Mie scattering by an anisotropic object. Part I. Homogeneous sphere

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Establishing a vector spherical harmonic expansion of the electromagnetic field propagating inside an arbitrary anisotropic medium, we extend Mie theory to the diffraction by an anisotropic sphere, with or without losses. The particular case of a uniaxial material leads to a simpler analysis. This work opens the way to the construction of a differential theory of diffraction by a three-dimensional object with arbitrary shape, filled by an arbitrary anisotropic material. © 2006 Optical Society of America

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1. INTRODUCTION

Resonant scattering from anisotropic particles is a field of growing interest due to an increasing number of technological and biological applications. By "resonant scattering" we mean particles comparable in size to the wavelength of the incident radiation. By "comparable in size," we mean any particle size approaching an order of magnitude smaller than the wavelength and within a few orders of magnitude larger than the wavelength. Scattering from anisotropic particles much smaller than the wavelength is well understood from dipolar considerations,[1] while one generally considers that particles a few orders of magnitude larger than the wavelength can be reasonably well treated with geometric optics[2] (despite some notable exceptions already known from scattering by large isotropic scatterers.[3]) Scattering of electromagnetic radiation from a homogeneous isotropic sphere as originally addressed by Lorenz[4,5] and later by Mie[6] has been the source of a vast quantity of scientific and technological studies over the last 50 years (at least). The Lorenz–Mie solution is expressed analytically as an infinite series involving spherical Bessel functions. The complexity involved in evaluating these special functions largely prevented detailed studies from being performed before the availability of electronic calculators.

In view of the wide popularity and success of studies based on Mie theory and the numerous questions posed by anisotropic scattering, a number of attempts have been made in the literature to extend Mie theory to the problem of scattering by a sphere composed of anisotropic media. Studies involving analytical calculations have usually chosen to simplify the problem by addressing some particular geometries and/or anisotropic configurations in order to facilitate analytic or near analytic calculations (anisotropy in a spherical layer,[7] radial or uniform,[8] radial anisotropy in a sphere.[9]) A notable exception is the recent paper by Geng *et al.*,[10] who presented an analytic solution for the uniaxial anisotropic sphere and of which we became aware during the preparation of this paper. Concerning general homogeneous anisotropy, however, the recent work of Ref. 10 declares it to be not "exactly soluble," while the well-known book of Bohren and Huffman[11] says only that no exact solution has been published and concentrates on the Rayleigh–Gans approximation. In this paper, we solve the problem of scattering by a sphere composed of an *arbitrary* homogeneous anisotropic medium. By arbitrary, we mean that the sphere is composed of a medium described by an arbitrary permittivity tensor, including the possibility of absorption. This solution, like the Mie solution, is analytic in the sense that it involves only mathematical formulas that can be readily evaluated on a computer so that the only source of error comes from selection of a finite partial wave cutoff (as in ordinary Mie theory), as well as machine errors.

2. ELECTRIC PERMITTIVITY IN SPHERICAL COORDINATES

In Cartesian coordinates, the tensor of relative permittivity has the most general form:

$$\bar{\bar{\epsilon}} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix}, \tag{1}$$

where no restricted symmetry properties are assigned and the elements may be complex numbers. The sphere is assumed to be homogeneous, which means that the elements of the permittivity tensor are independent of the spatial position. In spherical coordinates, its expression $\tilde{\tilde{\epsilon}}$ can be derived through the Cartesian-to-spherical transformation matrix $\mathfrak{R}$ using the formula

$$\tilde{\tilde{\epsilon}} = \mathfrak{R}\bar{\bar{\epsilon}}\mathfrak{R}^{\mathrm{T}} \tag{2}$$

where T stands for transpose.

We denote with a circumflex the unit vectors along the coordinate axis. The transformation matrix $\mathfrak{R}$ is expressed using the scalar products of these unit vectors:

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$$\mathfrak{R} = \begin{pmatrix} \hat{\mathbf{r}}\cdot\hat{\mathbf{x}} & \hat{\mathbf{r}}\cdot\hat{\mathbf{y}} & \hat{\mathbf{r}}\cdot\hat{\mathbf{z}} \\ \hat{\boldsymbol{\theta}}\cdot\hat{\mathbf{x}} & \hat{\boldsymbol{\theta}}\cdot\hat{\mathbf{y}} & \hat{\boldsymbol{\theta}}\cdot\hat{\mathbf{z}} \\ \hat{\boldsymbol{\varphi}}\cdot\hat{\mathbf{x}} & \hat{\boldsymbol{\varphi}}\cdot\hat{\mathbf{y}} & \hat{\boldsymbol{\varphi}}\cdot\hat{\mathbf{z}} \end{pmatrix}. \tag{3}$$

The unit vectors are linked by the relations

$$\hat{\mathbf{r}} = \hat{\mathbf{x}}\cos\varphi\sin\theta + \hat{\mathbf{y}}\sin\varphi\sin\theta + \hat{\mathbf{z}}\cos\theta,$$

$$\hat{\boldsymbol{\varphi}} = -\hat{\mathbf{x}}\sin\varphi + \hat{\mathbf{y}}\cos\varphi,$$

$$\hat{\boldsymbol{\theta}} = -\hat{\mathbf{r}}\times\hat{\boldsymbol{\varphi}} = \hat{\mathbf{x}}\cos\varphi\cos\theta + \hat{\mathbf{y}}\sin\varphi\cos\theta - \hat{\mathbf{z}}\sin\theta, \tag{4}$$

and thus the matrix $\mathfrak{R}$ takes the form

$$\mathfrak{R} = \begin{pmatrix} \cos\varphi\sin\theta & \sin\varphi\sin\theta & \cos\theta \\ \cos\varphi\cos\theta & \sin\varphi\cos\theta & -\sin\theta \\ -\sin\varphi & \cos\varphi & 0 \end{pmatrix}. \tag{5}$$

Equations (1), (2), and (5) give the elements $\tilde{\tilde{\epsilon}}_{ij}, i,j = r,\theta,\varphi$ of $\tilde{\tilde{\epsilon}}$. Since the spherical coordinate system is orthogonal, it is not necessary to distinguish between covariant and contravariant components, and all vector and tensor components will be denoted by subscripts. It is worth noticing that the elements of $\tilde{\tilde{\epsilon}}$ depend on (θ,φ), contrary to Ref. 9, but do not depend on (x,y,z), as already mentioned.

3. PROPAGATION EQUATION OF PLANE WAVES

The monochromatic propagation equation has the form

$$\operatorname{curl}\operatorname{curl}\mathbf{E} - k_0^2\tilde{\tilde{\epsilon}}\mathbf{E} = 0, \tag{6}$$

where $k_0=\omega/c$ is the vacuum wavenumber, ω is the angular frequency, and c the speed of light in vacuum. As is well known, this equation permits solutions in the form of plane waves,

$$\mathbf{E}(\mathbf{k},\mathbf{r}_{OM}) = \mathbf{A}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r}_{OM}) \tag{7}$$

where $\mathbf{r}_{OM}$ is the radius vector of an arbitrary point M and $\mathbf{k}$ is the wave vector of this wave with $\mathbf{k}=|\mathbf{k}|\hat{\mathbf{r}}$. In the case of isotropic media, $\mathbf{E}$ is a solution of the Helmholtz equation, and the wave vector $\mathbf{k}$ becomes isotropic, its norm being independent of the direction of propagation. Anisotropy complicates the form of the solution, since $|\mathbf{k}|$ then depends on the direction of propagation. Nevertheless $|\mathbf{k}|$ can be determined analytically from the elements of the permittivity tensor. Noting that

$$\operatorname{curl}[\mathbf{A}\exp(i\mathbf{k}\cdot\mathbf{r}_{OM})] = i\mathbf{k}\times\mathbf{A}\exp(i\mathbf{k}\cdot\mathbf{r}_{OM}), \tag{8}$$

one obtains from Eq. (6) that $\mathbf{A}$ must satisfy

$$\mathbf{k}\times(\mathbf{k}\times\mathbf{A}) + k_0^2\tilde{\tilde{\epsilon}}\mathbf{A} = 0. \tag{9}$$

Introducing the tensor $(\mathbf{kk})$ whose (i, j) element is equal to $k_i k_j$, Eq. (9) can be written in the form

$$[k^2\mathbb{I} - (\mathbf{kk}) - k_0^2\tilde{\tilde{\epsilon}}]\mathbf{A}(\mathbf{k}) = 0, \tag{10}$$

where $k^2=|\mathbf{k}|^2=\mathrm{Tr}(\mathbf{kk})$ and $\mathbb{I}$ is the unit matrix. Equation (10) shows that k^2 must be a nonlinear eigenvalue of the operator $(\mathbf{kk})+k_0^2\tilde{\tilde{\epsilon}}$ and that $\mathbf{A}(\mathbf{k})$ is the corresponding eigenvector. The eigenvalue equation reads

$$\det[k^2\mathbb{I} - (\mathbf{kk}) - k_0^2\tilde{\tilde{\epsilon}}] = 0. \tag{11}$$

4. SOLUTION OF THE EIGENPROBLEM

A. Eigenvalues

Following the work of Papadakis *et al.*,[12] we express Eq. (11) in spherical coordinates. As the wave vector $\mathbf{k}$ of the plane wave is invariant with respect to translation, its only nonzero component is along $\hat{\mathbf{r}}$; however, in anisotropic media $k_r=k_r(\theta,\varphi)$ depends only on the direction of propagation, as already discussed. This fact considerably simplifies the form of the tensor $(\mathbf{kk})$ in spherical coordinates:

$$(\mathbf{kk}) = k^2\mathbb{I}_{1/3} \tag{12}$$

with

$$\mathbb{I}_{1/3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{13}$$

and Eq. (11) then reads

$$\det\left[\frac{k^2}{k_0^2}(\mathbb{I} - \mathbb{I}_{1/3}) - \tilde{\tilde{\epsilon}}\right] = 0 \Leftrightarrow \begin{vmatrix} \epsilon_{rr} & \epsilon_{r\theta} & \epsilon_{r\varphi} \\ \epsilon_{\theta r} & \epsilon_{\theta\theta} - \hat{k}^2 & \epsilon_{\theta\varphi} \\ \epsilon_{\varphi r} & \epsilon_{\varphi\theta} & \epsilon_{\varphi\varphi} - \hat{k}^2 \end{vmatrix} = 0, \tag{14}$$

where $\hat{k} \equiv k/k_0$.

