1

Basic Theory of Electromagnetic Scattering

This chapter is devoted to present the fundamentals of the electromagnetic scattering theory which are relevant in the analysis of the null-field method. We begin with a brief discussion on the physical background of Maxwell's equations and establish vector spherical wave expansions for the incident field. We then derive new systems of vector functions for internal field approximations by analyzing wave propagation in isotropic, anisotropic and chiral media, and present the $\boldsymbol{T}$-matrix formulation for electromagnetic scattering. We decided to leave out some technical details in the presentation. Therefore, the integral and orthogonality relations, the addition theorems and the basic properties of the scalar and vector spherical wave functions are reviewed in Appendices A and B.

1.1 Maxwell's Equations and Constitutive Relations

In this section, we formulate the Maxwell equations that govern the behavior of the electromagnetic fields. We present the fundamental laws of electromagnetism, derive the boundary conditions and describe the properties of isotropic, anisotropic and chiral media by constitutive relations. Our presentation follows the treatment of Kong [122] and Mishchenko et al. [169]. Other excellent textbooks on classical electrodynamics and optics have been given by Stratton [215], Tsang et al. [228], Jackson [110], van de Hulst [105], Kerker [115], Bohren and Huffman [17], and Born and Wolf [19].

The behavior of the macroscopic field at interior points in material media is governed by Maxwell's equations:

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t} \quad \text{(Faraday's induction law)}, \qquad (1.1)$$

$$\nabla \times \boldsymbol{H} = \boldsymbol{J} + \frac{\partial \boldsymbol{D}}{\partial t} \quad \text{(Maxwell–Ampere law)}, \qquad (1.2)$$

$$\nabla \cdot \boldsymbol{D} = \rho \quad \text{(Gauss' electric field law)}, \qquad (1.3)$$

$$\nabla \cdot \boldsymbol{B} = 0 \quad \text{(Gauss' magnetic field law)}, \qquad (1.4)$$

where t is time, $\boldsymbol{E}$ the electric field, $\boldsymbol{H}$ the magnetic field, $\boldsymbol{B}$ the magnetic induction, $\boldsymbol{D}$ the electric displacement and ρ and $\boldsymbol{J}$ the electric charge density and current density, respectively. The first three equations in Maxwell's theory are independent, because the Gauss magnetic field law can be obtained from Faraday's law by taking the divergence and by setting the integration constant with respect to time equal to zero. Analogously, taking the divergence of Maxwell–Ampere law and using the Gauss electric field law we obtain the continuity equation:

$$\nabla \cdot \boldsymbol{J} + \frac{\partial \rho}{\partial t} = 0, \qquad (1.5)$$

which expresses the conservation of electric charge. The Gauss magnetic field law and the continuity equation should be treated as auxiliary or dependent equations in the entire system of equations (1.1)–(1.5). The charge and current densities are associated with the so-called "free" charges, and for a source-free medium, $\boldsymbol{J} = 0$ and $\rho = 0$. In this case, the Gauss electric field law can be obtained from Maxwell–Ampere law and only the first two equations in Maxwell's theory are independent.

In our analysis we will assume that all fields and sources are time harmonic. With ω being the angular frequency and $\text{j} = \sqrt{-1}$, we write

$$\boldsymbol{E}(\boldsymbol{r}, t) = \text{Re}\left\{ \boldsymbol{E}(\boldsymbol{r}) \text{e}^{-\text{j}\omega t} \right\}$$

and similarly for other field quantities. The vector field $\boldsymbol{E}(\boldsymbol{r})$ in the frequency domain is a complex quantity, while $\boldsymbol{E}(\boldsymbol{r}, t)$ in the time domain is real. As a result of the Fourier component Ansatz, the Maxwell equations in the frequency domain become

$$\nabla \times \boldsymbol{E} = \text{j}\,\omega \boldsymbol{B},$$

$$\nabla \times \boldsymbol{H} = \boldsymbol{J} - \text{j}\,\omega \boldsymbol{D},$$

$$\nabla \cdot \boldsymbol{D} = \rho,$$

$$\nabla \cdot \boldsymbol{B} = 0.$$

Taking into account the continuity equation in the frequency domain $\nabla \cdot \boldsymbol{J} - \text{j}\,\omega\rho = 0$, we may express the Maxwell–Ampere law and the Gauss electric field law as

$$\nabla \times \boldsymbol{H} = -\text{j}\,\omega \boldsymbol{D}_{\text{t}},$$

$$\nabla \cdot \boldsymbol{D}_{\text{t}} = 0,$$

where

$$\boldsymbol{D}_{\text{t}} = \boldsymbol{D} + \frac{\text{j}}{\omega}\boldsymbol{J}$$

is the total electric displacement.

Across the interface separating two different media the fields may be discontinuous and a boundary condition is associated with each of Maxwell's equations. To derive the boundary conditions, we consider a regular domain D enclosed by a surface S with outward normal unit vector $\boldsymbol{n}$, and use the *curl* theorem

$$\int_D \nabla \times \boldsymbol{a}\, \mathrm{d}V = \int_S \boldsymbol{n} \times \boldsymbol{a}\, \mathrm{d}S \,,$$

to obtain

$$\int_S \boldsymbol{n} \times \boldsymbol{E}\, \mathrm{d}S = \mathrm{j}\,\omega \int_D \boldsymbol{B}\, \mathrm{d}V \,,$$

$$\int_S \boldsymbol{n} \times \boldsymbol{H}\, \mathrm{d}S = \int_D \boldsymbol{J}\, \mathrm{d}V - \mathrm{j}\,\omega \int_D \boldsymbol{D}\, \mathrm{d}V \,,$$

and the Gauss theorem

$$\int_D \nabla \cdot \boldsymbol{a}\, \mathrm{d}V = \int_S \boldsymbol{n} \cdot \boldsymbol{a}\, \mathrm{d}S \,,$$

to derive

$$\int_S \boldsymbol{n} \cdot \boldsymbol{D}\, \mathrm{d}S = \int_D \rho\, \mathrm{d}V \,,$$

$$\int_S \boldsymbol{n} \cdot \boldsymbol{B}\, \mathrm{d}S = 0 \,.$$

Note that the *curl* theorem follows from Gauss theorem applied to the vector field $\boldsymbol{c} \times \boldsymbol{a}$, where $\boldsymbol{c}$ is a constant vector, and the identity $\nabla \cdot (\boldsymbol{c} \times \boldsymbol{a}) = -\boldsymbol{c} \cdot (\nabla \times \boldsymbol{a})$. We then consider a surface boundary joining two different media 1 and 2, denote by $\boldsymbol{n}_1$ the surface normal pointing toward medium 2, and assume that the surface of discontinuity is contained in D. We choose the domain of analysis in the form of a thin slab with thickness h and area ΔS, and let the volume approach zero by letting h go to zero and then letting ΔS go to zero (Fig. 1.1). Terms involving vector or dot product by $\boldsymbol{n}$ will be dropped except when $\boldsymbol{n}$ is in the direction of $\boldsymbol{n}_1$ or $-\boldsymbol{n}_1$. Assuming that $\boldsymbol{D}$ and $\boldsymbol{B}$ are finite in the region of integration, and that the boundary may support a surface current $\boldsymbol{J}_\mathrm{s}$ such that $\boldsymbol{J}_\mathrm{s} = \lim_{h\to 0} h\boldsymbol{J}$, and a surface charge
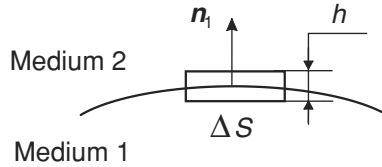
Fig. 1.1. The surface of discontinuity and a thin slab of thickness h and area ΔS

density ρ_s such that $\rho_\mathrm{s} = \lim_{h \to 0} h\rho$, we see that the tangential component of $\boldsymbol{E}$ is continuous:

$$\boldsymbol{n}_1 \times (\boldsymbol{E}_2 - \boldsymbol{E}_1) = 0\,,$$

the tangential component of $\boldsymbol{H}$ is discontinuous:

$$\boldsymbol{n}_1 \times (\boldsymbol{H}_2 - \boldsymbol{H}_1) = \boldsymbol{J}_\mathrm{s}\,,$$

the normal component of $\boldsymbol{B}$ is continuous:

$$\boldsymbol{n}_1 \cdot (\boldsymbol{B}_2 - \boldsymbol{B}_1) = 0\,,$$

and the normal component of $\boldsymbol{D}$ is discontinuous:

$$\boldsymbol{n}_1 \cdot (\boldsymbol{D}_2 - \boldsymbol{D}_1) = \rho_\mathrm{s}\,.$$

Energy conservation follows from Maxwell's equations. The vector identity

$$\nabla \cdot (\boldsymbol{a} \times \boldsymbol{b}) = \boldsymbol{b} \cdot (\nabla \times \boldsymbol{a}) - \boldsymbol{a} \cdot (\nabla \times \boldsymbol{b})$$

yields the Poynting theorem in the time domain:

$$\nabla \cdot (\boldsymbol{E} \times \boldsymbol{H}) + \boldsymbol{H} \cdot \frac{\partial \boldsymbol{B}}{\partial t} + \boldsymbol{E} \cdot \frac{\partial \boldsymbol{D}}{\partial t} = -\boldsymbol{E} \cdot \boldsymbol{J},$$

and the Poynting vector defined as

$$\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}$$

is interpreted as the power flow density. Integrating over a finite domain D with boundary S, and using the Gauss theorem, yields

$$-\int_D \boldsymbol{E} \cdot \boldsymbol{J}\,\mathrm{d}V = \int_S \boldsymbol{S} \cdot \boldsymbol{n}\,\mathrm{d}S + \int_D \left(\boldsymbol{H} \cdot \frac{\partial \boldsymbol{B}}{\partial t} + \boldsymbol{E} \cdot \frac{\partial \boldsymbol{D}}{\partial t} \right) \mathrm{d}V\,,$$

where as before, $\boldsymbol{n}$ is the outward normal unit vector to the surface S. The above equation states that the power supplied by the sources within a volume is equal to the sum of the increase in electromagnetic energy and the Poynting's power flowing out through the volume boundary. Poynting's theorem can also be derived in the frequency domain:

$$\nabla \cdot (\boldsymbol{E} \times \boldsymbol{H}^*) = \mathrm{j}\omega (\boldsymbol{B} \cdot \boldsymbol{H}^* - \boldsymbol{E} \cdot \boldsymbol{D}^*) - \boldsymbol{E} \cdot \boldsymbol{J}^*\,,$$

where the asterisk denotes a complex-conjugate value. The complex Poynting vector is defined as $\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}^*$ and the term $-\int_D \boldsymbol{E} \cdot \boldsymbol{J}^*\,\mathrm{d}V$ is interpreted as the complex power supplied by the source.

