$\xi_n'(z)=\frac{(n+1)}{z}\xi_n(z)-\xi_{n+1}(z). \quad \text{(E2)}$$

We note, for example, the elements of the $p^{(j)}$ and $q^{(j)}$ matrices of Eq. (152) are simply the logarithmic derivatives of the Ricatti–Bessel functions:

$$p_{p,q}^{(j)}\equiv\delta_{pq}\Phi_n(k_M r_j)\equiv\left.\delta_{pq}\frac{\psi_n'(z)}{\psi_n(z)}\right|_{z=k_M r_j},$$

$$q_{p,q}^{(j)}\equiv\delta_{pq}\Psi_n(k_M r_j)\equiv\left.\delta_{pq}\frac{\xi_n'(z)}{\xi_n(z)}\right|_{z=k_M r_j}, \quad \text{(E3)}$$

which can be rapidly and reliably calculated[1] from recurrence relations derived from Eqs. (E2),

$$\Phi_{n-1}(z)=\frac{n}{z}-\frac{1}{\Phi_n(z)+n/z},$$

or

$$\Psi_n(z)=\frac{1}{n/z-\Psi_{n-1}(z)}-\frac{n}{z}, \quad \text{(E4)}$$

so that Ricatti–Bessel functions simplify the initialization of the shooting method. Of course, the partition of the modulated area should be done in such a way that no value of r_j coincides with a zero of a Ricatti $\psi_n(z)$ function.

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scattering matrix. It is essentially the S_{12} block of the $S^{(M-1)}$ matrix appearing later on in Eq. (158); see also Eqs. (163) and (165).

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