Equation (14) represents a biquadratic algebraic equation for $\hat{k}$, which can be written in the form

$$\alpha\hat{k}^4 - \beta\hat{k}^2 + \gamma = 0, \tag{15}$$

where

$$\alpha = \epsilon_{rr},$$

$$\beta = \epsilon_{rr}(\epsilon_{\theta\theta} + \epsilon_{\varphi\varphi}) - \epsilon_{r\theta}\epsilon_{\theta r} - \epsilon_{r\varphi}\epsilon_{\varphi r},$$

$$\gamma = \det(\tilde{\tilde{\epsilon}}). \tag{16}$$

Defining $\Delta=\beta^2-4\alpha\gamma$, Eq. (15) has two roots for $\hat{k}^2$, $(\hat{k}^2)' = (\beta+\sqrt{\Delta})/2\alpha$ and $(\hat{k}^2)''=(\beta-\sqrt{\Delta})/2\alpha$. From there, we obtain four eigenvalues of $\hat{k}$ noted $\hat{k}_j$ $(j=1-4)$, which give four values of k_j:

$$k_1/k_0 = \hat{k}_1 = \sqrt{(\hat{k}^2)'} = -\hat{k}_3 = -k_3/k_0,$$

$$k_2/k_0 = \hat{k}_2 = \sqrt{(\hat{k}^2)''} = -\hat{k}_4 = -k_4/k_0. \tag{17}$$

For lossless materials, energy conservation requires that the tensor $\bar{\bar{\epsilon}}$ (and thus $\tilde{\tilde{\epsilon}}$) is real and symmetric. It can be shown that for each real direction of propagation (θ,φ), two real positive values k_1 and k_2 exist, which, in general, depend on (θ,φ). The other two values correspond to waves propagating in the opposite direction.

For lossy materials, $\bar{\bar{\epsilon}}$ and $\tilde{\bar{\epsilon}}$ have complex elements, and their real and imaginary parts cannot in general be diagonalized in the same basis. However, the analysis of this subsection can be directly generalized to lossy media by searching for complex solutions of Eq. (11). This could be done numerically, but by applying a simple procedure, one can directly use Eqs. (17). To that end, it is necessary to define a complex spherical coordinate system in the following manner. A complex unit vector $\hat{\mathbf{r}}_{\mathrm{C}}=\mathbf{k}/|k|$ is introduced, from which two complex angles θ_{C} and φ_{C} are derived using the simple trigonometric relations:

$$\cos(\theta_{\mathrm{C}}) = \hat{\mathbf{r}}_{\mathrm{C}} \cdot \hat{\mathbf{z}}$$

$$\cos(\varphi_{\mathrm{C}}) = \hat{\mathbf{r}}_{\mathrm{C}} \cdot \hat{\mathbf{x}}/\sin(\theta_{\mathrm{C}}) \tag{18}$$

A complex orthogonal basis is then constructed by extending the second and the third of Eqs. (4) to complex angles. Using this coordinate system, Eqs. (12)–(14), (5), and (16) are still valid and Eq. (17) holds for lossy media as well, taking $\sqrt{\Delta}$, k_1, and k_2 with nonnegative imaginary parts.

B. Eigenvectors

1. Arbitrary Anisotropy

As solutions of a linear homogeneous equation, all eigenvector are determined through interrelations among their components. Let us take as an independent component $A_{j,r}=\mathbf{A}(k_j\hat{\mathbf{r}})\cdot\hat{\mathbf{r}}$, $j=1,2$ (the case when this component is zero is discussed further on). Due to the fact that $\mathbf{A}(k_j\hat{\mathbf{r}})$ depends on k^2 only, Eq. (10), the eigenvectors can be separated into two pairs, each corresponding to $+k_j$ and $-k_j$ and having the same vector components. However, these vector components are expressed in two opposite local trihedrals (r,θ,φ), so that $\mathbf{A}(k_3\hat{\mathbf{r}})=-\mathbf{A}(k_1\hat{\mathbf{r}})$ and $\mathbf{A}(k_4\hat{\mathbf{r}})=-\mathbf{A}(k_2\hat{\mathbf{r}})$. Equation (10) reads

$$\left|\begin{array}{l} \epsilon_{rr}A_{j,r} + \epsilon_{r\theta}A_{j,\theta} + \epsilon_{r\varphi}A_{j,\varphi} = 0, \\ \epsilon_{\theta r}A_{j,r} + (\epsilon_{\theta\theta} - \hat{k}_j^2)A_{j,\theta} + \epsilon_{\theta\varphi}A_{j,\varphi} = 0, \\ \epsilon_{\varphi r}A_{j,r} + \epsilon_{\varphi\theta}A_{j,\theta} + (\epsilon_{\varphi\varphi} - \hat{k}_j^2)A_{j,\varphi} = 0. \end{array}\right. \tag{19}$$

The first two equations give the relations

$$A_{j,\theta} = \frac{\begin{vmatrix} -\epsilon_{rr} & \epsilon_{r\varphi} \\ -\epsilon_{\theta r} & \epsilon_{\theta\varphi} \end{vmatrix}}{\begin{vmatrix} \epsilon_{r\theta} & \epsilon_{r\varphi} \\ \epsilon_{\theta\theta} - \hat{k}_j^2 & \epsilon_{\theta\varphi} \end{vmatrix}} A_{j,r}, \tag{20}$$

$$A_{j,\varphi} = \frac{\begin{vmatrix} \epsilon_{rr} & -\epsilon_{r\theta} \\ \epsilon_{\theta r} & \hat{k}_j^2 - \epsilon_{\theta\theta} \end{vmatrix}}{\begin{vmatrix} \epsilon_{r\theta} & \epsilon_{r\varphi} \\ \epsilon_{\theta\theta} - \hat{k}_j^2 & \epsilon_{\theta\varphi} \end{vmatrix}} A_{j,r}. \tag{21}$$

Denoting $A_{j,r}$ by $A_{j,r}=\tilde{A}_j$, Eqs. (20) and (21) provide the components of the eigenvectors $\mathbf{A}(k_j\hat{\mathbf{r}})$ as functions of $\tilde{A}_j$. Moreover, all the particular cases discussed in the next subsections enable us to define known vectors $\mathbf{\Gamma}_j$, which allow the eigenvector components to be expressed in terms of one free parameter $\tilde{A}_j$:

$$\mathbf{A}_j = \tilde{A}_j\mathbf{\Gamma}_j. \tag{22}$$

As mentioned before, this analysis excludes the possibility of having $A_{j,r}=0$. However, this is a quite common situation, since it corresponds to a transverse wave, when the electric field vector has no component along the direction of propagation. This concerns all waves in isotropic homogeneous media, ordinary waves in uniaxial materials, and extraordinary waves traveling along the optic axis of uniaxial materials. These cases require a special analysis.

2. Uniaxial Materials

If the z axis is chosen to be parallel to the optic axis, the permittivity tensor of a uniaxial material has a diagonal form in Cartesian coordinates:

$$\bar{\bar{\epsilon}} = \begin{pmatrix} \epsilon_x & 0 & 0 \\ 0 & \epsilon_x & 0 \\ 0 & 0 & \epsilon_z \end{pmatrix}. \tag{23}$$

Its form in spherical coordinates is obtained by applying the transformation defined by Eqs. (2) and (3):

$$\tilde{\bar{\epsilon}} = \begin{pmatrix} \epsilon_x \sin^2\theta + \epsilon_z \cos^2\theta & (\epsilon_x - \epsilon_z)\sin\theta\cos\theta & 0 \\ (\epsilon_x - \epsilon_z)\sin\theta\cos\theta & \epsilon_z \sin^2\theta + \epsilon_x \cos^2\theta & 0 \\ 0 & 0 & \epsilon_x \end{pmatrix}, \tag{24}$$

i.e., $\epsilon_{r\varphi}=\epsilon_{\varphi r}=\epsilon_{\varphi\theta}=\epsilon_{\theta\varphi}=0$. The set of equations (19) then reduces to

$$\epsilon_{rr}A_{j,r} + \epsilon_{r\theta}A_{j,\theta} = 0, \tag{25}$$

$$\epsilon_{\theta r}A_{j,r} + (\epsilon_{\theta\theta} - \hat{k}_j^2)A_{j,\theta} = 0, \tag{26}$$

$$(\epsilon_{\varphi\varphi} - \hat{k}_j^2)A_{j,\varphi} = 0. \tag{27}$$

There are two possible classes of solutions. The ordinary wave is characterized by refractive index $\hat{k}_1=\sqrt{\epsilon_x}\equiv\sqrt{\epsilon_{\varphi\varphi}}$ and eigenvalue $k_1=k_0\hat{k}_1$; i.e., the coefficient in Eq. (27) vanishes for the ordinary wave:

$$\epsilon_{\varphi\varphi} = \hat{k}_1^2 = 0, \tag{28}$$

and it is then possible to have

$$A_{1,\varphi} \neq 0. \tag{29}$$

If we take into account that for uniaxial materials $\epsilon_x \neq \epsilon_z$, then it can be shown that Eqs. (25) and (26) are incompatible under condition (28), leading to $A_{1,r}=A_{1,\theta}=0$, and thus the ordinary eigenvector has the form

$$\mathbf{A}_1 = \tilde{A}_1\mathbf{\Gamma}_1, \quad \text{with } \mathbf{\Gamma}_1 = \hat{\boldsymbol{\varphi}} \text{ and } \tilde{A}_1 = A_{1,\varphi}. \tag{30}$$

The extraordinary wave is described by the second solution of Eqs. (25)–(27), characterized by

$$A_{j,\varphi} \equiv A_{2,\varphi} = 0. \tag{31}$$

The corresponding eigenvalue ($k_2=k_0\hat{k}_2$) is obtained provided that there exists a nontrivial solution of Eqs. (25) and (26), i.e., provided that

$$\begin{vmatrix} \epsilon_{rr} & \epsilon_{r\theta} \\ \epsilon_{\theta r} & \epsilon_{\theta\theta} - \hat{k}_2^2 \end{vmatrix} = 0, \tag{32}$$

which provides the value of the extraordinary refractive index $\hat{k}_2$ (Ref. 13), which depends on the polar angle:

$$\frac{1}{\hat{k}_2^2(\theta)} = \frac{\sin^2\theta}{\epsilon_z} + \frac{\cos^2\theta}{\epsilon_x}. \tag{33}$$

The extraordinary eigenvector $\mathbf{A}_2$ can then be obtained within a multiplicative constant $A_{2,\theta} \equiv \tilde{A}_2$. We get from Eq. (25)

$$A_{2,r} = -\frac{\epsilon_{r\theta}}{\epsilon_{rr}} A_{2,\theta} \equiv \frac{(\epsilon_z - \epsilon_x)\sin\theta\cos\theta}{\epsilon_x \sin^2\theta + \epsilon_z\cos^2\theta}\tilde{A}_2 \Rightarrow \mathbf{A}_2 = \tilde{A}_2 \boldsymbol{\Gamma}_2,$$

$$\text{with } \boldsymbol{\Gamma}_2 = \frac{(\epsilon_z - \epsilon_x)\sin\theta\cos\theta}{\epsilon_x\sin^2\theta + \epsilon_z\cos^2\theta}\hat{\mathbf{r}} + \hat{\boldsymbol{\theta}}, \qquad \tilde{A}_2 = A_{2,\theta}. \tag{34}$$

Along the optic axis ($\theta=0$), $\Gamma_{2,r}=0$ and the extraordinary solution becomes a transverse wave like the ordinary one, since then $\boldsymbol{\Gamma}_2 = \hat{\boldsymbol{\theta}}$. However, the polarizations of the ordinary and extraordinary waves are orthogonal.