In practice, the angular frequency ω is such high that a measuring instrument is not capable of following the rapid oscillations of the power flow but

rather responds to a time average power flow. Considering the time-harmonic vector fields $\boldsymbol{a}$ and $\boldsymbol{b}$,

$$\boldsymbol{a}(\boldsymbol{r},t) = \frac{1}{2}\left[\boldsymbol{a}(\boldsymbol{r})\mathrm{e}^{-\mathrm{j}\omega t} + \boldsymbol{a}^*(\boldsymbol{r})\mathrm{e}^{\mathrm{j}\omega t}\right] ,$$

$$\boldsymbol{b}(\boldsymbol{r},t) = \frac{1}{2}\left[\boldsymbol{b}(\boldsymbol{r})\mathrm{e}^{-\mathrm{j}\omega t} + \boldsymbol{b}^*(\boldsymbol{r})\mathrm{e}^{\mathrm{j}\omega t}\right] ,$$

we express the dot product of the vectors as

$$\begin{aligned} c(\boldsymbol{r},t) &= \boldsymbol{a}(\boldsymbol{r},t) \cdot \boldsymbol{b}(\boldsymbol{r},t) \\ &= \frac{1}{2}\mathrm{Re}\left\{\boldsymbol{a}(\boldsymbol{r}) \cdot \boldsymbol{b}^*(\boldsymbol{r}) + \boldsymbol{a}(\boldsymbol{r}) \cdot \boldsymbol{b}(\boldsymbol{r})\mathrm{e}^{-2\mathrm{j}\omega t}\right\} . \end{aligned}$$

Defining the time average of c as

$$\langle c(\boldsymbol{r})\rangle = \lim_{T\to\infty} \frac{1}{T}\int_0^{\mathrm{T}} c(\boldsymbol{r},t)\,\mathrm{d}t ,$$

where T is a time interval, we derive

$$\langle c(\boldsymbol{r})\rangle = \frac{1}{2}\mathrm{Re}\left\{\boldsymbol{a}(\boldsymbol{r}) \cdot \boldsymbol{b}^*(\boldsymbol{r})\right\} ,$$

while for the cross product of the vectors

$$\boldsymbol{c}(\boldsymbol{r},t) = \boldsymbol{a}(\boldsymbol{r},t) \times \boldsymbol{b}(\boldsymbol{r},t) ,$$

we similarly obtain

$$\langle \boldsymbol{c}(\boldsymbol{r})\rangle = \frac{1}{2}\mathrm{Re}\left\{\boldsymbol{a}(\boldsymbol{r}) \times \boldsymbol{b}^*(\boldsymbol{r})\right\} .$$

Thus, the time average of the dot or cross product of two time-harmonic complex quantities is equal to half of the real part of the respective product of one quantity and the complex conjugate of the other. In this regard, the time-averaged Poynting vector is given by

$$\langle \boldsymbol{S}\rangle = \frac{1}{2}\mathrm{Re}\left\{\boldsymbol{E} \times \boldsymbol{H}^*\right\} .$$

The three independent vector equations (1.1)–(1.3) are equivalent to seven scalar differential equations, while the number of unknown scalar functions is 16. Obviously, the three independent equations are not sufficient to form a complete systems of equations to solve for the unknown functions, and for this reason, the equations given by (1.1)–(1.4) are known as the indefinite form of the Maxwell equations. Note that for a free-source medium, we have six scalar differential equations with 12 unknown scalar functions. To make the Maxwell equations definite we need more information and this additional

information is given by the constitutive relations. The constitutive relations provide a description of media and give functional dependence among vector fields. For isotropic media, the constitutive relations read as

$$\boldsymbol{D} = \varepsilon \boldsymbol{E} \,,$$

$$\boldsymbol{B} = \mu \boldsymbol{H} \,,$$

$$\boldsymbol{J} = \sigma \boldsymbol{E} \quad \text{(Ohm's law)} \,, \tag{1.6}$$

where ε is the electric permittivity, μ is the magnetic permeability and σ is the electric conductivity. The above equations provide nine scalar relations that make the number of unknowns and the number of equations compatible, while for a source-free medium, the first two constitutive relations guarantee this compatibility. When the constitutive relations between the vector fields are specified, Maxwell equations become definite. In free space $\varepsilon_0 = 8.85 \times 10^{-12} \, \text{F m}^{-1}$ and $\mu_0 = 4\pi \times 10^{-7} \, \text{H m}^{-1}$, while in a material medium, the permittivity and permeability are determined by the electrical and magnetic properties of the medium. A dielectric material can be characterized by a free-space part and a part depending on the polarization vector $\boldsymbol{P}$ such that

$$\boldsymbol{D} = \varepsilon_0 \boldsymbol{E} + \boldsymbol{P} \,.$$

The polarization $\boldsymbol{P}$ symbolizes the average electric dipole moment per unit volume and is given by

$$\boldsymbol{P} = \varepsilon_0 \chi_{\text{e}} \boldsymbol{E} \,,$$

where χ_{e} is the electric susceptibility. A magnetic material can also be characterized by a free-space part and a part depending on the magnetization vector $\boldsymbol{M}$,

$$\boldsymbol{B} = \mu_0 \boldsymbol{H} + \mu_0 \boldsymbol{M} \,,$$

where $\boldsymbol{M}$ symbolizes the average magnetic dipole moment per unit volume,

$$\boldsymbol{M} = \chi_{\text{m}} \boldsymbol{H} \,,$$

and χ_{m} is the magnetic susceptibility. A medium is diamagnetic if $\mu < \mu_0$ and paramagnetic if $\mu > \mu_0$, while for a nonmagnetic medium we have $\mu = \mu_0$. The permittivity and permeability of isotropic media can be written as

$$\varepsilon = \varepsilon_0 \varepsilon_{\text{r}} = \varepsilon_0 \left(1 + \chi_{\text{e}} \right) \,,$$

$$\mu = \mu_0 \mu_{\text{r}} = \mu_0 \left(1 + \chi_{\text{m}} \right) \,,$$

where ε_{r} and μ_{r} stand for the corresponding relative quantities. The constitutive relation for the total electric displacement is

$$\boldsymbol{D}_{\text{t}} = \varepsilon_{\text{t}} \boldsymbol{E} \,,$$

where the complex permittivity ε_t is given by

$$\varepsilon_t = \varepsilon_0\varepsilon_{rt} = \varepsilon_0\left(1 + \chi_e + \frac{j\sigma}{\omega\varepsilon_0}\right)$$

with ε_{rt} being the complex relative permittivity. Both the conductivity and the susceptibility contribute to the imaginary part of the permittivity, $\text{Im}\{\varepsilon_t\} = \varepsilon_0\text{Im}\{\chi_e\} + \text{Re}\{\sigma/\omega\}$, and a complex value for ε_t means that the medium is absorbing. Usually, $\text{Im}\{\chi_e\}$ is associated with the "bound" charge current density and $\text{Re}\{\sigma/\omega\}$ with the "free" charge current density, and absorption is determined by the sum of these two quantities. Note that for a free-source medium, $\sigma = 0$ and $\varepsilon_{rt} = \varepsilon_r = 1 + \chi_e$. The simplest solution to Maxwell's equations in source-free media is the vector plane wave solution. The behavior of a vector plane wave in an isotropic medium is characterized by the dispersion relation

$$k = \omega\sqrt{\varepsilon\mu}\,,$$

which relates the wave number k to the properties of the medium and to the angular frequency ω of the wave. The dimensionless quantity

$$m = c\sqrt{\varepsilon\mu}$$

is the refractive index of the medium, where $c = 1/\sqrt{\varepsilon_0\mu_0}$ is the speed of light in vacuum, and if $k_0 = \omega\sqrt{\varepsilon_0\mu_0}$ is the wave number in free space, we see that

$$m = \frac{k}{k_0}\,.$$

The constitutive relations for anisotropic media are

$$\boldsymbol{D} = \overline{\varepsilon}\boldsymbol{E}\,,$$
$$\boldsymbol{B} = \overline{\mu}\boldsymbol{H}\,, \tag{1.7}$$

where $\overline{\varepsilon}$ and $\overline{\mu}$ are the permittivity and permeability tensors, respectively. In our analysis we will consider electrically anisotropic media for which the permittivity is a tensor and the permeability is a scalar. Except for amorphous materials and crystals with cubic symmetry, the permittivity is always a tensor, and in general, the permittivity tensor of a crystal is symmetric. Since there exists a coordinate transformation that transforms a symmetric matrix into a diagonal matrix, we can take this coordinate system as reference frame and we have

$$\overline{\varepsilon} = \begin{bmatrix} \varepsilon_x & 0 & 0 \\ 0 & \varepsilon_y & 0 \\ 0 & 0 & \varepsilon_z \end{bmatrix}\,. \tag{1.8}$$

This reference frame is called the principal coordinate system and the three coordinate axes are known as the principal axes of the crystal. If $\varepsilon_x \neq \varepsilon_y \neq \varepsilon_z$,

the medium is biaxial, and if $\varepsilon = \varepsilon_x = \varepsilon_y$ and $\varepsilon \neq \varepsilon_z$, the medium is uniaxial. Orthorhombic, monoclinic and triclinic crystals are biaxial, while tetragonal, hexagonal and rhombohedral crystals are uniaxial. For uniaxial crystals, the principal axis that exhibits the anisotropy is called the optic axis. The crystal is positive uniaxial if $\varepsilon_z > \varepsilon$ and negative uniaxial if $\varepsilon_z < \varepsilon$.