3. Isotropic Medium

The isotropic case is obtained from the uniaxial one by stating that $\epsilon_x = \epsilon_z$. The tensor of permittivity is proportional to the unit tensor, and from Eq. (25) it is evident that the wave has a transversal character with $A_{1,r} = A_{2,r} = 0$. The eigensystem is degenerate, i.e., the eigenvalues are equal with $k_1 = k_2 = k_0\sqrt{\epsilon_x}$, as obtained from Eqs. (15) and (16) or, more directly, from Eqs. (26) and (27). Equations (30) and (34), respectively, provide two independent eigenvectors, transverse to the direction of the wave vector:

$$\mathbf{A}_1 = \tilde{A}_1 \hat{\boldsymbol{\varphi}},$$

$$\mathbf{A}_2 = \tilde{A}_2 \hat{\boldsymbol{\theta}}. \tag{35}$$

5. GENERAL FORM OF THE PLANE WAVE EXPANSION

At an arbitrary point M in space with radius vector $\mathbf{r}_{\mathrm{OM}}$, the nondiverging electric field vector can be expressed as a superposition of plane waves propagating in each direction. For each given direction, the wave vector can take two possible values; thus the general form of the field is given by a three-dimensional Fourier transform (having only two Fourier components along $\mathbf{k}$),

$$\mathbf{E}(\mathbf{r}_{OM}) = \sum_{j=1}^{2} \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\varphi \mathbf{A}_j(\theta,\varphi) \times \exp[ik_j(\theta,\varphi)\hat{\mathbf{r}} \cdot \mathbf{r}_{OM}], \tag{36}$$

where the different components of $\mathbf{A}_j$ are interrelated as discussed in Section 4, each vector being determined within a multiplicative factor. During the numerical treatment of the problem, this double integral has to be discretized into N_θ values along θ and N_φ values along φ. In Section 6 we introduce a multipole expansion of the field. Let n_{Max} be the cutoff associated with the multipole cutoff of the n index [see Eq. (52) below]. We shall discretize the Fourier integral by defining a generalized Fourier space discretization index $\nu \in [1,\ldots,N_\nu]$. As we demonstrate in what follows, the two cutoffs have to be linked by the relation $N_\nu = (n_{\mathrm{Max}}+1)^2$ to obtain a well-determined system of equations for the unknown field amplitudes $\mathbf{A}_j$. Each value of ν will specify a unique direction in k space associated with a unique pair of indices n_θ and n_φ. The polar index goes over a range

$$n_\theta = 1, 2, \ldots, 2n_{\mathrm{Max}} + 1, \tag{37}$$

with the Fourier polar angle θ_ν associated with its discretization index given by

$$\theta_\nu = \pi \frac{n_\theta - 1}{2n_{\mathrm{Max}}}. \tag{38}$$

We thus realize that this yields values for θ_ν that are evenly spaced over the interval $\theta \in [0, \pi]$:

$$\theta_\nu = 0, \frac{\pi}{2n_{\mathrm{Max}}}, \frac{2\pi}{2n_{\mathrm{Max}}}, \ldots, \pi \tag{39}$$

and that when $n_\theta = n_{\mathrm{Max}}+1$, then $\theta = \pi/2$.

For the same density of discretization directions to be preserved, the number of discretization points along φ must depend on θ. In the upper half-space, the polar index n_θ is in the range $n_\theta \leqslant n_{\max}+1$ and the azimuthal index n_φ covers the range

$$n_\varphi = 1, \ldots, n_\theta, \tag{40}$$

while the azimuthal angle φ_ν is given by

$$\varphi_\nu = 2\pi \frac{n_\varphi}{n_\theta + 1} \tag{41}$$

and the generalized index ν in the range $n_\theta \leqslant n_{\mathrm{Max}}+1$, $n_\varphi \leqslant n_\theta$, is given by

$$\nu = n_\varphi + \frac{n_\theta(n_\theta - 1)}{2}. \tag{42}$$

The inverse relations for going from the generalized index ν to n_θ and n_φ provided that the index ν is in the range

$$\nu = \leqslant \frac{(n_{\mathrm{Max}}+1)(n_{\mathrm{Max}}+2)}{2} \tag{43}$$

are

$$n_\theta = \mathrm{Int}\left(\frac{1+\sqrt{8\nu - 7}}{2}\right),$$

$$n_\varphi = \nu - \frac{n_\theta(n_\theta - 1)}{2}. \tag{44}$$

In the lower half-space where $n_\theta > n_{\mathrm{Max}}+1$, to obtain the same density of discretized directions as in the upper half-space, the azimuthal index covers the range

$$n_\varphi = 1, \ldots, 2(n_{\mathrm{Max}}+1) - n_\theta \tag{45}$$

and the associated azimuthal angle φ_ν is given by

$$\varphi_\nu = \frac{2\pi n_\varphi}{2(n_{\mathrm{Max}}+1) - n_\theta + 1}, \tag{46}$$

while the generalized index ν in this range is given by the expression

$$\nu = (n_{\mathrm{Max}}+1)^2 + n_\varphi - \frac{(2n_{\mathrm{Max}} - n_\theta + 3)(2n_{\mathrm{Max}} - n_\theta + 2)}{2},$$

$$n_\theta > n_{\mathrm{Max}} + 1, \qquad n_\varphi \leqslant 2(n_{\mathrm{Max}}+1) - n_\theta. \tag{47}$$

The inverse relations are

$$n_\theta = 2(n_{\mathrm{Max}}+1) - \mathrm{Int}\left(\frac{1+\sqrt{8(n_{\mathrm{Max}}+1)^2 - 8\nu + 1}}{2}\right),$$

$$n_\varphi = \nu + \frac{(2n_{\mathrm{Max}} - n_\theta + 3)(2n_{\mathrm{Max}} - n_\theta + 2)}{2} - (n_{\mathrm{Max}}+1)^2. \tag{48}$$

These rules might seem a bit complicated at first, but they are easy to program. The total number N_ν of discretized values of ν can be obtained by taking into account that the maximum value taken by n_φ is equal to n_θ in the upper half-space, Eq. (40), where n_θ varies from 1 to n_{Max}. Thus the number of discretized directions in the upper half-space is equal to $N_{\mathrm{up}} = \Sigma_1^{n_{\mathrm{Max}}} n_\theta = (n_{\mathrm{Max}}/2)(n_{\mathrm{Max}}+1)$. In the lower half-space, as already explained, we preserve the same number of discretized directions as in the upper half. In the equatorial plane the number of discretizations is equal to $(n_{\mathrm{Max}}+1)$. Thus the total number N_ν is the sum of the numbers in the upper and lower half-spaces and in the equatorial plane:

$$N_\nu = 2N_{\mathrm{up}} + (n_{\mathrm{Max}}+1) = (n_{\mathrm{Max}}+1)^2. \tag{49}$$

By explicitly writing out the values of ν and its corresponding n_θ and n_φ values as illustrated in Tables 1 and 2, we can easily see that the rules of discretization create a rather symmetric sampling of the phase space integral.

In its discretized form, Eq. (36) can be written as

$$\mathbf{E}(\mathbf{r}_{OM}) = \sum_{j=1}^{2}\sum_{\nu=1}^{N_\nu} \mathbf{A}_{j,\nu} \exp(ik_{j,\nu}\hat{\mathbf{r}}_\nu \cdot \mathbf{r}_{OM})$$
$$= \sum_{j=1}^{2}\sum_{\nu=1}^{N_\nu} \tilde{A}_{j,\nu}\boldsymbol{\Gamma}_{j,\nu} \exp(ik_{j,\nu}\hat{\mathbf{r}}_\nu \cdot \mathbf{r}_{OM}), \tag{50}$$

with

Table 1. Discretization Corresponding to a Dipolar Representation ($n_{\mathrm{Max}}=1$)

ν	1	2	3	4
n_θ, n_φ	1, 1	2, 1	2, 2	3, 1
θ_ν, φ_ν	$0, \pi$	$\frac{\pi}{2}, \frac{2\pi}{3}$	$\frac{\pi}{2}, \frac{4\pi}{3}$	π, π

$$\tilde{A}_{j,\nu} = \tilde{A}_j(\theta_\nu, \varphi_\nu)\sin\theta_\nu,$$

$$\boldsymbol{\Gamma}_{j,\nu} = \boldsymbol{\Gamma}_j(\theta_\nu, \varphi_\nu),$$

$$k_{j,\nu} = k_j(\theta_\nu, \varphi_\nu),$$

$$\hat{\mathbf{r}}_\nu = \hat{\mathbf{r}}(\theta_\nu, \varphi_\nu). \tag{51}$$

Thus, the general form of the field in Eq. (50) depends on $2N_\nu$ coefficients $\tilde{A}_{j,\nu}$, which determine the norm of each eigenvector. These unknown field amplitudes could be obtained by matching the tangential field components on the boundaries between different physical regions, in particular on the surface of the optically anisotropic sphere under study. However, this standard procedure requires separation between incident (known) and diffracted (unknown) waves. While it is evident how to do this in Cartesian coordinates and isotropic media, anisotropy and spherical geometry complicate considerably the separation into incident and diffracted waves, in particular inside the sphere. To this aim, we first project the field onto the basis of vector spherical harmonic functions $\mathbf{Y}_{nm}(\theta,\varphi)$, $\mathbf{X}_{nm}(\theta,\varphi)$, and $\mathbf{Z}_{nm}(\theta,\varphi)$. This enables us to explicitly separate the field into two parts, proportional to the spherical Bessel functions j_n and h_n^+. The second part, which diverges at the origin of coordinates has to be eliminated inside the sphere.

6. FIELD EXPANSION ON VECTOR SPHERICAL HARMONICS

In spherical coordinates, several different bases are available to represent the electromagnetic field in any isotropic or anisotropic material. We shall use the basis of vector spherical harmonic functions $\mathbf{Y}_{nm}(\theta,\varphi)$, $\mathbf{X}_{nm}(\theta,\varphi)$, and $\mathbf{Z}_{nm}(\theta,\varphi)$ (Ref. 14), in which basis the electric field takes the form

$$\mathbf{E}(r,\theta,\varphi) = \sum_{n=0}^{n_{\mathrm{Max}}}\sum_{m=-n}^{n} [E_{Ynm}(r)\mathbf{Y}_{nm}(\theta,\varphi) + E_{Xnm}(r)\mathbf{X}_{nm}(\theta,\varphi)$$
$$+ E_{Znm}(r)\mathbf{Z}_{nm}(\theta,\varphi)]. \tag{52}$$

Appendix A establishes the development of the field of a single plane wave on the basis of vector spherical harmonic functions. Each term in Eq. (50) can then be represented by an expansion having the form of Eq. (A20). As it was done in Section 5, we simplify the notation by introducing a single summation index p defined in terms of the two integers n and m through the relations

$$p = n(n+1) + m + 1,$$

$$p_{\mathrm{Max}} = (n_{\mathrm{Max}}+1)^2, \tag{53}$$

or vice versa:

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

$$m(p) = p - 1 - n(p)[n(p)+1], \tag{54}$$

with $\mathrm{Int}(x)$ standing for the integer part of x.