In our analysis, we will investigate the electromagnetic response of isotropic, chiral media exposed to arbitrary external excitations. The lack of geometric symmetry between a particle and its mirror image is referred to as chirality or optical activity. A chiral medium is characterized by either a left- or a right-handedness in its microstructure, and as a result, left- and right-hand circularly polarized fields propagate through it with differing phase velocities. For a source-free, isotropic, chiral medium, the constitutive relations read as

$$\boldsymbol{D} = \varepsilon \boldsymbol{E} + \beta \varepsilon \nabla \times \boldsymbol{E} \,,$$

$$\boldsymbol{B} = \mu \boldsymbol{H} + \beta \mu \nabla \times \boldsymbol{H} \,,$$

where the real number β is known as the chirality parameter. The Maxwell equations can be written compactly in matrix form as

$$\nabla \times \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix} = \boldsymbol{K} \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix} \,, \quad \nabla \cdot \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix} = 0 \,, \tag{1.9}$$

where

$$\boldsymbol{K} = \frac{1}{1 - \beta^2 k^2} \begin{bmatrix} \beta k^2 & \mathrm{j}\omega\mu \\ -\mathrm{j}\omega\varepsilon & \beta k^2 \end{bmatrix}$$

and $k = \omega\sqrt{\varepsilon\mu}$.

Without loss of generality and so as to simplify our notations we make the following transformations:

$$\boldsymbol{E} \to \frac{1}{\sqrt{\varepsilon_0}} \boldsymbol{E}, \boldsymbol{H} \to \frac{1}{\sqrt{\mu_0}} \boldsymbol{H} \,,$$

$$\boldsymbol{D} \to \sqrt{\varepsilon_0} \boldsymbol{D}, \boldsymbol{B} \to \sqrt{\mu_0} \boldsymbol{B} \,.$$

As a result, the Maxwell equations for a free-source medium become more "symmetric":

$$\nabla \times \boldsymbol{E} = \mathrm{j}k_0 \boldsymbol{B} \,,$$
$$\nabla \times \boldsymbol{H} = -\mathrm{j}k_0 \boldsymbol{D} \,,$$
$$\nabla \cdot \boldsymbol{D} = 0 \,,$$
$$\nabla \cdot \boldsymbol{B} = 0 \,, \tag{1.10}$$

the constitutive relations are given by (1.6) and (1.7) with ε and μ being the relative permittivity and permeability, respectively, the wave number is $k = k_0\sqrt{\varepsilon\mu}$, and the $\boldsymbol{K}$ matrix in (1.9) takes the form

$$\boldsymbol{K} = \frac{1}{1 - \beta^2 k^2} \begin{bmatrix} \beta k^2 & \mathrm{j}k_0\mu \\ -\mathrm{j}k_0\varepsilon & \beta k^2 \end{bmatrix} \,. \tag{1.11}$$

1.2 Incident Field

In this section, we characterize the polarization state of vector plane waves and derive vector spherical wave expansions for the incident field. The first topic is relevant in the analysis of the scattered field, while the second one plays an important role in the derivation of the transition matrix.

1.2.1 Polarization

In addition to intensity and frequency, a monochromatic (time harmonic) electromagnetic wave is characterized by its state of polarization. This concept is useful when we discuss the polarization of the scattered field since the polarization state of a beam is changed on interaction with a particle.

We consider a right-handed Cartesian coordinate system $OXYZ$ with a fixed spatial orientation. This reference frame will be referred to as the global coordinate system or the laboratory coordinate system. The direction of propagation of the vector plane wave is specified by the unit vector $\boldsymbol{e}_k$, or equivalently, by the zenith and azimuth angles β and α, respectively (Fig. 1.2). The polarization state of the incident wave will be described in terms of the vertical polarization unit vector $\boldsymbol{e}_\alpha = \boldsymbol{e}_z \times \boldsymbol{e}_k / |\boldsymbol{e}_z \times \boldsymbol{e}_k|$ and the horizontal polarization vector $\boldsymbol{e}_\beta = \boldsymbol{e}_\alpha \times \boldsymbol{e}_k$. Note that other names for vertical polarization are TM polarization, parallel polarization and p polarization, while other names for horizontal polarization are TE polarization, perpendicular polarization and s polarization.
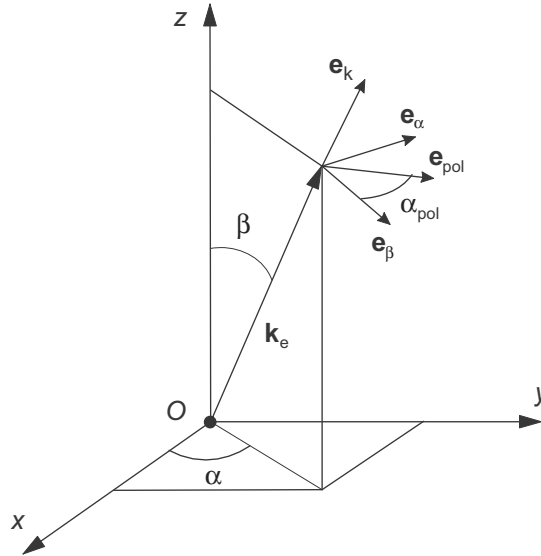

Fig. 1.2. Wave vector in the global coordinate system

In the frequency domain, a vector plane wave propagating in a medium with constant wave number $k_\mathrm{s} = k_0 \sqrt{\varepsilon_\mathrm{s} \mu_\mathrm{s}}$ is given by

$$\boldsymbol{E}_\mathrm{e}(\boldsymbol{r}) = \boldsymbol{E}_\mathrm{e0} \mathrm{e}^{\mathrm{j} \boldsymbol{k}_\mathrm{e} \cdot \boldsymbol{r}}, \quad \boldsymbol{E}_\mathrm{e0} \cdot \boldsymbol{e}_k = 0, \tag{1.12}$$

where k_0 is the wave number in free space, $\boldsymbol{k}_\mathrm{e}$ is the wave vector, $\boldsymbol{k}_\mathrm{e} = k_\mathrm{s} \boldsymbol{e}_k$, $\boldsymbol{E}_\mathrm{e0}$ is the complex amplitude vector,

$$\boldsymbol{E}_\mathrm{e0} = E_{\mathrm{e0},\beta} \boldsymbol{e}_\beta + E_{\mathrm{e0},\alpha} \boldsymbol{e}_\alpha,$$

and $E_{\mathrm{e0},\beta}$ and $E_{\mathrm{e0},\alpha}$ are the complex amplitudes in the β- and α-direction, respectively. An equivalent representation for $\boldsymbol{E}_\mathrm{e0}$ is

$$\boldsymbol{E}_\mathrm{e0} = |\boldsymbol{E}_\mathrm{e0}| \, \boldsymbol{e}_\mathrm{pol}, \tag{1.13}$$

where $\boldsymbol{e}_\mathrm{pol}$ is the complex polarization unit vector, $|\boldsymbol{e}_\mathrm{pol}| = 1$, and

$$\boldsymbol{e}_\mathrm{pol} = \frac{1}{|\boldsymbol{E}_\mathrm{e0}|} \left(E_{\mathrm{e0},\beta} \boldsymbol{e}_\beta + E_{\mathrm{e0},\alpha} \boldsymbol{e}_\alpha \right).$$

Inserting (1.13) into (1.12), gives the representation

$$\boldsymbol{E}_\mathrm{e}(\boldsymbol{r}) = |\boldsymbol{E}_\mathrm{e0}| \, \boldsymbol{e}_\mathrm{pol} \mathrm{e}^{\mathrm{j} \boldsymbol{k}_\mathrm{e} \cdot \boldsymbol{r}}, \quad \boldsymbol{e}_\mathrm{pol} \cdot \boldsymbol{e}_k = 0,$$

and obviously, $|\boldsymbol{E}_\mathrm{e}(\boldsymbol{r})| = |\boldsymbol{E}_\mathrm{e0}|$.

There are three ways of describing the polarization state of vector plane waves.

1. Setting

$$\begin{aligned} E_{\mathrm{e0},\beta} &= a_\beta \mathrm{e}^{\mathrm{j}\delta_\beta}, \\ E_{\mathrm{e0},\alpha} &= a_\alpha \mathrm{e}^{\mathrm{j}\delta_\alpha}, \end{aligned} \tag{1.14}$$

where a_β and a_α are the real non-negative amplitudes, and δ_β and δ_α are the real phases, we characterize the polarization state of a vector plane wave by a_β, a_α and the phase difference $\Delta\delta = \delta_\beta - \delta_\alpha$.

2. Taking into account the representation of a vector plane wave in the time domain

$$\boldsymbol{E}_\mathrm{e}(\boldsymbol{r},t) = \mathrm{Re}\left\{ \boldsymbol{E}_\mathrm{e}(\boldsymbol{r}) \mathrm{e}^{-\mathrm{j}\omega t} \right\} = \mathrm{Re}\left\{ \boldsymbol{E}_\mathrm{e0} \mathrm{e}^{\mathrm{j}(\boldsymbol{k}_\mathrm{e} \cdot \boldsymbol{r} - \omega t)} \right\},$$

where $\boldsymbol{E}_\mathrm{e}(\boldsymbol{r},t)$ is the real electric vector, we deduce that (cf. (1.14))

$$\begin{aligned} E_{\mathrm{e},\beta}(\boldsymbol{r},t) &= a_\beta \cos\left(\delta_\beta + \boldsymbol{k}_\mathrm{e} \cdot \boldsymbol{r} - \omega t\right), \\ E_{\mathrm{e},\alpha}(\boldsymbol{r},t) &= a_\alpha \cos\left(\delta_\alpha + \boldsymbol{k}_\mathrm{e} \cdot \boldsymbol{r} - \omega t\right), \end{aligned}$$

where

$$\boldsymbol{E}_\mathrm{e}(\boldsymbol{r},t) = E_{\mathrm{e},\beta}(\boldsymbol{r},t) \boldsymbol{e}_\beta + E_{\mathrm{e},\alpha}(\boldsymbol{r},t) \boldsymbol{e}_\alpha.$$

At any fixed point in space the endpoint of the real electric vector describes an ellipse which is also known as the vibration ellipse [17]. The vibration ellipse can be traced out in two opposite senses: clockwise and anticlockwise. If the real electric vector rotates clockwise, as viewed by an observer looking in the direction of propagation, the polarization of the ellipse is right-handed and the polarization is left-handed if the electric vector rotates anticlockwise. The two opposite senses of rotation lead to a classification of vibration ellipses according to their handedness. In addition to its handedness, a vibration ellipse is characterized by $E_0 = \sqrt{a^2 + b^2}$, where a and b are the semi-major and semi-minor axes of the ellipse, the orientation angle ψ and the ellipticity angle χ (Fig. 1.3). The orientation angle ψ is the angle between the α-axis and the major axis, and $\psi \in [0, \pi)$. The ellipticity angle χ is usually expressed as $\tan \chi = \pm b/a$, where the plus sign corresponds to right-handed elliptical polarization, and $\chi \in [-\pi/4, \pi/4]$.