Table 2. Discretization Corresponding to a Quadrupolar Representation for $n_{\mathrm{Max}}=2$

ν	1	2	3	4	5	6	7	8	9
n_θ, n_φ	1, 1	2, 1	2, 2	3, 1	3, 2	3, 3	4, 1	4, 2	5, 1
θ_ν, φ_ν	$0, \pi$	$\frac{\pi}{4}, \frac{2\pi}{3}$	$\frac{\pi}{4}, \frac{4\pi}{3}$	$\frac{\pi}{2}, \frac{\pi}{2}$	$\frac{\pi}{2}, \pi$	$\frac{\pi}{2}, \frac{3\pi}{2}$	$\frac{3\pi}{4}, \frac{2\pi}{3}$	$\frac{3\pi}{4}, \frac{4\pi}{3}$	π, π

Thus, each term in Eq. (50) takes the form of Eq. (A20) with a summation with respect to the simple subscript p:

$$\begin{aligned}\mathbf{\Gamma}_{j,\nu} \exp(ik_{j,\nu}\hat{\mathbf{r}}_{j,\nu}\cdot\mathbf{r}_{OM}) &= \sum_{p=1}^{p_{\mathrm{Max}}} \Bigg\{ a_{h,p,j,\nu}(k_{j,\nu} r_{OM})\mathbf{X}_p(\theta_{OM},\varphi_{OM}) \\ &+ \left[a_p a_{e,p,j,\nu} \frac{j_n(k_{j,\nu} r_{OM})}{k_{j,\nu} r_{OM}} + a_{o,p,j,\nu} j_n'(k_{j,\nu} r_{OM}) \right] \\ &\times \mathbf{Y}_p(\theta_{OM},\varphi_{OM}) + \left[a_{e,p,j,\nu} \frac{(k_{j,\nu} r_{OM} j_n(k_{j,\nu} r_{OM}))'}{k_{j,\nu} r_{OM}} \right. \\ &\left. + a_p a_{o,p,j,\nu} \frac{j_n(k_{j,\nu} r_{OM})}{k_{j,\nu} r_{OM}} \right] \mathbf{Z}_p(\theta_{OM},\varphi_{OM}) \Bigg\}, \end{aligned} \tag{55}$$

where r_{OM}, θ_{OM}, φ_{OM} are the spherical coordinates of M, $a_p = \sqrt{n(p)[n(p)-1]}$, and

$$a_{h,p,j,\nu} = 4\pi i^n \mathbf{X}_p^*(\hat{\mathbf{r}}_\nu)\cdot\mathbf{\Gamma}_{j,\nu}, \qquad a_{e,p,j,\nu} = 4\pi i^{n-1}\mathbf{Z}_p^*(\hat{\mathbf{r}}_\nu)\cdot\mathbf{\Gamma}_{j,\nu},$$

$$a_{o,p,j,\nu} = 4\pi i^{n-1}\mathbf{Y}_p^*(\hat{\mathbf{r}}_\nu)\cdot\mathbf{\Gamma}_{j,\nu}. \tag{56}$$

In a region that does not contain the origin (for example, outside the sphere or in an additional separate layer covering the sphere), there exist other solutions of the Maxwell equations, containing terms that would diverge at the origin. These solutions represent fields radiated from the origin and propagating outward in the direction $r \to \infty$. They can be described in terms of h_n^+, another set of spherical Bessel functions, as mentioned at the end of Section 5. These solutions can be obtained as a linear combination with amplitudes $\tilde{A}_{j,\nu}^{(d)}$ of the terms participating in the expansion given on the right-hand side of Eq. (55) by substituting j_n with h_n^+. Inside the inner region, these amplitudes are null in order to avoid field divergence at the origin. Outside the sphere, they represent the outgoing (scattered, diffracted) solutions; thus the use of superscript (d). The bounded part, containing j_n, plays the role of incident waves in the outermost region and will have amplitudes $\tilde{A}_{j,\nu}^{(i)}$, the superscript (i) standing for incident, which are known outside the sphere from the amplitude and polarization of the incident wave. If the sphere is covered by a layer(s), both $\tilde{A}_{j,\nu}^{(i)}$ and $\tilde{A}_{j,\nu}^{(d)}$ will be unknown constants. Thus the most general form of the electric field vector will contain two terms:

$$\mathbf{E} = \mathbf{E}^{(i)} + \mathbf{E}^{(d)}, \tag{57}$$

The incident (bounded) part has the form, resulting from Eqs. (50) and (55),

$$\begin{aligned}\mathbf{E}^{(i)}(\mathbf{r}_{OM}) = \sum_{p=1}^{p_{\mathrm{Max}}} \sum_{\nu=1}^{N_\nu-1} \sum_{j=1}^{2} \tilde{A}_{j,\nu}^{(i)} \Bigg\{ & a_{h,p,j,\nu} j_n(k_{j,\nu} r_{OM})\mathbf{X}_p(\theta_{OM},\varphi_{OM}) + \left[a_p a_{e,p,j,\nu} \frac{j_n(k_{j,\nu} r_{OM})}{k_{j,\nu} r_{OM}} + a_{o,p,j,\nu} j_n'(k_{j,\nu} r_{OM}) \right] \mathbf{Y}_p(\theta_{OM},\varphi_{OM}) \\ & + \left[a_{e,p,j,\nu} \frac{(k_{j,\nu} r_{OM} j_n(k_{j,\nu} r_{OM}))'}{k_{j,\nu} r_{OM}} + a_p a_{o,p,j,\nu} \frac{j_n(k_{j,\nu} r_{OM})}{k_{j,\nu} r_{OM}} \right] \mathbf{Z}_p(\theta_{OM},\varphi_{OM}) \Bigg\}, \end{aligned} \tag{58}$$

while the scattered (diverging at the origin) part can be obtained by replacing (i) by (d), and j_n by h_n^+:

$$\begin{aligned}\mathbf{E}^{(d)}(\mathbf{r}_{OM}) = \sum_{p=1}^{p_{\mathrm{Max}}} \sum_{\nu=1}^{N_\nu-1} \sum_{j=1}^{2} \tilde{A}_{j,\nu}^{(d)} \Bigg\{ & a_{h,p,j,\nu} h_n^+(k_{j,\nu} r_{OM})\mathbf{X}_p(\theta_{OM},\varphi_{OM}) + \left[a_p a_{e,p,j,\nu} \frac{h_n^+(k_{j,\nu} r_{OM})}{k_{j,\nu} r_{OM}} + a_{o,p,j,\nu} h_n^{+\prime}(k_{j,\nu} r_{OM}) \right] \mathbf{Y}_p(\theta_{OM},\varphi_{OM}) \\ & + \left[a_{e,p,j,\nu} \frac{(k_{j,\nu} r_{OM} h_n^+(k_{j,\nu} r_{OM}))'}{k_{j,\nu} r_{OM}} + a_p a_{o,p,j,\nu} \frac{h_n^+(k_{j,\nu} r_{OM})}{k_{j,\nu} r_{OM}} \right] \mathbf{Z}_p(\theta_{OM},\varphi_{OM}) \Bigg\}. \end{aligned} \tag{59}$$

Given the definition of vector spherical harmonics (Appendix A), it can be observed that $\mathbf{X}_1 = \mathbf{Z}_1 = 0$, while $\mathbf{Y}_1 \neq 0$. In isotropic media the longitudinal field components are null, so the sum in p starts from 2 instead of 1. If we consider that the outside medium is isotropic (having refractive index n_{out}), the eigenvalues are equal to $k_1 = k_2 = n_{\mathrm{out}} k_0$, and the incident and the diffracted eigenvectors are given by Eq. (35). The orthogonality between $\mathbf{Y}_{nm}(\theta,\varphi)$ (parallel to $\mathbf{r}$) and $\mathbf{\Gamma}_{j,\nu}$ [Eq. (35)] leads to $a_{o,nm,j,\nu}^{(i)} = a_{o,nm,j,\nu}^{(d)} = 0$.

7. RESOLUTION OF THE BOUNDARY-VALUE PROBLEM

The unknown field amplitudes $\tilde{A}_{j,\nu}^{(d)}$ and $\tilde{A}_{j,\nu}$ can be found as functions of the incident field amplitudes $\tilde{A}_{j,\nu}^{(i)}$ by applying the boundary conditions on the surface of the sphere. They imply the continuity of the tangential field components. Here we can take advantage of the orthogonality of the basis functions. First, we observe that $\mathbf{Y}_p(\theta_{\mathrm{OM}},\varphi_{\mathrm{OM}})$ is parallel to $\mathbf{r}_{\mathrm{OM}}$, while $\mathbf{X}_p(\theta_{\mathrm{OM}},\varphi_{\mathrm{OM}})$ and $\mathbf{Z}_p(\theta_{\mathrm{OM}},\varphi_{\mathrm{OM}})$ are perpendicular to it. Second, the latter functions are mutually orthogonal for different values of their indices n and m and thus of p. Consequently, it suffices, for each value of p, to consider the continuity of $E_{X,p}$, $E_{Z,p}$, $H_{X,p}$, and $H_{Z,p}$ at $|\mathbf{r}_{\mathrm{OM}}|=R$, radius of the sphere.

The continuity of $E_{X,p}$ gives

$$\sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}^{(i)}a_{h,p,j,\nu}j_n(n_{\mathrm{out}}k_0R) + \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}^{(d)}a_{h,p,j,\nu}h_n^{+}(n_{\mathrm{out}}k_0R) = \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}a_{h,p,j,\nu}j_n(k_{j,\nu}R), \qquad \forall\, p=2,\ldots,p_{\mathrm{Max}}. \tag{60}$$

Since $\mathbf{X}_1=0$, it is evident from Eq. (56) that for $p=1$, Eq. (60) is written $0=0$ and thus has to be excluded from the set. The requirement to preserve an equal number of unknowns and equations leads to disregarding one term in the sum in ν, too. However, we are not losing information concerning the longitudinal field components carried by the terms proportional to $a_{o,l,j,\nu}$ in Eqs. (58) and (59), because the amplitudes $\tilde{A}_{j,\nu}$ are independent of the subscript p and once determined can be used to obtain the longitudinal terms corresponding to $p=1$.

Equation (60) can be further simplified by using the fact that the argument of the spherical Bessel functions j_n and h_n^{+} in the isotropic medium does not depend on the direction of propagation, i.e., on ν. We can thus introduce new amplitudes of the field in the isotropic region outside the sphere, which amplitudes contain the sum over j and ν:

$$A_{h,p}^{(i)} = \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}^{(i)}a_{h,p,j,\nu} \equiv \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}^{(i)}4\pi i^{n}\mathbf{X}_p^{*}(\hat{\mathbf{r}}_\nu)\cdot\boldsymbol{\Gamma}_{j,\nu},$$

$$A_{e,p}^{(i)} = \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}^{(i)}a_{e,p,j,\nu} \equiv \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}^{(i)}4\pi i^{n-1}\mathbf{Z}_p^{*}(\hat{\mathbf{r}}_\nu)\cdot\boldsymbol{\Gamma}_{j,\nu},$$

$$B_{h,p} = \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}^{(d)}a_{h,p,j,\nu} \equiv \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}^{(d)}4\pi i^{n}\mathbf{X}_p^{*}(\hat{\mathbf{r}}_\nu)\cdot\boldsymbol{\Gamma}_{j,\nu},$$

$$B_{e,p} = \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}^{(d)}a_{e,p,j,\nu} \equiv \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}^{(d)}4\pi i^{n-1}\mathbf{Z}_p^{*}(\hat{\mathbf{r}}_\nu)\cdot\boldsymbol{\Gamma}_{j,\nu}. \tag{61}$$

Here, $\tilde{A}_{j,\nu}^{(i)}$ are derived from the amplitude and the polarization of the incident wave. For example, a plane incident wave has a non-null amplitude $\tilde{A}^{(i)}$ only in its direction of propagation (θ_i,φ_i). Denoting its polarization vector by $\hat{\mathbf{e}}^{(i)}$, the first two of Eqs. (61) simply give $A_{h,p}^{(i)}=4\pi i^{n}\mathbf{X}_p^{*}(\theta_i,\varphi_i)\cdot\hat{\mathbf{e}}^{(i)}\tilde{A}^{(i)}$ and $A_{e,p}^{(i)}=4\pi i^{n-1}\mathbf{Z}_p^{*}(\theta_i,\varphi_i)\cdot\hat{\mathbf{e}}^{(i)}\tilde{A}^{(i)}$, as seen in Eqs. (134) and (135) of Ref. 14.

Finally, the field inside the isotropic medium takes the same form as in Ref. 14, and Eq. (60) takes the form

$$A_{h,p}^{(i)}j_n(n_{\mathrm{out}}k_0R) + B_{h,p}h_n^{+}(n_{\mathrm{out}}k_0R) = \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}a_{h,p,j,\nu}j_n(k_{j,\nu}R), \qquad \forall\, p=2,\ldots p_{\mathrm{Max}}. \tag{62}$$

The continuity of $E_{Z,nm}$ gives

$$A_{e,p}^{(i)}\frac{[n_{\mathrm{out}}k_0Rj_n(n_{\mathrm{out}}k_0R)]'}{n_{\mathrm{out}}k_0R} + B_{e,p}\frac{[n_{\mathrm{out}}k_0Rh_n^{+}(n_{\mathrm{out}}k_0R)]'}{n_{\mathrm{out}}k_0R} = \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}\left\{a_{e,p,j,\nu}\frac{[k_{j,\nu}Rj_n(k_{j,\nu}R)]'}{k_{j,\nu}R} + a_pa_{o,p,j,\nu}\frac{j_n(k_{j,\nu}R)}{k_{j,\nu}R}\right\}, \qquad \forall\, p=2,\ldots p_{\mathrm{Max}}. \tag{63}$$

Equation (63) can be expressed in a different form, more common in the studies using spherical coordinates:

$$A_{e,p}^{(i)}\frac{\psi_n'(n_{\mathrm{out}}k_0R)}{n_{\mathrm{out}}k_0R} + B_{e,p}\frac{\xi_n'(n_{\mathrm{out}}k_0R)}{n_{\mathrm{out}}k_0R} = \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}\left[a_{e,p,j,\nu}\frac{\psi_n'(k_{j,\nu}R)}{k_{j,\nu}R} + a_pa_{o,p,j,\nu}\frac{j_n(k_{j,\nu}R)}{k_{j,\nu}R}\right], \tag{64}$$

where ψ_n and ξ_n are Ricatti–Bessel functions,[14] which are linked, respectively, with j_n and h_n^{+} by

$$\psi_n(z)=zj_n(z), \qquad \xi_n(z)=zh_n^{+}(z). \tag{65}$$

The second two sets of equations are obtained from Maxwell equations projected onto the vector spherical harmonic basis:

$$a_p\frac{E_{X,p}}{r} = i\omega\mu_0H_{Y,p}, \tag{66}$$

$$a_p\frac{E_{Y,p}}{r} - \frac{E_{Z,p}}{r} - \frac{\mathrm{d}E_{Z,p}}{\mathrm{d}r} = i\omega\mu_0H_{X,p}, \tag{67}$$

$$\frac{E_{X,p}}{r} + \frac{\mathrm{d}E_{X,p}}{\mathrm{d}r} = i\omega\mu_0H_{Z,p}, \tag{68}$$

$$a_p\frac{H_{X,p}}{r} = -i\omega D_{Y,p}, \tag{69}$$

$$a_p\frac{H_{Y,p}}{r} - \frac{H_{Z,p}}{r} - \frac{\mathrm{d}H_{Z,p}}{\mathrm{d}r} = -i\omega D_{X,p}, \tag{70}$$

$$\frac{H_{X,p}}{r}+\frac{\mathrm{d}H_{X,p}}{\mathrm{d}r}=-i\omega D_{Z,p}. \tag{71}$$

Equations (67), (58) and (59) enable us to express $H_{X,p}$ as a function of $E_{Z,p}$. After some transformations using the properties of j_n, h_n^+, ξ_n, and ψ_n (described in detail in Ref. 14), the continuity of $H_{X,nm}$ gives the third relation:

$$n_{\mathrm{out}}k_0[A_{e,p}^{(i)}j_n(n_{\mathrm{out}}k_0R)+B_{e,p}h_n^+(n_{\mathrm{out}}k_0R)] = \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\widetilde{A}_{j,\nu}a_{e,p,j,\nu}k_{j,\nu}j_n(k_{j,\nu}R). \tag{72}$$

Equation (68) represents $H_{Z,p}$ as a function of $E_{X,p}$, and its continuity gives

$$A_{h,p}^{(i)}\psi_n'(n_{\mathrm{out}}k_0R)+B_{h,p}\xi_n'(n_{\mathrm{out}}k_0R) = \sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\widetilde{A}_{j,\nu}a_{h,p,j,\nu}\psi_n'(k_{j,\nu}R). \tag{73}$$

Equations (62), (64), (72), and (73) form a set of equations sufficient to find the unknown diffracted amplitudes $\widetilde{A}_{j,\nu}$, $B_{e,p}$, and $B_{h,p}$ when the incident field amplitudes $A_{e,p}^{(i)}$ and $A_{h,p}^{(i)}$ are given, a set that contains $4p_{\mathrm{Max}}-4$ equations. In order that the number of unknowns be equal to the number of equations, it is necessary to impose that $N_\nu=p_{\mathrm{Max}}$; i.e., the number of unknowns in the outside medium must be equal to the number of unknowns inside the sphere. It is worth noticing that the system of $4p_{\mathrm{Max}}-4$ equations is decoupled with respect to the subscript p, i.e., with respect to the angular coordinates of the observation point M. For each value of p, it is possible to eliminate half of the unknowns, $B_{e,p}$ and $B_{h,p}$, and to obtain a linear system for $\widetilde{A}_{j,\nu}$. In order to simplify the formulas and to obtain relations similar in form to Mie coefficients, let us introduce the symbolic notation. First, we define four diagonal matrices with elements given by

$$(\Psi_0)_{pq}=\delta_{pq}\psi_n(n_{\mathrm{out}}k_0R),\qquad (\Psi_0')_{pq}=\delta_{pq}\psi_n'(n_{\mathrm{out}}k_0R),$$
$$(\xi_0)_{pq}=\delta_{pq}\xi_n(n_{\mathrm{out}}k_0R),\qquad (\xi_0')_{pq}=\delta_{pq}\xi_n'(n_{\mathrm{out}}k_0R), \tag{74}$$

Second, we introduce five matrices,

$$\Psi_{h,a}=(\Psi_{h,a_1},\Psi_{h,a_2}),\quad \text{with } (\Psi_{h,a_j})_{p\nu}=a_{h,p,j,\nu}\psi_n(k_{j,\nu}R),$$
$$\Psi_{h,a}'=(\Psi_{h,a_1}',\Psi_{h,a_2}'),\quad \text{with } (\Psi_{h,a_j}')_{p\nu}=a_{h,p,j,\nu}\psi_n'(k_{j,\nu}R),$$
$$\xi_{h,a}=(\xi_{h,a_1},\xi_{h,a_2}),\quad \text{with } (\xi_{h,a_j})_{p\nu}=a_{h,p,j,\nu}\xi_n(k_{j,\nu}R),$$
$$\xi_{h,a}'=(\xi_{h,a_1}',\xi_{h,a_2}'),\quad \text{with } (\xi_{h,a_j}')_{p\nu}=a_{h,p,j,\nu}\xi_n'(k_{j,\nu}R),$$
$$J_{o,a}=(J_{o,a_1},J_{o,a_2}),\quad \text{with } (J_{o,a_j})_{p\nu}=a_pa_{o,p,j,\nu}j_n(k_{j,\nu}R), \tag{75}$$

and similar definitions by exchanging the subscript h with e and o. Third, the wavenumbers of different waves are grouped in a diagonal matrix:

$$\left(\frac{k_{\mathrm{out}}}{k_{\mathrm{in}}}\right)=\begin{pmatrix}\left(\frac{k_{\mathrm{out}}}{k_{\mathrm{in},1}}\right) & 0\\ 0 & \left(\frac{k_{\mathrm{out}}}{k_{\mathrm{in},2}}\right)\end{pmatrix}\quad \text{with } \left(\frac{k_{\mathrm{out}}}{k_{\mathrm{in},j}}\right)_{\tau\nu}=\delta_{\tau\nu}\frac{n_{\mathrm{out}}k_0}{k_{j,\nu}}. \tag{76}$$

With this notation, the four equations (62), (73), (64), and (72) take the matrix form

$$\Psi_0[A_h^{(i)}]+\xi_0[B_h]=\Psi_{h,a}\left(\frac{k_{\mathrm{out}}}{k_{\mathrm{in}}}\right)[\widetilde{A}], \tag{77}$$

$$\Psi_0'[A_h^{(i)}]+\xi_0'[B_h]=\Psi_{h,a}'[\widetilde{A}], \tag{78}$$

$$\Psi_0'[A_e^{(i)}]+\xi_0'[B_e]=(\Psi_{e,a}'+J_{o,a})\left(\frac{k_{\mathrm{out}}}{k_{\mathrm{in}}}\right)[\widetilde{A}], \tag{79}$$

$$\Psi_0[A_e^{(i)}]+\xi_0[B_e]=\Psi_{e,a}[\widetilde{A}], \tag{80}$$

where the columns in the square brackets contain the corresponding field amplitudes, for example $[B_e]_p=B_{e,p}$.