We now proceed to relate the complex amplitudes $E_{e0,\beta}$ and $E_{e0,\alpha}$ to the ellipsometric parameters E_0, ψ and χ. Representing the semi-axes of the vibration ellipse as

$$
\begin{aligned}
b &= \pm E_0 \sin \chi \,, \\
a &= E_0 \cos \chi \,,
\end{aligned}
\tag{1.15}
$$

where the plus sign corresponds to right-handed polarization, and taking into account the parametric representation of the ellipse in the principal coordinate system $O\alpha'\beta'$

$$
\begin{aligned}
E'_{e,\beta}(\boldsymbol{r}, t) &= \pm b \sin\left(\boldsymbol{k}_e \cdot \boldsymbol{r} - \omega t\right) \,, \\
E'_{e,\alpha}(\boldsymbol{r}, t) &= a \cos\left(\boldsymbol{k}_e \cdot \boldsymbol{r} - \omega t\right) \,,
\end{aligned}
$$
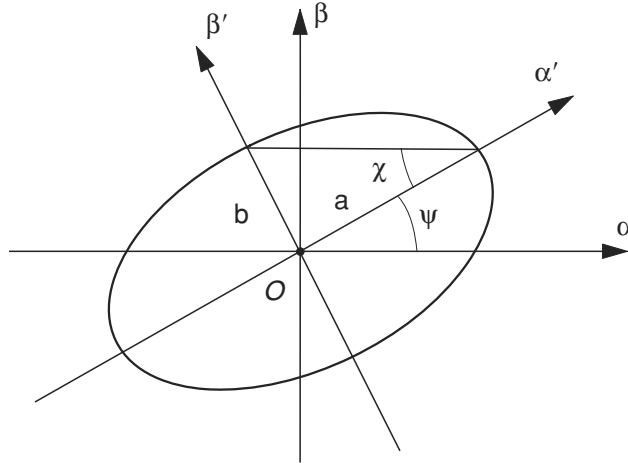
Fig. 1.3. Vibration ellipse

we obtain

$$E'_{e,\beta}(\boldsymbol{r},t) = E_0 \sin\chi \sin\left(\boldsymbol{k}_e \cdot \boldsymbol{r} - \omega t\right) = E_0 \sin\chi \cos\left(\boldsymbol{k}_e \cdot \boldsymbol{r} - \omega t - \frac{\pi}{2}\right),$$

$$E'_{e,\alpha}(\boldsymbol{r},t) = E_0 \cos\chi \cos\left(\boldsymbol{k}_e \cdot \boldsymbol{r} - \omega t\right).$$

In the frequency domain, the complex amplitude vector $\boldsymbol{E}'_{e0}$ defined as

$$\boldsymbol{E}'_e(\boldsymbol{r},t) = \mathrm{Re}\left\{\boldsymbol{E}'_{e0}\mathrm{e}^{\mathrm{j}(\boldsymbol{k}_e \cdot \boldsymbol{r} - \omega t)}\right\},$$

where

$$\boldsymbol{E}'_e(\boldsymbol{r},t) = E'_{e,\beta}(\boldsymbol{r},t)\boldsymbol{e}'_\beta + E'_{e,\alpha}(\boldsymbol{r},t)\boldsymbol{e}'_\alpha,$$

has the components

$$E'_{e0,\beta} = -\mathrm{j}E_0 \sin\chi,$$

$$E'_{e0,\alpha} = E_0 \cos\chi.$$

Using the transformation rule for rotation of a two-dimensional coordinate system we obtain the desired relations

$$E_{e0,\beta} = E_0\left(\cos\chi \sin\psi - \mathrm{j}\sin\chi \cos\psi\right),$$

$$E_{e0,\alpha} = E_0\left(\cos\chi \cos\psi + \mathrm{j}\sin\chi \sin\psi\right),$$

and

$$\boldsymbol{e}_{\mathrm{pol}} = \left(\cos\chi \sin\psi - \mathrm{j}\sin\chi \cos\psi\right)\boldsymbol{e}_\beta$$
$$+ \left(\cos\chi \cos\psi + \mathrm{j}\sin\chi \sin\psi\right)\boldsymbol{e}_\alpha. \tag{1.16}$$

If $b = 0$, the ellipse degenerates into a straight line and the wave is linearly polarized. In this specific case $\chi = 0$ and

$$E_{e0,\beta} = E_0 \sin\psi = E_0 \cos\left(\frac{\pi}{2} - \psi\right) = E_0 \cos\alpha_{\mathrm{pol}},$$

$$E_{e0,\alpha} = E_0 \cos\psi = E_0 \sin\left(\frac{\pi}{2} - \psi\right) = E_0 \sin\alpha_{\mathrm{pol}},$$

where α_{pol} is the polarization angle and

$$\alpha_{\mathrm{pol}} = \pi/2 - \psi, \quad \alpha_{\mathrm{pol}} \in (-\pi/2, \pi/2]. \tag{1.17}$$

In view of (1.16) and (1.17) it is apparent that the polarization unit vector is real and is given by

$$\boldsymbol{e}_{\mathrm{pol}} = \cos\alpha_{\mathrm{pol}}\boldsymbol{e}_\beta + \sin\alpha_{\mathrm{pol}}\boldsymbol{e}_\alpha. \tag{1.18}$$

If $a = b$, the ellipse is a circle and the wave is circularly polarized. We have $\tan \chi = \pm 1$, which implies $\chi = \pm \pi/4$, and choosing $\psi = \pi/2$, we obtain

$$E_{\mathrm{e}0,\beta} = \frac{\sqrt{2}}{2} E_0 \,,$$

$$E_{\mathrm{e}0,\alpha} = \pm \mathrm{j} \frac{\sqrt{2}}{2} E_0 \,.$$

The polarization unit vectors of right- and left-circularly polarized waves then become

$$\boldsymbol{e}_{\mathrm{R}} = \frac{\sqrt{2}}{2} \left(\boldsymbol{e}_\beta + \mathrm{j} \boldsymbol{e}_\alpha \right) \,,$$

$$\boldsymbol{e}_{\mathrm{L}} = \frac{\sqrt{2}}{2} \left(\boldsymbol{e}_\beta - \mathrm{j} \boldsymbol{e}_\alpha \right) \,,$$

and we see that these basis vectors are orthonormal in the sense that $\boldsymbol{e}_{\mathrm{R}} \cdot \boldsymbol{e}_{\mathrm{R}}^* = 1$, $\boldsymbol{e}_{\mathrm{L}} \cdot \boldsymbol{e}_{\mathrm{L}}^* = 1$ and $\boldsymbol{e}_{\mathrm{R}} \cdot \boldsymbol{e}_{\mathrm{L}}^* = 0$.

3. The polarization characteristics of the incident field can also be described by the coherency and Stokes vectors. Although the ellipsometric parameters completely specify the polarization state of a monochromatic wave, they are difficult to measure directly (with the exception of the intensity E_0^2). In contrast, the Stokes parameters are measurable quantities and are of greater usefulness in scattering problems. The coherency vector is defined as

$$\boldsymbol{J}_{\mathrm{e}} = \frac{1}{2} \sqrt{\frac{\varepsilon_{\mathrm{s}}}{\mu_{\mathrm{s}}}} \begin{bmatrix} E_{\mathrm{e}0,\beta} E_{\mathrm{e}0,\beta}^* \\ E_{\mathrm{e}0,\beta} E_{\mathrm{e}0,\alpha}^* \\ E_{\mathrm{e}0,\alpha} E_{\mathrm{e}0,\beta}^* \\ E_{\mathrm{e}0,\alpha} E_{\mathrm{e}0,\alpha}^* \end{bmatrix} \,, \tag{1.19}$$

while the Stokes vector is given by

$$\boldsymbol{I}_{\mathrm{e}} = \begin{bmatrix} I_{\mathrm{e}} \\ Q_{\mathrm{e}} \\ U_{\mathrm{e}} \\ V_{\mathrm{e}} \end{bmatrix} = \boldsymbol{D} \boldsymbol{J}_{\mathrm{e}} = \frac{1}{2} \sqrt{\frac{\varepsilon_{\mathrm{s}}}{\mu_{\mathrm{s}}}} \begin{bmatrix} \left| E_{\mathrm{e}0,\beta} \right|^2 + \left| E_{\mathrm{e}0,\alpha} \right|^2 \\ \left| E_{\mathrm{e}0,\beta} \right|^2 - \left| E_{\mathrm{e}0,\alpha} \right|^2 \\ -E_{\mathrm{e}0,\alpha} E_{\mathrm{e}0,\beta}^* - E_{\mathrm{e}0,\beta} E_{\mathrm{e}0,\alpha}^* \\ \mathrm{j} \left(E_{\mathrm{e}0,\alpha} E_{\mathrm{e}0,\beta}^* - E_{\mathrm{e}0,\beta} E_{\mathrm{e}0,\alpha}^* \right) \end{bmatrix} \,, \tag{1.20}$$

where $\boldsymbol{D}$ is a transformation matrix and

$$\boldsymbol{D} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 0 \\ 0 & -\mathrm{j} & \mathrm{j} & 0 \end{bmatrix} \,. \tag{1.21}$$