Let us at first eliminate the amplitudes $B_{h,p}$ and $B_{e,p}$. To this end, Eqs. (77) and (78) are multiplied, respectively, by ξ_0' and ξ_0 and the results subtracted. With the Wronskian identity,

$$\psi_n(x)\xi_n'(x)-\psi_n'(x)\xi_n(x)=i,\qquad \forall\, n, \tag{81}$$

the resulting equation takes the form

$$i[A_h^{(i)}]=\left[\xi_0'\Psi_{h,a}\left(\frac{k_{\mathrm{out}}}{k_{\mathrm{in}}}\right)-\xi_0\Psi_{h,a}'\right][\widetilde{A}]. \tag{82}$$

By multiplying Eqs. (79) and (80) by ξ_0 and ξ_0' and subtracting them, we can eliminate $B_{e,p}$, and the result has a similar form:

$$i[A_e^{(i)}]=\left[\xi_0'\Psi_{e,a}-\xi_0(\Psi_{e,a}'+J_{o,a})\left(\frac{k_{\mathrm{out}}}{k_{\mathrm{in}}}\right)\right][\widetilde{A}]. \tag{83}$$

Equations (82) and (83) form a set of $2(N_\nu-1)$ equations that can be solved by a unique matrix inversion,

$$[\widetilde{A}]=iU^{-1}\begin{pmatrix}[A_h^{(i)}]\\ [A_e^{(i)}]\end{pmatrix}, \tag{84}$$

where

$$U=\begin{pmatrix}\xi_0'\Psi_{h,a}\left(\frac{k_{\mathrm{out}}}{k_{\mathrm{in}}}\right)-\xi_0\Psi_{h,a}'\\ \xi_0'\Psi_{e,a}-\xi_0(\Psi_{e,a}'+J_{o,a})\left(\frac{k_{\mathrm{out}}}{k_{\mathrm{in}}}\right)\end{pmatrix}. \tag{85}$$

Multiplying Eqs. (77) and (78) respectively by Ψ_0' and Ψ_0 and subtracting the results permits the elimination of $[A_h^{(i)}]$:

$$i[B_h]=\left[\Psi_0\Psi'_{h,a}-\Psi'_0\Psi_{h,a}\left(\frac{k_{\rm out}}{k_{\rm in}}\right)\right][\tilde{A}]. \quad (86)$$

By multiplying Eqs. (79) and (80) by Ψ_0 and Ψ'_0 and subtracting them we can eliminate $[A_e^{(i)}]$:

$$i[B_e]=\left[\Psi_0(\Psi'_{e,a}+J_{o,a})\left(\frac{k_{\rm out}}{k_{\rm in}}\right)-\Psi'_0\Psi_{e,a}\right][\tilde{A}]. \quad (87)$$

Combining Eqs. (84), (86), and (87) gives the link between $B_{h,p}$ $B_{e,p}$ and $A_{h,p}^{(i)}$, $A_{e,p}^{(i)}$ in a matrix form,

$$\begin{pmatrix}[B_h]\\ [B_e]\end{pmatrix}=\begin{pmatrix}T_{hh} & T_{he}\\ T_{eh} & T_{ee}\end{pmatrix}\begin{pmatrix}[A_h^{(i)}]\\ [A_e^{(i)}]\end{pmatrix}, \quad (88)$$

where the T matrix is equal to

$$T=\begin{pmatrix}T_{hh} & T_{he}\\ T_{eh} & T_{ee}\end{pmatrix}=\begin{pmatrix}\Psi_0\Psi'_{h,a}-\Psi'_0\Psi_{h,a}\left(\frac{k_{\rm out}}{k_{\rm in}}\right)\\ \Psi_0(\Psi'_{e,a}+J_{o,a})\left(\frac{k_{\rm out}}{k_{\rm in}}\right)-\Psi'_0\Psi_{e,a}\end{pmatrix}$$
$$\times\begin{pmatrix}\xi'_0\Psi_{h,a}\left(\frac{k_{\rm out}}{k_{\rm in}}\right)-\xi_0\Psi'_{h,a}\\ \xi'_0\Psi_{e,a}-\xi_0(\Psi'_{e,a}+J_{o,a})\left(\frac{k_{\rm out}}{k_{\rm in}}\right)\end{pmatrix}^{-1}. \quad (89)$$

Thus the field is determined everywhere. The amplitudes $B_{e,p}$ and $B_{h,p}$ serve to obtain the physical quantities, such as total scattering, extinction and absorption cross section, and radar and differential cross section, using classical formulas, as recalled in Ref. 14.

In the case when the sphere is optically isotropic, the wavenumber does not depend on the direction of propagation, and it is possible to make the same change of unknowns inside the sphere as was done in the outer region using Eq. (61). We thus introduce the amplitudes $A_{h,p}^{(1)}$ and $A_{e,p}^{(1)}$ given by

$$A_{h,p}^{(1)}=\sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}a_{h,p,j,\nu},$$

$$A_{e,p}^{(1)}=\sum_{\nu=1}^{N_\nu-1}\sum_{j=1}^{2}\tilde{A}_{j,\nu}a_{e,p,j,\nu}. \quad (90)$$

Moreover, as $a_{o,p,j,\nu}=0$, the matrix $J_{o,a}$ becomes null. The product of matrices $\Psi_{h,a}$ and $\Psi_{e,a}$ with $[\tilde{A}]$ gives diagonal matrices equal to

$$(\Psi_{h,a}[\tilde{A}])_p=\psi_n(n_1k_0R)A_{h,p}^{(1)},$$

$$(\Psi_{e,a}[\tilde{A}])_p=\psi_n(n_1k_0R)A_{e,p}^{(1)}, \quad (91)$$

and similar expressions for $\Psi'_{h,a}$ and $\Psi'_{e,a}$. Equations (82) and (83) become diagonal and yield

$$iA_{h,p}^{(i)}=\left[\xi'_n(n_{\rm out}k_0R)\psi_n(n_1k_0R)\frac{n_{\rm out}}{n_1}-\xi_n(n_{\rm out}k_0R)\psi'_n(n_1k_0R)\right]A_{h,p}^{(1)},$$

$$iA_{e,p}^{(i)}=\left[\xi'_n(n_{\rm out}k_0R)\psi_n(n_1k_0R)-\xi_n(n_{\rm out}k_0R)\psi'_n(n_1k_0R)\frac{n_{\rm out}}{n_1}\right]A_{e,p}^{(1)}. \quad (92)$$

The same is valid for Eqs. (86) and (87):

$$iB_{h,p}=\left[\psi_n(n_{\rm out}k_0R)\psi'_n(n_1k_0R)-\psi'_n(n_{\rm out}k_0R)\psi_n(n_1k_0R)\frac{n_{\rm out}}{n_1}\right]A_{h,p}^{(1)},$$

$$iB_{e,p}=\left[\psi_n(n_{\rm out}k_0R)\psi'_n(n_1k_0R)\frac{n_{\rm out}}{n_1}-\psi'_n(n_{\rm out}k_0R)\psi_n(n_1k_0R)\right]A_{e,p}^{(1)}. \quad (93)$$

Matrix $\mathbf{U}$ becomes diagonal, and thus the T matrix takes a diagonal form with elements generally referred to as Mie coefficients:

$$(T_{hh})_{pq}=\frac{\psi_n(n_{\rm out}k_0R)\psi'_n(n_1k_0R)-\psi'_n(n_{\rm out}k_0R)\psi_n(n_1k_0R)\frac{n_{\rm out}}{n_1}}{\xi'_n(n_{\rm out}k_0R)\psi_n(n_1k_0R)\frac{n_{\rm out}}{n_1}-\xi_n(n_{\rm out}k_0R)\psi'_n(n_1k_0R)}\delta_{pq},$$

$$(T_{ee})_{pq}=\frac{\psi_n(n_{\rm out}k_0R)\psi'_n(n_1k_0R)\frac{n_{\rm out}}{n_1}-\psi'_n(n_{\rm out}k_0R)\psi_n(n_1k_0R)}{\xi'_n(n_{\rm out}k_0R)\psi_n(n_1k_0R)-\xi_n(n_{\rm out}k_0R)\psi'_n(n_1k_0R)\frac{n_{\rm out}}{n_1}}\delta_{pq}.$$

$$T_{eh}=T_{he}=0. \quad (94)$$

In that case, there is no coupling between the two fundamental polarizations nor between different p components. In other words, scattering by an isotropic sphere does not mix electric and magnetic degrees of freedom, nor does it mix multipole orders. On the other hand, anisotropy can mix multipole orders as well as electric and magnetic degrees of freedom.

8. UNIAXIAL MATERIALS

As already observed in Subsection 4.B.2, the equations are simplified for a uniaxial material. First, the wavenumber of the ordinary wave does not depend on the direction of propagation, $k_{1,\nu}=k_0\sqrt{\epsilon_x}, \forall \nu$. Second, the ordinary wave is transverse, and thus $a_{o,p,l,\nu}=0$. Third, the ordinary-wave eigenvector does not depend on θ, $\mathbf{\Gamma}_{1,\nu}=\hat{\boldsymbol{\varphi}}$. The fourth simplification concerns the extraordinary wave. Its eigenvalue and eigenvector are independent of φ, as obtained from Eqs. (33) and (34). As a result, the φ dependence in Eqs. (58) and (59) remains only in the unknown amplitudes $\tilde{A}_{j,\nu}=\tilde{A}_j(\theta_\nu,\varphi_\nu)\sin\theta_\nu$ and in the coefficients $a_{h,p,j,\nu}$, $a_{e,p,j,\nu}$, and $a_{o,p,j,\nu}$. However, the φ dependence of these coefficients has a very simple form when the eigenvectors $\mathbf{\Gamma}_{j,\nu}$ do not depend on φ. This can be observed in Eqs. (7)–(10) and (13)–(17) of Ref. 14, summarized here in Eq. (A22). Taking them into account, as well as the above-mentioned arguments, it is possible to separate the variables in the coefficients defined in Eq. (56):

$$a_{h,p,1,\nu}=4\pi i^n\mathbf{X}_p^*(\hat{\mathbf{r}}_\nu)\cdot\mathbf{\Gamma}_{1,\nu}=4\pi i^n\mathbf{X}_p^*(\theta_\nu,\varphi_\nu)\cdot\hat{\boldsymbol{\varphi}}_\nu=2\pi\alpha_{h,p,1}(\theta_\nu)\exp[im(p)\varphi_\nu],$$

$$a_{e,p,1,\nu}=4\pi i^{n-1}\mathbf{Z}_p^*(\hat{\mathbf{r}}_\nu)\cdot\mathbf{\Gamma}_{1,\nu}=4\pi i^{n-1}\mathbf{Z}_p^*(\theta_\nu,\varphi_\nu)\,.\,\hat{\boldsymbol{\varphi}}_\nu=2\pi\alpha_{e,p,1}(\theta_\nu)\exp[im(p)\varphi_\nu],$$

$$a_{o,p,1,\nu}=4\pi i^{n-1}\mathbf{Y}_p^*(\hat{\mathbf{r}}_\nu)\cdot\mathbf{\Gamma}_{1,\nu}=4\pi i^{n-1}\mathbf{Y}_p^*(\theta_\nu,\varphi_\nu)\cdot\hat{\boldsymbol{\varphi}}_\nu=0,$$

$$a_{h,p,2,\nu}=4\pi i^n\mathbf{X}_p^*(\hat{\mathbf{r}}_\nu)\cdot\mathbf{\Gamma}_{2,\nu}=4\pi i^n\mathbf{X}_p^*(\theta_{n_\theta},\varphi_\nu)\,.\,\hat{\boldsymbol{\theta}}_\nu=2\pi\alpha_{h,p,2}(\theta_\nu)\exp[im(p)\varphi_\nu],$$

$$a_{e,p,2,\nu}=4\pi i^{n-1}\mathbf{Z}_p^*(\hat{\mathbf{r}}_\nu)\cdot\mathbf{\Gamma}_{2,\nu}=4\pi i^{n-1}\mathbf{Z}_p^*(\theta_\nu,\varphi_\nu)\cdot\hat{\boldsymbol{\theta}}_\nu=2\pi\alpha_{e,p,2}(\theta_\nu)\exp[im(p)\varphi_\nu],$$

$$a_{o,p,2,\nu}=4\pi i^{n-1}\mathbf{Y}_p^*(\hat{\mathbf{r}}_\nu)\cdot\mathbf{\Gamma}_{2,\nu}=4\pi i^{n-1}Y_p^*(\theta_\nu,\varphi_\nu)\Gamma_{2,\nu,r}=2\pi\alpha_{o,p,2}(\theta_\nu)\exp[im(p)\varphi_\nu]. \quad (95)$$