The first Stokes parameter I_e,

$$I_\mathrm{e} = \frac{1}{2}\sqrt{\frac{\varepsilon_\mathrm{s}}{\mu_\mathrm{s}}}\,|\boldsymbol{E}_{\mathrm{e}0}|^2$$

is the intensity of the wave, while the Stokes parameters Q_e, U_e and V_e describe the polarization state of the wave. The Stokes parameters are defined with respect to a reference plane containing the direction of wave propagation, and Q_e and U_e depend on the choice of the reference frame. If the unit vectors $\boldsymbol{e}_\beta$ and $\boldsymbol{e}_\alpha$ are rotated through an angle φ (Fig. 1.4), the transformation from the Stokes vector $\boldsymbol{I}_\mathrm{e}$ to the Stokes vector $\boldsymbol{I}'_\mathrm{e}$ (relative to the rotated unit vectors $\boldsymbol{e}'_\beta$ and $\boldsymbol{e}'_\alpha$) is given by

$$\boldsymbol{I}'_\mathrm{e} = \boldsymbol{L}\left(\varphi\right)\boldsymbol{I}_\mathrm{e}\,, \tag{1.22}$$

where the Stokes rotation matrix $\boldsymbol{L}$ is

$$\boldsymbol{L}\left(\varphi\right) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\varphi & -\sin 2\varphi & 0 \\ 0 & \sin 2\varphi & \cos 2\varphi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\,. \tag{1.23}$$

The Stokes parameters can be expressed in terms of a_β, a_α and $\Delta\delta$ as (omitting the factor $\frac{1}{2}\sqrt{\varepsilon_\mathrm{s}/\mu_\mathrm{s}}$)

$$I_\mathrm{e} = a_\beta^2 + a_\alpha^2\,,$$
$$Q_\mathrm{e} = a_\beta^2 - a_\alpha^2\,,$$
$$U_\mathrm{e} = -2a_\beta a_\alpha \cos\Delta\delta\,,$$
$$V_\mathrm{e} = 2a_\beta a_\alpha \sin\Delta\delta\,,$$
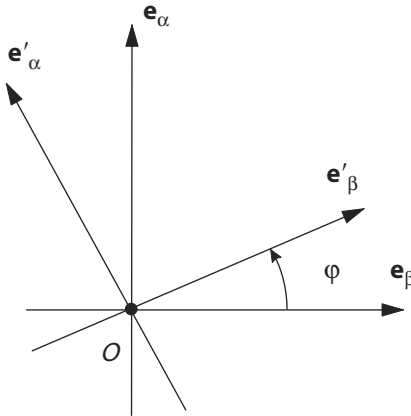
Fig. 1.4. Rotation of the polarization unit vectors through the angle φ

and in terms of E_0, ψ and χ, as

$$I_{\mathrm{e}} = E_0^2 \,,$$

$$Q_{\mathrm{e}} = -E_0^2 \cos 2\chi \cos 2\psi \,,$$

$$U_{\mathrm{e}} = -E_0^2 \cos 2\chi \sin 2\psi \,,$$

$$V_{\mathrm{e}} = -E_0^2 \sin 2\chi \,.$$

The above relations show that the Stokes parameters carry information about the amplitudes and the phase difference, and are operationally defined in terms of measurable quantities (intensities). For a linearly polarized plane wave, $\chi = 0$ and $V_{\mathrm{e}} = 0$, while for a circularly polarized plane wave, $\chi = \pm \pi/4$ and $Q_{\mathrm{e}} = U_{\mathrm{e}} = 0$. Thus, the Stokes vector of a linearly polarized wave of unit amplitude is given by $\boldsymbol{I}_{\mathrm{e}} = [1, \cos 2\alpha_{\mathrm{pol}}, -\sin 2\alpha_{\mathrm{pol}}, 0]^{\mathrm{T}}$, while the Stokes vector of a circularly polarized wave of unit amplitude is $\boldsymbol{I}_{\mathrm{e}} = [1, 0, 0, \mp 1]^{\mathrm{T}}$.

The Stokes parameters of a monochromatic plane wave are not independent since

$$I_{\mathrm{e}}^2 = Q_{\mathrm{e}}^2 + U_{\mathrm{e}}^2 + V_{\mathrm{e}}^2 \,, \tag{1.24}$$

and we may conclude that only three parameters are required to characterize the state of polarization. For quasi-monochromatic light, the amplitude of the electric field fluctuate in time and the Stokes parameters are expressed in terms of the time-averaged quantities $\langle E_{\mathrm{e}0,p} E_{\mathrm{e}0,q}^* \rangle$, where p and q stand for β and α. In this case, the equality in (1.24) is replaced by the inequality

$$I_{\mathrm{e}}^2 \geq Q_{\mathrm{e}}^2 + U_{\mathrm{e}}^2 + V_{\mathrm{e}}^2 \,,$$

and the quantity

$$P = \frac{\sqrt{Q_{\mathrm{e}}^2 + U_{\mathrm{e}}^2 + V_{\mathrm{e}}^2}}{I_{\mathrm{e}}}$$

is known as the degree of polarization of the quasi-monochromatic beam. For natural (unpolarized) light, $P = 0$, while for fully polarized light $P = 1$. The Stokes vector defined by (1.20) is one possible representation of polarization. Other representations are discussed by Hovenier and van der Mee [101], while a detailed discussion of the polarimetric definitions can be found in [17,169,171].

1.2.2 Vector Spherical Wave Expansion

The derivation of the transition matrix in the framework of the null-field method requires the expansion of the incident field in terms of (localized) vector spherical wave functions. This expansion must be provided in the particle coordinate system, where in general, the particle coordinate system $Oxyz$ is obtained by rotating the global coordinate system $OXYZ$ through the Euler angles α_{p}, β_{p} and γ_{p} (Fig. 1.5). In our analysis, vector plane waves and Gaussian beams are considered as external excitations.
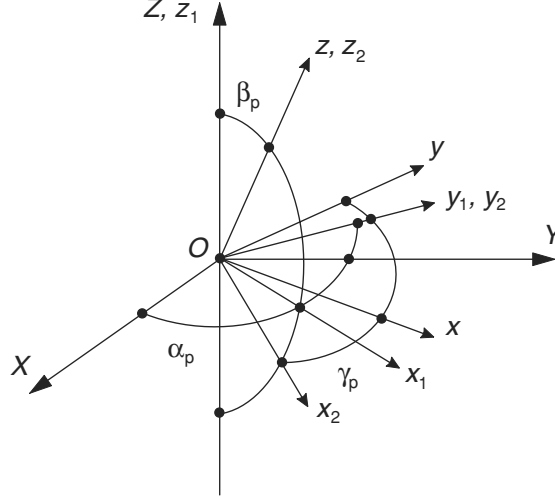
Fig. 1.5. Euler angles α_{p}, β_{p} and γ_{p} specifying the orientation of the particle coordinate system $Oxyz$ with respect to the global coordinate system $OXYZ$. The transformation $OXYZ \rightarrow Oxyz$ is achieved by means of three successive rotations: (1) rotation about the Z-axis through α_{p}, $OXYZ \rightarrow Ox_1y_1z_1$, (2) rotation about the y_1-axis through β_{p}, $Ox_1y_1z_1 \rightarrow Ox_2y_2z_2$ and (3) rotation about the z_2-axis through γ_{p}, $Ox_2y_2z_2 \rightarrow Oxyz$

Vector Plane Wave

We consider a vector plane wave of unit amplitude propagating in the direction $(\beta_{\mathrm{g}}, \alpha_{\mathrm{g}})$ with respect to the global coordinate system. Passing from spherical coordinates to Cartesian coordinates and using the transformation rules under coordinate rotations we may compute the spherical angles β and α of the wave vector in the particle coordinate system. Thus, in the particle coordinate system we have the representation

$$\boldsymbol{E}_{\mathrm{e}}(\boldsymbol{r}) = \boldsymbol{e}_{\mathrm{pol}}\mathrm{e}^{\mathrm{j}\boldsymbol{k}_{\mathrm{e}}\cdot\boldsymbol{r}}\,, \quad \boldsymbol{e}_{\mathrm{pol}}\cdot\boldsymbol{e}_k = 0\,,$$

where as before, $\boldsymbol{k}_{\mathrm{e}} = k_{\mathrm{s}}\boldsymbol{e}_k$.

The vector spherical waves expansion of the incident field reads as

$$\boldsymbol{E}_{\mathrm{e}}(\boldsymbol{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} a_{mn}\boldsymbol{M}_{mn}^1\left(k_{\mathrm{s}}\boldsymbol{r}\right) + b_{mn}\boldsymbol{N}_{mn}^1\left(k_{\mathrm{s}}\boldsymbol{r}\right)\,, \qquad (1.25)$$

where the expansion coefficients are given by [9, 228]

$$a_{mn} = 4\mathrm{j}^n\boldsymbol{e}_{\mathrm{pol}}\cdot\boldsymbol{m}_{mn}^*(\beta,\alpha)$$

$$= -\frac{4\mathrm{j}^n}{\sqrt{2n(n+1)}}\boldsymbol{e}_{\mathrm{pol}}\cdot\left[\mathrm{j}m\pi_n^{|m|}(\beta)\boldsymbol{e}_\beta + \tau_n^{|m|}(\beta)\boldsymbol{e}_\alpha\right]\mathrm{e}^{-\mathrm{j}m\alpha}\,,$$

$$b_{mn} = -4\mathrm{j}^{n+1}\boldsymbol{e}_{\mathrm{pol}} \cdot \boldsymbol{n}_{mn}^*(\beta, \alpha)$$

$$= -\frac{4\mathrm{j}^{n+1}}{\sqrt{2n(n+1)}}\boldsymbol{e}_{\mathrm{pol}} \cdot \left[\tau_n^{|m|}(\beta)\boldsymbol{e}_\beta - \mathrm{j}m\pi_n^{|m|}(\beta)\boldsymbol{e}_\alpha\right]\mathrm{e}^{-\mathrm{j}m\alpha}. \quad (1.26)$$

To give a justification of the above expansion we consider the integral representation

$$\boldsymbol{e}_{\mathrm{pol}}(\beta, \alpha)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_{\mathrm{e}}(\beta,\alpha)\cdot\boldsymbol{r}} = \int_0^{2\pi}\int_0^\pi \boldsymbol{e}_{\mathrm{pol}}(\beta, \alpha)\mathrm{e}^{\mathrm{j}\boldsymbol{k}(\beta',\alpha')\cdot\boldsymbol{r}}$$

$$\times\delta(\alpha' - \alpha)\delta(\cos\beta' - \cos\beta)\sin\beta'\,\mathrm{d}\beta'\,\mathrm{d}\alpha', \quad (1.27)$$

and expand the tangential field

$$\boldsymbol{f}(\beta, \alpha, \beta', \alpha') = \boldsymbol{e}_{\mathrm{pol}}(\beta, \alpha)\delta(\alpha' - \alpha)\delta(\cos\beta' - \cos\beta) \quad (1.28)$$

in vector spherical harmonics

$$\boldsymbol{f}(\beta, \alpha, \beta', \alpha') = \frac{1}{4\pi\mathrm{j}^n}\sum_{n=1}^\infty\sum_{m=-n}^n a_{mn}\boldsymbol{m}_{mn}(\beta', \alpha') + \mathrm{j}b_{mn}\boldsymbol{n}_{mn}(\beta', \alpha'). \quad (1.29)$$

Using the orthogonality relations of vector spherical harmonics we see that the expansion coefficients a_{mn} and b_{mn} are given by

$$a_{mn} = 4\mathrm{j}^n\int_0^{2\pi}\int_0^\pi \boldsymbol{f}(\beta, \alpha, \beta', \alpha') \cdot \boldsymbol{m}_{mn}^*(\beta', \alpha')\sin\beta'\,\mathrm{d}\beta'\,\mathrm{d}\alpha'$$

$$= 4\mathrm{j}^n\boldsymbol{e}_{\mathrm{pol}}(\beta, \alpha) \cdot \boldsymbol{m}_{mn}^*(\beta, \alpha),$$

$$b_{mn} = -4\mathrm{j}^{n+1}\int_0^{2\pi}\int_0^\pi \boldsymbol{f}(\beta, \alpha, \beta', \alpha') \cdot \boldsymbol{n}_{mn}^*(\beta', \alpha')\sin\beta'\,\mathrm{d}\beta'\,\mathrm{d}\alpha'$$

$$= -4\mathrm{j}^{n+1}\boldsymbol{e}_{\mathrm{pol}}(\beta, \alpha) \cdot \boldsymbol{n}_{mn}^*(\beta, \alpha).$$

Substituting (1.28) and (1.29) into (1.27) and taking into account the integral representations for the regular vector spherical wave functions (cf. (B.26) and (B.27)) yields (1.25).

The polarization unit vector of a linearly polarized vector plane wave is given by (1.18). If the vector plane wave propagates along the z-axis we have $\beta = \alpha = 0$ and for $\beta = 0$, the spherical vector harmonics are zero unless $m = \pm 1$. Using the special values of the angular functions π_n^1 and τ_n^1 when $\beta = 0$,

$$\pi_n^1(0) = \tau_n^1(0) = \frac{1}{2\sqrt{2}}\sqrt{n(n+1)(2n+1)},$$

we obtain

$$a_{\pm 1n} = -\mathrm{j}^n\sqrt{2n+1}\left(\pm\mathrm{j}\cos\alpha_{\mathrm{pol}} + \sin\alpha_{\mathrm{pol}}\right),$$

$$b_{\pm 1n} = -\mathrm{j}^{n+1}\sqrt{2n+1}\left(\cos\alpha_{\mathrm{pol}} \mp \mathrm{j}\sin\alpha_{\mathrm{pol}}\right).$$

Thus, for a vector plane wave polarized along the x-axis we have

$$a_{1n} = -a_{-1n} = \mathrm{j}^{n-1}\sqrt{2n+1}\,,$$
$$b_{1n} = b_{-1n} = \mathrm{j}^{n-1}\sqrt{2n+1}\,,$$

while for a vector plane wave polarized along the y-axis we have

$$a_{1n} = a_{-1n} = \mathrm{j}^{n-2}\sqrt{2n+1}\,,$$
$$b_{1n} = -b_{-1n} = \mathrm{j}^{n-2}\sqrt{2n+1}\,.$$

Gaussian Beam

Many optical particle sizing instruments and particle characterization methods are based on scattering by particles illuminated with laser beams. A laser beam has a Gaussian intensity distribution and the often used appellation Gaussian beam appears justified. A mathematical description of a Gaussian beam relies on Davis approximations [45]. An nth Davis beam corresponds to the first n terms in the series expansion of the exact solution to the Maxwell equations in power of the beam parameter s,

$$s = \frac{w_0}{l}\,,$$

where w_0 is the waist radius and l is the diffraction length, $l = k_{\mathrm{s}}w_0^2$. According to Barton and Alexander [9], the first-order approximation is accurate to $s < 0.07$, while the fifth-order is accurate to $s < 0.02$, if the maximum percent error of the solution is less than 1.2%. Each nth Davis beam appears under three versions which are: the mathematical conservative version, the L-version and the symmetrized version [145]. None of these beams are exact solutions to the Maxwell equations, so that each nth Davis beam can be considered as a "pseudo-electromagnetic" field.

In the $\boldsymbol{T}$-matrix method a Gaussian beam is expanded in terms of vector spherical wave functions by replacing the pseudo-electromagnetic field of an nth Davis beam by an equivalent electromagnetic field, so that both fields have the same values on a spherical surface [81, 83, 85]. As a consequence of the equivalence method, the expansion coefficients (or the beam shape coefficients) are computed by integrating the incident field over the spherical surface. Because these fields are rapidly varying, the evaluation of the coefficients by numerical integration requires dense grids in both the θ- and φ-direction and the computer run time is excessively long.

For weakly focused Gaussian beams, the generalized localized approximation to the beam shape coefficients represents a pleasing alternative (see, for instance, [84, 87]). The form of the analytical approximation was found in part by analogy to the propagation of geometrical light rays and in part by numerical experiments. This is not a rigorous method but its use simplifies and significantly speeds up the numerical computations. A justification of

the localized approximations for both on- and off-axis beams has been given by Lock and Gouesbet [145] and Gouesbet and Lock [82]. We note that the focused beam generated by the localized approximation is a good approximation to a Gaussian beam for $s \leq 0.1$.

We consider the geometry depicted in Fig. 1.6 and assume that the middle of the beam waist is located at the point O_b. The particle coordinate system $Oxyz$ and the beam coordinate system $O_b x_b y_b z_b$ have identical spatial orientation, and the position vector of the particle center O in the system $O_b x_b y_b z_b$ is denoted by $\boldsymbol{r}_0$. The Gaussian beam is of unit amplitude, propagates along the z_b-axis and is linearly polarized along the x_b-axis. In the particle coordinate system, the expansion of the Gaussian beam in vector spherical wave functions is given by

$$\boldsymbol{E}_e(\boldsymbol{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \widetilde{a}_{mn} \boldsymbol{M}_{mn}^1 (k_s \boldsymbol{r}) + \widetilde{b}_{mn} \boldsymbol{N}_{mn}^1 (k_s \boldsymbol{r}) \ ,$$

and the generalized localized approximation to the Davis first-order beam is

$$\widetilde{a}_{mn} = K_{mn} \Psi_0 e^{j k_s z_0} \left[e^{j(m-1)\varphi_0} J_{m-1}(u) - e^{j(m+1)\varphi_0} J_{m+1}(u) \right] ,$$

$$\widetilde{b}_{mn} = K_{mn} \Psi_0 e^{j k_s z_0} \left[e^{j(m-1)\varphi_0} J_{m-1}(u) + e^{j(m+1)\varphi_0} J_{m+1}(u) \right] ,$$

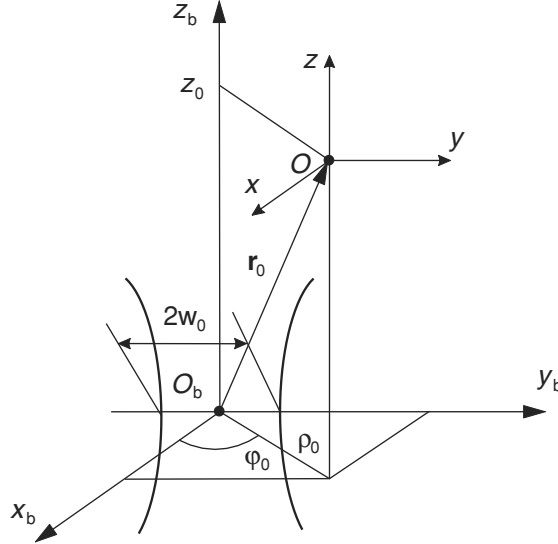**Fig. 1.6.** The particle coordinate system $Oxyz$ and the beam coordinate system $Ox_b y_b z_b$ have the same spatial orientation

where (ρ_0, φ_0, z_0) are the cylindrical coordinates of $\boldsymbol{r}_0$,

$$\Psi_0 = \mathrm{j}Q \exp\left(-\mathrm{j}Q\frac{\rho_0^2 + \rho_n^2}{w_0^2}\right) , \quad Q = \frac{1}{\mathrm{j} - 2z_0/l} , \quad \rho_n = \frac{1}{k_s}\left(n + \frac{1}{2}\right) ,$$

and

$$u = 2Q\frac{\rho_0\rho_n}{w_0^2} .$$

The normalization constant K_{mn} is given by

$$K_{mn} = 2\mathrm{j}^n\sqrt{\frac{n(n+1)}{2n+1}}$$

for $m = 0$, and by

$$K_{mn} = (-1)^{|m|}\frac{\mathrm{j}^{n+|m|}}{\left(n + \frac{1}{2}\right)^{|m|-1}}\sqrt{\frac{2n+1}{n(n+1)} \cdot \frac{(n+|m|)!}{(n-|m|)!}}$$

for $m \neq 0$. If both coordinate systems coincide ($\rho_0 = 0$), all expansion coefficients are zero unless $m = \pm 1$ and

$$\widetilde{a}_{1n} = -\widetilde{a}_{-1n} = \mathrm{j}^{n-1}\sqrt{2n+1}\exp\left(-\frac{\rho_n^2}{w_0^2}\right) ,$$

$$\widetilde{b}_{1n} = \widetilde{b}_{-1n} = \mathrm{j}^{n-1}\sqrt{2n+1}\exp\left(-\frac{\rho_n^2}{w_0^2}\right) .$$

The Gaussian beam becomes a plane wave if w_0 tends to infinity and for this specific case, the expressions of the expansion coefficients reduce to those of a vector plane wave.