The new coefficients α can be obtained by using Eqs. (A22) and are expressed by using the normalized associated Legendre functions $\bar{P}_n^m(\cos\theta_\nu)$:

$$\alpha_{h,p,1}(\theta_\nu)=-\frac{2i^n}{a_p}\frac{\mathrm{d}\bar{P}_n^m(\cos\theta_\nu)}{\mathrm{d}\theta_\nu},$$

$$\alpha_{e,p,1}(\theta_\nu)=-\frac{2i^n m}{a_p\sin\theta_\nu}\bar{P}_n^m(\cos\theta_\nu),$$

$$\alpha_{h,p,2}(\theta_\nu)=-\frac{2i^{n+1}}{a_p\sin\theta_\nu}\bar{P}_n^m(\cos\theta_\nu),$$

$$\alpha_{e,p,2}(\theta_\nu)=-\frac{2i^{n-1}}{a_p}\frac{\mathrm{d}\bar{P}_n^m(\cos\theta_\nu)}{\mathrm{d}\theta_\nu},$$

$$\alpha_{o,p,2}(\theta_\nu)=2i^{n-1}\bar{P}_n^m(\cos\theta_\nu)\frac{(\epsilon_z-\epsilon_x)\sin\theta_\nu\cos\theta_\nu}{\epsilon_x\sin^2\theta_\nu+\epsilon_z\cos^2\theta_\nu}, \quad (96)$$

where n and m are determined from p through Eq. (54). Quite important is that the new coefficients α depend on θ_ν but not on φ_ν. This fact enables us to reduce significantly the size of the set of equations to solve by introducing new amplitudes in a manner similar to the way they are used in Eqs. (61), which are, in fact, Fourier transforms of $\tilde{A}_{j,\nu}$ with respect to φ:

$$\tilde{A}_{j,p,n_\theta}=\frac{1}{2\pi}\sum_{n_\varphi=1}^{n_\theta}\tilde{A}_{j,\nu(n_\theta,n_\varphi)}\exp[im(p)\varphi_{n_\varphi}]. \quad (97)$$

With this substitution, the set of Eqs. (82) and (83) changes into a set having a much smaller number of unknowns. When explicitly written, it takes the form

$$iA_{h,p}^{(i)}=\sum_{n_\theta=1}^{2n_{\mathrm{Max}}}\sum_{j=1}^{2}\tilde{A}_{j,p,n_\theta}\alpha_{h,p,j,n_\theta}\left[\xi_n'(n_{\mathrm{out}}k_0R)\psi_n(k_{j,n_\theta}R)\frac{n_{\mathrm{out}}k_0}{k_{j,n_\theta}}-\xi_n(n_{\mathrm{out}}k_0R)\psi_n'(k_{j,n_\theta}R)\right],$$

$$iA_{e,p}^{(i)}=\sum_{n_\theta=1}^{2n_{\mathrm{Max}}}\sum_{j=1}^{2}\tilde{A}_{j,p,n_\theta}\left\{\alpha_{e,p,j,n_\theta}\xi_n'(n_{\mathrm{out}}k_0R)\psi_n(k_{j,n_\theta}R)-\xi_n(n_{\mathrm{out}}k_0R)[\alpha_{e,p,j,n_\theta}\psi_n'(k_{j,n_\theta}R)+a_p\alpha_{o,p,j,n_\theta}j_n(k_{j,n_\theta}R)]\frac{n_{\mathrm{out}}k_0}{k_{j,n_\theta}}\right\}. \quad (98)$$

In addition to the change of the coefficients $a\to\alpha$, much more important is to notice that the summation in ν generally containing $N_\nu-1=n_{\mathrm{Max}}(n_{\mathrm{Max}}+2)$ terms has been reduced to only $2n_{\mathrm{Max}}$ terms for each p, i.e., almost n_{Max} times. Since $p_{\mathrm{Max}}=N_\nu$, a significant reduction of the required number of vector spherical harmonics is achieved.

After the amplitudes $\tilde{A}_{j,p,n_\theta}$ are determined by solving the linear system of algebraic equations, the diffracted amplitudes in the outermost medium, $B_{e,p}$ and $B_{h,p}$, are found by using Eqs. (72) and (73). In addition, the inverse Fourier transform of Eq. (97) gives the amplitudes of each plane wave $\tilde{A}_{j,p,\nu(n_\theta,n_\varphi)}$ inside the uniaxial material.

9. CONCLUSIONS

Using vector spherical harmonic functions as a basis, we succeeded in obtaining the general form of the electromagnetic field in an arbitrary anisotropic homogeneous medium. Applying the boundary conditions across the surface of a sphere allows us to find the components of the diffracted field from those of the incident field through a matrix inversion. This semianalytical method reduces, of course, to the analytic Mie theory when the sphere is filled with isotropic medium. The case of uniaxial material, characterized by a φ-independent permittivity tensor, leads to some simplifications and to a significant reduction of the size of the matrix to be inverted.

This work presents the first step toward resolving the problem of diffraction by an arbitrary-shaped anisotropic object or an inhomogeneous anisotropic sphere, for which the permittivity tensor is a function of the Cartesian coordinates. This problem is treated in detail in Part II (this issue):[16] its solution is based on this work and extends the differential theory, published in Ref. 14 to anisotropic bodies.

APPENDIX A: VECTOR SPHERICAL HARMONICS DEVELOPMENT OF AN ARBITRARY PLANE WAVE

In order to establish the development of an arbitrary vector plane wave, let us recall that it is well known that an arbitrary scalar plane wave can be represented in terms of Legendre polynomials,

$$\exp(i\mathbf{k}\cdot\mathbf{r})=\sum_{q=0}^{\infty}(2q+1)i^q j_q(kr)P_q(\hat{\mathbf{r}}_k\cdot\hat{\mathbf{r}}), \tag{A1}$$

where P_q are the Legendre polynomials, $\hat{\mathbf{r}}=\mathbf{r}/r$, and $\hat{\mathbf{r}}_k \equiv \hat{\mathbf{k}}=\mathbf{k}/k$.

The addition theorem for Legendre polynomials represents them in terms of scalar spherical harmonics $Y_{qm}(\theta,\varphi)$:

$$P_q(\hat{\mathbf{r}}_k\cdot\hat{\mathbf{r}})=\frac{4\pi}{2q+1}\sum_{m=-q}^{q}Y^*_{qm}(\hat{\mathbf{r}}_k)Y_{qm}(\hat{\mathbf{r}}). \tag{A2}$$

The scalar spherical harmonics are expressed in terms of associated Legendre functions P_q^m or of normalized associated Legendre functions $\bar{P}_q^m$:

$$\begin{aligned}Y_{qm}(\theta,\varphi)&=\left[\frac{2m+1}{4\pi}\frac{(q-m)!}{(q+m)!}\right]^{1/2}P_q^m(\cos\theta)\exp(im\varphi)\\&=\bar{P}_q^m(\cos\theta)\exp(im\varphi).\end{aligned} \tag{A3}$$

Equation (A2) allows us to write the expansion of a scalar plane wave in terms of the scalar spherical harmonics:

$$\exp(i\mathbf{k}\cdot\mathbf{r})=4\pi\sum_{q=0}^{\infty}\sum_{m=-q}^{q}i^q j_q(kr)Y_{qm}(\hat{\mathbf{r}})Y^*_{qm}(\mathbf{r}_k). \tag{A4}$$

The next step is to generalize these expressions to a vector plane wave with arbitrary vector amplitude. To this end we invoke a set of vector spherical harmonics. The first set, denoted $\mathbf{Y}^m_{n,n+1}$, $\mathbf{Y}^m_{n,n}$, $\mathbf{Y}^m_{n,n-1}$ is obtained through the so-called angular coupling formalism [15] by using the Cartesian spherical unit vectors:

$$\hat{\boldsymbol{\chi}}_1=-\frac{1}{\sqrt{2}}(\hat{\mathbf{x}}+i\hat{\mathbf{y}}),$$

$$\hat{\boldsymbol{\chi}}_0=\hat{\mathbf{z}},$$

$$\hat{\boldsymbol{\chi}}_{-1}=\frac{1}{\sqrt{2}}(\hat{\mathbf{x}}-i\hat{\mathbf{y}}). \tag{A5}$$

They form a complete orthogonal basis for the three-dimensional vectors:

$$\sum_{\mu=-1}^{1}\hat{\boldsymbol{\chi}}^*_\mu\hat{\boldsymbol{\chi}}_\mu=\mathbb{I},\qquad \hat{\boldsymbol{\chi}}^*_\mu\cdot\hat{\boldsymbol{\chi}}_\tau=\delta_{\mu\tau}. \tag{A6}$$

Making use of Clebsch–Gordon coefficients, we define the first set of vector spherical harmonics in terms of the scalar spherical harmonics:

$$\mathbf{Y}^m_{n,q}=\sum_{\mu=-1}^{1}(q,m-\mu;1,\mu|n,m)Y_{q,m-\mu}\hat{\boldsymbol{\chi}}_\mu,$$

$$q=n-1,n,n+1. \tag{A7}$$

These vectors form a complete and orthogonal basis for functions depending on angular variables:

$$\int_0^{4\pi}\mathrm{d}\Omega\,Y^{*m}_{n,q}(\hat{\mathbf{r}})\cdot Y^{m'}_{n',q'}(\hat{\mathbf{r}})=\delta_{nn'}\delta_{mm'}\delta_{qq'},$$

$$\sum_{n,m,q}Y^{*m}_{n,q}(\hat{\mathbf{r}})Y^{*m}_{n,q}(\hat{\mathbf{r}}')=\mathbb{I}\delta_\Omega(\hat{\mathbf{r}},\hat{\mathbf{r}}'). \tag{A8}$$

The vector analog of the scalar addition theorem, Eq. (A2) is

$$\mathbb{I}P_q(\hat{\mathbf{r}}_k\cdot\hat{\mathbf{r}})=\frac{4\pi}{2q+1}\sum_{n,m}\mathbf{Y}^{*m}_{nq}(\hat{\mathbf{r}}_k)\mathbf{Y}^m_{nq}(\hat{\mathbf{r}}), \tag{A9}$$

which allows us to write the vector analog of Eq. (A4):

$$\mathbb{I}\exp(i\mathbf{k}\cdot\mathbf{r})=4\pi\sum_{n,m,q}i^q j_q(kr)\mathbf{Y}^{*m}_{nq}(\hat{\mathbf{r}}_k)\mathbf{Y}^m_{nq}(\hat{\mathbf{r}}). \tag{A10}$$

This expression can be used to express the vector plane wave polarized in direction $\boldsymbol{\Gamma}$ in the following form:

$$\begin{aligned}\boldsymbol{\Gamma}\exp(i\mathbf{k}\cdot\mathbf{r})&=\mathbb{I}\cdot\boldsymbol{\Gamma}\exp(i\mathbf{k}\cdot\mathbf{r})\\&=4\pi\sum_{n,m,q}i^q j_q(kr)\mathbf{Y}^{*m}_{nq}(\hat{\mathbf{r}}_k)\mathbf{Y}^m_{nq}(\hat{\mathbf{r}})\cdot\boldsymbol{\Gamma}.\end{aligned} \tag{A11}$$