We next consider the general situation depicted in Fig. 1.7 and assume that the auxiliary coordinate system $O_{\mathrm{b}}X_{\mathrm{b}}Y_{\mathrm{b}}Z_{\mathrm{b}}$ and the global coordinate system $OXYZ$ have the same spatial orientation. The Gaussian beam propagates in a direction characterized by the zenith and azimuth angles β_{g} and α_{g}, respectively, while the polarization unit vector encloses the angle α_{pol} with the x_{b}-axis of the beam coordinate system $O_{\mathrm{b}}x_{\mathrm{b}}y_{\mathrm{b}}z_{\mathrm{b}}$. As before, the particle coordinate system is obtained by rotating the global coordinate system through the Euler angles α_{p}, β_{p} and γ_{p}. The expansion of the Gaussian beam in the particle coordinate system is obtained by using the addition theorem for vector spherical wave functions under coordinate rotations (cf. (B.52) and (B.53)), and the result is

$$\boldsymbol{E}_{\mathrm{e}}(\boldsymbol{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} a_{mn}\boldsymbol{M}_{mn}^1(k_{\mathrm{s}}\boldsymbol{r}) + b_{mn}\boldsymbol{N}_{mn}^1(k_{\mathrm{s}}\boldsymbol{r}) ,$$
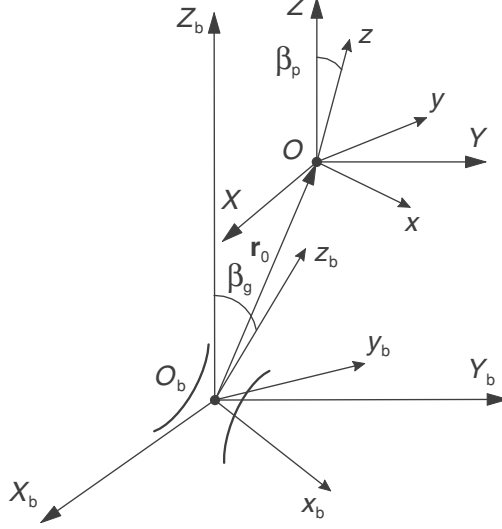
Fig. 1.7. General orientations of the particle and beam coordinate systems

where

$$a_{mn} = \sum_{m'=-n}^{n} \sum_{m''=-n}^{n} D_{m'm''}^{n}\left(-\alpha_{\mathrm{pol}}, -\beta_{\mathrm{g}}, -\alpha_{\mathrm{g}}\right) D_{m''m}^{n}\left(\alpha_{p}, \beta_{p}, \gamma_{p}\right) \widetilde{a}_{m'n},$$

$$b_{mn} = \sum_{m'=-n}^{n} \sum_{m''=-n}^{n} D_{m'm''}^{n}\left(-\alpha_{\mathrm{pol}}, -\beta_{\mathrm{g}}, -\alpha_{\mathrm{g}}\right) D_{m''m}^{n}\left(\alpha_{p}, \beta_{p}, \gamma_{p}\right) \widetilde{b}_{m'n},$$

and the Wigner D-functions $D_{m''m}^{n}$ are given by (B.34).

Remark. Another representation of a Gaussian beam is the integral representation over plane waves [48, 116]. This can be obtained by using Fourier analysis and by replacing the pseudo-vector potential of a nth Davis beam by an equivalent vector potential (satisfying the wave equation), so that both vector fields have the same values in a plane $z = \mathrm{const}$.

1.3 Internal Field

To solve the scattering problem in the framework of the null-field method it is necessary to approximate the internal field by a suitable system of vector functions. For isotropic particles, regular vector spherical wave functions of the interior wave equation are used for internal field approximations. In this section we derive new systems of vector functions for anisotropic and chiral particles by representing the electromagnetic fields (propagating in anisotropic

and chiral media) as integrals over plane waves. For each plane wave, we solve the Maxwell equations and derive the dispersion relation following the treatment of Kong [122]. The dispersion relation which relates the amplitude of the wave vector $\boldsymbol{k}$ to the properties of the medium enable us to reduce the three-dimensional integrals to two-dimensional integrals over the unit sphere. The integral representations are then transformed into series representations by expanding appropriate tangential vector functions in vector spherical harmonics. The new basis functions are the vector quasi-spherical wave functions (for anisotropic media) and the vector spherical wave functions of left- and right-handed type (for chiral media).

1.3.1 Anisotropic Media

Maxwell equations describing electromagnetic wave propagation in a source-free, electrically anisotropic medium are given by (1.10), while the constitutive relations are given by (1.7) with the scalar permeability μ in place of the permeability tensor $\overline{\mu}$. In the principal coordinate system, the first constitutive relation can be written as

$$\boldsymbol{E} = \overline{\lambda}\boldsymbol{D}\,,$$

where the impermittivity tensor $\overline{\lambda}$ is given by

$$\overline{\lambda} = \begin{bmatrix} \lambda_x & 0 & 0 \\ 0 & \lambda_y & 0 \\ 0 & 0 & \lambda_z \end{bmatrix}\,,$$

and $\lambda_x = 1/\varepsilon_x$, $\lambda_y = 1/\varepsilon_y$ and $\lambda_z = 1/\varepsilon_z$.

The electromagnetic fields can be expressed as integrals over plane waves by considering the inverse Fourier transform (excepting the factor $1/(2\pi)^3$):

$$\boldsymbol{A}(\boldsymbol{r}) = \int \mathcal{A}(\boldsymbol{k})\,\mathrm{e}^{\mathrm{j}\boldsymbol{k}\cdot\boldsymbol{r}}\,\mathrm{d}V(\boldsymbol{k})\,,$$

where $\boldsymbol{A}$ stands for $\boldsymbol{E}$, $\boldsymbol{D}$, $\boldsymbol{H}$ and $\boldsymbol{B}$, and $\mathcal{A}$ stands for the Fourier transforms $\mathcal{E}$, $\mathcal{D}$, $\mathcal{H}$ and $\mathcal{B}$. Using the identities

$$\nabla \times \boldsymbol{A}(\boldsymbol{r}) = \mathrm{j} \int \boldsymbol{k} \times \mathcal{A}(\boldsymbol{k})\,\mathrm{e}^{\mathrm{j}\boldsymbol{k}\cdot\boldsymbol{r}}\,\mathrm{d}V(\boldsymbol{k})\,,$$

$$\nabla \cdot \boldsymbol{A}(\boldsymbol{r}) = \mathrm{j} \int \boldsymbol{k} \cdot \mathcal{A}(\boldsymbol{k})\,\mathrm{e}^{\mathrm{j}\boldsymbol{k}\cdot\boldsymbol{r}}\,\mathrm{d}V(\boldsymbol{k})\,,$$

we see that the Maxwell equations for the Fourier transforms take the forms

$$\boldsymbol{k} \times \mathcal{E} = k_0\mathcal{B}\,, \quad \boldsymbol{k} \times \mathcal{H} = -k_0\mathcal{D}\,,$$

$$\boldsymbol{k} \cdot \mathcal{D} = 0\,, \quad \boldsymbol{k} \cdot \mathcal{B} = 0\,,$$

and the plane wave solutions read as

$$\mathcal{E}_\beta = \frac{k_0}{k}\mathcal{B}_\alpha\,, \quad \mathcal{E}_\alpha = -\frac{k_0}{k}\mathcal{B}_\beta\,,$$

$$\mathcal{H}_\beta = -\frac{k_0}{k}\mathcal{D}_\alpha\,, \quad \mathcal{H}_\alpha = \frac{k_0}{k}\mathcal{D}_\beta\,,$$

$$\mathcal{D}_k = 0\,, \quad \mathcal{B}_k = 0\,, \tag{1.30}$$

where (k, β, α) and $(\boldsymbol{e}_k, \boldsymbol{e}_\beta, \boldsymbol{e}_\alpha)$ are the spherical coordinates and the spherical unit vectors of the wave vector $\boldsymbol{k}$, respectively, and in general, $(\mathcal{A}_k, \mathcal{A}_\beta, \mathcal{A}_\alpha)$ are the spherical coordinates of the vector $\mathcal{A}$. The constitutive relations for the transformed fields $\mathcal{E} = \bar{\lambda}\mathcal{D}$ and $\mathcal{H} = (1/\mu)\mathcal{B}$ can be written in spherical coordinates by using the transformation

$$\begin{bmatrix} \mathcal{A}_x \\ \mathcal{A}_y \\ \mathcal{A}_z \end{bmatrix} = \begin{bmatrix} \cos\alpha\sin\beta & \cos\alpha\cos\beta & -\sin\alpha \\ \sin\alpha\sin\beta & \sin\alpha\cos\beta & \cos\alpha \\ \cos\beta & -\sin\beta & 0 \end{bmatrix} \begin{bmatrix} \mathcal{A}_k \\ \mathcal{A}_\beta \\ \mathcal{A}_\alpha \end{bmatrix}\,,$$

and the result is

$$\mathcal{E}_k = \lambda_{k\beta}\mathcal{D}_\beta + \lambda_{k\alpha}\mathcal{D}_\alpha\,,$$

$$\mathcal{E}_\beta = \lambda_{\beta\beta}\mathcal{D}_\beta + \lambda_{\beta\alpha}\mathcal{D}_\alpha\,,$$

$$\mathcal{E}_\alpha = \lambda_{\alpha\beta}\mathcal{D}_\beta + \lambda_{\alpha\alpha}\mathcal{D}_\alpha\,, \tag{1.31}$$