When working in spherical coordinates, it is convenient to define a second set of vector spherical harmonics $\mathbf{Y}_{nm}$, $\mathbf{X}_{nm}$, $\mathbf{Z}_{nm}$, sometimes known as $\mathbf{Y}^{(o)}_{n,m}$, $\mathbf{Y}^{(m)}_{n,m}$, $\mathbf{Y}^{(e)}_{n,m}$. These are related to $\mathbf{Y}^m_{n,n+1}$, $\mathbf{Y}^m_{n,n}$, $\mathbf{Y}^m_{n,n-1}$ via the relations

$$\mathbf{X}_{nm} \equiv \mathbf{Y}^{(m)}_{n,m} \equiv \frac{1}{i}\mathbf{Y}^{m}_{n,n},$$

$$\mathbf{Z}_{nm} \equiv \mathbf{Y}^{(e)}_{n,m} \equiv \left(\frac{n+1}{2n+1}\right)^{1/2}\mathbf{Y}^{m}_{n,n-1} + \left(\frac{n}{2n+1}\right)^{1/2}\mathbf{Y}^{m}_{n,n+1},$$

$$\mathbf{Y}_{nm} \equiv \mathbf{Y}^{(o)}_{n,m} \equiv \left(\frac{n}{2n+1}\right)^{1/2}\mathbf{Y}^{m}_{n,n-1} - \left(\frac{n+1}{2n+1}\right)^{1/2}\mathbf{Y}^{m}_{n,n+1}, \tag{A12}$$

with inverse relations

$$\frac{1}{i}\mathbf{Y}^{m}_{n,n} = i\mathbf{X}_{nm},$$

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

$$\mathbf{Y}^{m}_{n,n+1} = \left(\frac{n}{2n+1}\right)^{1/2}\mathbf{Z}_{nm} - \left(\frac{n+1}{2n+1}\right)^{1/2}\mathbf{Y}_{nm}. \tag{A13}$$

With these new vector spherical harmonics, the three terms in the sum in $q=n-1,n,n+1$ in Eq. (A10) become

$q=n-1$

$$\begin{aligned}4\pi\sum_{n,m} i^{n-1}j_{n-1}(kr)\mathbf{Y}^{*m}_{n,n-1}(\hat{\mathbf{k}})\mathbf{Y}^{m}_{n,n-1}(\hat{\mathbf{r}}) &= 4\pi\sum_{n,m} i^{n-1}j_{n-1}(kr)\\ &\times\left\{\frac{n+1}{2n+1}\mathbf{Z}_{nm}(\hat{\mathbf{r}})\mathbf{Z}^{*}_{nm}(\hat{\mathbf{k}}) + \frac{n}{2n+1}\hat{\mathbf{Y}}_{nm}(\hat{\mathbf{r}})\hat{\mathbf{Y}}^{*}_{nm}(\hat{\mathbf{k}})\right.\\ &\left.+\frac{\sqrt{n(n+1)}}{2n+1}[\hat{\mathbf{Y}}_{nm}(\hat{\mathbf{r}})\mathbf{Z}^{*}_{nm}(\hat{\mathbf{k}}) + \mathbf{Z}_{nm}(\hat{\mathbf{r}})\hat{\mathbf{Y}}^{*}_{nm}(\hat{\mathbf{k}})]\right\},\end{aligned} \tag{A14}$$

$q=n$

$$4\pi\sum_{n,m} i^{n}j_{n}(kr)\mathbf{Y}^{*m}_{n,n}(\hat{\mathbf{k}})\mathbf{Y}^{m}_{n,n}(\hat{\mathbf{r}}) = 4\pi\sum_{n,m} i^{n}j_{n}(kr)\mathbf{X}_{nm}(\hat{\mathbf{r}})\mathbf{X}^{*}_{nm}(\hat{\mathbf{k}}), \tag{A15}$$

$q=n+1$

$$\begin{aligned}4\pi\sum_{n,m} i^{n+1}j_{n+1}(kr)\mathbf{Y}^{*m}_{n,n+1}(\hat{\mathbf{k}})\mathbf{Y}^{m}_{n,n+1}(\hat{\mathbf{r}}) &= 4\pi\sum_{n,m} i^{n+1}j_{n+1}(kr)\\ &\times\left\{\frac{n}{2n+1}\mathbf{Z}_{nm}(\hat{\mathbf{r}})\mathbf{Z}^{*}_{nm}(\hat{\mathbf{k}}) + \frac{n+1}{2n+1}\mathbf{Y}_{nm}(\hat{\mathbf{r}})\mathbf{Y}^{*}_{nm}(\hat{\mathbf{k}})\right.\\ &\left.-\frac{\sqrt{n(n+1)}}{2n+1}[\mathbf{Y}_{nm}(\hat{\mathbf{r}})\mathbf{Z}^{*}_{nm}(\hat{\mathbf{k}}) + \mathbf{Z}_{nm}(\hat{\mathbf{r}})\mathbf{Y}^{*}_{nm}(\hat{\mathbf{k}})]\right\}.\end{aligned} \tag{A16}$$

We thus obtain

$$\begin{aligned}\mathbb{I}\exp(i\mathbf{k}\cdot\mathbf{r}) &= 4\pi\sum_{n,m} i^{n}j_{n}(kr)\mathbf{X}_{nm}(\hat{\mathbf{r}})\mathbf{X}^{*}_{nm}(\hat{\mathbf{k}})\\ &+4\pi\sum_{n,m}\frac{i^{n-1}}{2n+1}[(n+1)j_{n-1}(kr)\\ &-nj_{n+1}(kr)]\mathbf{Z}_{nm}(\hat{\mathbf{r}})\mathbf{Z}^{*}_{nm}(\hat{\mathbf{k}})\\ &+4\pi\sum_{n,m}\frac{i^{n-1}}{2n+1}[nj_{n-1}(kr)-(n\\ &+1)j_{n+1}(kr)]\mathbf{Y}_{nm}(\hat{\mathbf{r}})\mathbf{Y}^{*}_{nm}(\hat{\mathbf{k}})\\ &+4\pi\sum_{n,m}\frac{i^{n-1}}{2n+1}\sqrt{n(n+1)}[j_{n-1}(kr)+j_{n+1}(kr)]\\ &\times[\mathbf{Y}_{nm}(\hat{\mathbf{r}})\mathbf{Z}^{*}_{nm}(\hat{\mathbf{k}}) + \mathbf{Z}_{nm}(\hat{\mathbf{r}})\mathbf{Y}^{*}_{nm}(\hat{\mathbf{k}})].\end{aligned} \tag{A17}$$

This formula can be simplified by invoking the spherical Bessel function recursion formulas,

$$j_{n-1}(x) + j_{n+1}(x) = \frac{2n+1}{x}j_{n}(x),$$

$$nj_{n-1}(x) - (n+1)j_{n+1}(x) = (2n+1)j'_{n}(x),$$

$$(n+1)j_{n-1}(x) - nj_{n+1}(x) = \frac{2n+1}{x}[xj_{n}(x)]', \tag{A18}$$

to obtain

$$\begin{aligned}\mathbb{I}\exp(i\mathbf{k}\cdot\mathbf{r}) = 4\pi\sum_{n,m}\Bigg\{ & i^{n}j_{n}(kr)\mathbf{X}_{nm}(\hat{\mathbf{r}})\mathbf{X}^{*}_{nm}(\hat{\mathbf{k}})\\ &+i^{n-1}\frac{[krj_{n}(kr)]'}{kr}\mathbf{Z}_{nm}(\hat{\mathbf{r}})\mathbf{Z}^{*}_{nm}(\hat{\mathbf{k}})\\ &+i^{n-1}j'_{n}(kr)\mathbf{Y}_{nm}(\hat{\mathbf{r}})\mathbf{Y}^{*}_{nm}(\hat{\mathbf{k}})\\ &+i^{n-1}\sqrt{n(n+1)}\frac{j_{n}(kr)}{kr}[\mathbf{Y}_{nm}(\hat{\mathbf{r}})\mathbf{Z}^{*}_{nm}(\hat{\mathbf{k}})\\ &+\mathbf{Z}_{nm}(\hat{\mathbf{r}})\mathbf{Y}^{*}_{nm}(\hat{\mathbf{k}})]\Bigg\}.\end{aligned} \tag{A19}$$

Equation (A11) is then written in the basis of $\mathbf{Y}_{nm}$, $\mathbf{X}_{nm}$, $\mathbf{Z}_{nm}$,

$$\begin{aligned}\exp(i\mathbf{k}\cdot\mathbf{r})\mathbf{\Gamma} = \sum_{n,m}\Bigg\{ & a_{h,nm}j_{n}(kr)\mathbf{X}_{nm}(\hat{\mathbf{r}})\\ &+\left[a_{e,nm}\frac{j_{n}(kr)}{kr}\sqrt{n(n+1)} + a_{o,nm}j'_{n}(kr)\right]\mathbf{Y}_{nm}(\hat{\mathbf{r}})\\ &+\left[a_{e,nm}\frac{[krj_{n}(kr)]'}{kr}\right.\\ &\left.+\sqrt{n(n+1)}a_{o,nm}\frac{j_{n}(kr)}{kr}\right]\mathbf{Z}_{nm}(\hat{\mathbf{r}})\Bigg\},\end{aligned} \tag{A20}$$

where

$$a_{h,nm} = 4\pi i^n \mathbf{X}^*_{nm}(\hat{\mathbf{k}}) \cdot \mathbf{\Gamma}, \qquad a_{e,nm} = 4\pi i^{n-1} \mathbf{Z}^*_{nm}(\hat{\mathbf{k}}) \cdot \mathbf{\Gamma},$$

$$a_{o,nm} = 4\pi i^{n-1} \mathbf{Y}^*_{nm}(\hat{\mathbf{k}}) \cdot \mathbf{\Gamma}. \tag{A21}$$

It is useful to recall the additional relations between the vector spherical harmonics and the normalized associated Legendre functions $\bar{P}_q^m$ established in Ref. 14:

$$\mathbf{Y}_{nm}(\theta,\varphi) = \hat{\mathbf{r}}\bar{P}_n^m(\cos\theta)\exp(im\varphi)$$

$$\begin{aligned}\mathbf{Z}_{nm}(\theta,\varphi) &= \frac{r}{\sqrt{n(n+1)}}\mathrm{grad}[\bar{P}_n^m(\cos\theta)\exp(im\varphi)] \\ &= \frac{\exp(im\varphi)}{\sqrt{n(n+1)}}\left[\hat{\boldsymbol{\varphi}}\frac{im}{\sin\theta} + \hat{\boldsymbol{\theta}}\frac{\mathrm{d}}{\mathrm{d}\theta}\right]\bar{P}_n^m(\cos\theta)\end{aligned}$$

$$\begin{aligned}\mathbf{X}_{nm}(\theta,\varphi) &= \mathbf{Z}_{nm}(\theta,\varphi) \times \hat{\mathbf{r}} \\ &= \frac{\exp(im\varphi)}{\sqrt{n(n+1)}}\left[\hat{\boldsymbol{\theta}}\frac{im}{\sin\theta} - \hat{\boldsymbol{\varphi}}\frac{\mathrm{d}}{\mathrm{d}\theta}\right]\bar{P}_n^m(\cos\theta).\end{aligned} \tag{A22}$$

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