and

$$\mathcal{H}_k = 0\,, \quad \mathcal{H}_\beta = \frac{1}{\mu}\mathcal{B}_\beta\,, \quad \mathcal{H}_\alpha = \frac{1}{\mu}\mathcal{B}_\alpha\,, \tag{1.32}$$

where

$$\lambda_{k\beta} = \left(\lambda_x\cos^2\alpha + \lambda_y\sin^2\alpha - \lambda_z\right)\sin\beta\cos\beta\,,$$

$$\lambda_{k\alpha} = (\lambda_y - \lambda_x)\sin\alpha\cos\alpha\sin\beta\,,$$

$$\lambda_{\beta\beta} = \left(\lambda_x\cos^2\alpha + \lambda_y\sin^2\alpha\right)\cos^2\beta + \lambda_z\sin^2\beta\,,$$

$$\lambda_{\beta\alpha} = (\lambda_y - \lambda_x)\sin\alpha\cos\alpha\cos\beta\,,$$

and

$$\lambda_{\alpha\beta} = \lambda_{\beta\alpha}\,,$$

$$\lambda_{\alpha\alpha} = \lambda_x\sin^2\alpha + \lambda_y\cos^2\alpha\,.$$

Equations (1.30) and (1.32) are then used to express $\mathcal{E}_\beta$, $\mathcal{E}_\alpha$ and $\mathcal{H}_\beta$, $\mathcal{H}_\alpha$ in terms of $\mathcal{D}_\beta$, $\mathcal{D}_\alpha$, and we obtain

$$\mathcal{E}_\beta = \mu\frac{k_0^2}{k^2}\mathcal{D}_\beta\,, \quad \mathcal{E}_\alpha = \mu\frac{k_0^2}{k^2}\mathcal{D}_\alpha\,,$$

$$\mathcal{H}_\beta = -\frac{k_0}{k}\mathcal{D}_\alpha\,, \quad \mathcal{H}_\alpha = \frac{k_0}{k}\mathcal{D}_\beta\,. \tag{1.33}$$

The last two equations in (1.31) and the first two equations in (1.33) yield a homogeneous system of equations for $\mathcal{D}_\beta$ and $\mathcal{D}_\alpha$

$$\begin{bmatrix} \lambda_{\beta\beta} - \mu \frac{k_0^2}{k^2} & \lambda_{\beta\alpha} \\ \lambda_{\beta\alpha} & \lambda_{\alpha\alpha} - \mu \frac{k_0^2}{k^2} \end{bmatrix} \begin{bmatrix} \mathcal{D}_\beta \\ \mathcal{D}_\alpha \end{bmatrix} = 0 \,. \tag{1.34}$$

Requiring nontrivial solutions we set the determinant equal to zero and obtain two values for the wave number k^2,

$$k_{1,2}^2 = k_0^2 \frac{\mu}{\lambda_{1,2}} \,,$$

where

$$\lambda_1 = \frac{1}{2} \left[(\lambda_{\beta\beta} + \lambda_{\alpha\alpha}) - \sqrt{(\lambda_{\beta\beta} - \lambda_{\alpha\alpha})^2 + 4\lambda_{\beta\alpha}^2} \right] \,,$$

and

$$\lambda_2 = \frac{1}{2} \left[(\lambda_{\beta\beta} + \lambda_{\alpha\alpha}) + \sqrt{(\lambda_{\beta\beta} - \lambda_{\alpha\alpha})^2 + 4\lambda_{\beta\alpha}^2} \right] \,.$$

The above relations are the dispersion relations for the extraordinary waves, which are the permissible characteristic waves in anisotropic media. For an extraordinary wave, the magnitude of the wave vector depends on the direction of propagation, while for an ordinary wave, k is independent of β and α. Straightforward calculations show that for real values of λ_x, λ_y and λ_z, $\lambda_{\beta\beta}\lambda_{\alpha\alpha} > \lambda_{\beta\alpha}^2$ and as a result $\lambda_1 > 0$ and $\lambda_2 > 0$. The two characteristic waves, corresponding to the two values of k^2, have the $\mathcal{D}$ vectors orthogonal to each other, i.e., $\mathcal{D}^{(1)} \cdot \mathcal{D}^{(2)} = 0$. In view of (1.34) it is apparent that the components of the vectors $\mathcal{D}^{(1)}$ and $\mathcal{D}^{(2)}$ can be expressed in terms of two independent scalar functions $\mathcal{D}_\alpha$ and $\mathcal{D}_\beta$. For $k_1 = k_0\sqrt{\mu/\lambda_1}$ we set

$$\mathcal{D}_\beta^{(1)} = f\mathcal{D}_\alpha \,, \quad \mathcal{D}_\alpha^{(1)} = \mathcal{D}_\alpha \,,$$

while for $k_2 = k_0\sqrt{\mu/\lambda_2}$ we choose

$$\mathcal{D}_\beta^{(2)} = -\mathcal{D}_\beta \,, \quad \mathcal{D}_\alpha^{(2)} = f\mathcal{D}_\beta \,,$$

where

$$f = -\frac{\lambda_{\beta\alpha}}{\Delta\lambda}$$

and

$$\Delta\lambda = \frac{1}{2} \left[(\lambda_{\beta\beta} - \lambda_{\alpha\alpha}) + \sqrt{(\lambda_{\beta\beta} - \lambda_{\alpha\alpha})^2 + 4\lambda_{\beta\alpha}^2} \right] \,.$$

Next, we define the tangential fields

$$\boldsymbol{v}_\alpha = f\boldsymbol{e}_\beta + \boldsymbol{e}_\alpha \,,$$

$$\boldsymbol{v}_\beta = -\boldsymbol{e}_\beta + f\boldsymbol{e}_\alpha \,,$$

and note that the vectors $\boldsymbol{v}_\alpha$ and $\boldsymbol{v}_\beta$ are orthogonal to each other, $\boldsymbol{v}_\alpha \cdot \boldsymbol{v}_\beta = 0$, and $\boldsymbol{v}_\alpha = -\boldsymbol{e}_k \times \boldsymbol{v}_\beta$ and $\boldsymbol{v}_\beta = \boldsymbol{e}_k \times \boldsymbol{v}_\alpha$. Taking into account that $\boldsymbol{k}_1\left(\boldsymbol{e}_k\right) = k_1\left(\boldsymbol{e}_k\right)\boldsymbol{e}_k$ and $\boldsymbol{k}_2\left(\boldsymbol{e}_k\right) = k_2\left(\boldsymbol{e}_k\right)\boldsymbol{e}_k$, we find the following integral representation for the electric displacement:

$$\boldsymbol{D}(\boldsymbol{r}) = \int_\Omega \left[\mathcal{D}_\alpha\left(\boldsymbol{e}_k\right)\boldsymbol{v}_\alpha\left(\boldsymbol{e}_k\right)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_1(\boldsymbol{e}_k)\cdot\boldsymbol{r}} + \mathcal{D}_\beta\left(\boldsymbol{e}_k\right)\boldsymbol{v}_\beta\left(\boldsymbol{e}_k\right)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_2(\boldsymbol{e}_k)\cdot\boldsymbol{r}} \right] \mathrm{d}\Omega\left(\boldsymbol{e}_k\right) ,$$

with Ω being the unit sphere. The result, the integral representation for the electric field is

$$\boldsymbol{E}(\boldsymbol{r}) = \frac{1}{\varepsilon_{xy}}$$

$$\times \int_\Omega \left[\mathcal{D}_\alpha\left(\boldsymbol{e}_k\right)\boldsymbol{w}_\alpha^{\mathrm{e}}\left(\boldsymbol{e}_k\right)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_1(\boldsymbol{e}_k)\cdot\boldsymbol{r}} - \mathcal{D}_\beta\left(\boldsymbol{e}_k\right)\boldsymbol{w}_\beta^{\mathrm{e}}\left(\boldsymbol{e}_k\right)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_2(\boldsymbol{e}_k)\cdot\boldsymbol{r}} \right] \mathrm{d}\Omega\left(\boldsymbol{e}_k\right) ,$$

where

$$\varepsilon_{xy} = \frac{1}{2}\left(\varepsilon_x + \varepsilon_y\right) ,$$

and

$$\boldsymbol{w}_\alpha^{\mathrm{e}} = \varepsilon_{xy}\left[\left(\lambda_{k\beta}f + \lambda_{k\alpha}\right)\boldsymbol{e}_k + \lambda_1\boldsymbol{v}_\alpha\right] ,$$

$$\boldsymbol{w}_\beta^{\mathrm{e}} = \varepsilon_{xy}\left[\left(\lambda_{k\beta} - \lambda_{k\alpha}f\right)\boldsymbol{e}_k - \lambda_2\boldsymbol{v}_\beta\right] ,$$

while for the magnetic field, we have

$$\boldsymbol{H}(\boldsymbol{r}) = -\frac{1}{\sqrt{\varepsilon_{xy}\mu}}\int_\Omega \left[\mathcal{D}_\alpha\left(\boldsymbol{e}_k\right)\boldsymbol{w}_\alpha^{\mathrm{h}}\left(\boldsymbol{e}_k\right)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_1(\boldsymbol{e}_k)\cdot\boldsymbol{r}} \right.$$

$$\left. + \mathcal{D}_\beta\left(\boldsymbol{e}_k\right)\boldsymbol{w}_\beta^{\mathrm{h}}\left(\boldsymbol{e}_k\right)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_2(\boldsymbol{e}_k)\cdot\boldsymbol{r}} \right] \mathrm{d}\Omega\left(\boldsymbol{e}_k\right) ,$$

where

$$\boldsymbol{w}_\alpha^{\mathrm{h}} = -\sqrt{\varepsilon_{xy}\lambda_1}\boldsymbol{v}_\beta ,$$

$$\boldsymbol{w}_\beta^{\mathrm{h}} = \sqrt{\varepsilon_{xy}\lambda_2}\boldsymbol{v}_\alpha .$$

For uniaxial anisotropic media we set $\lambda = \lambda_x = \lambda_y$, derive the relations

$$\lambda_{k\beta} = \left(\lambda - \lambda_z\right)\sin\beta\cos\beta , \quad \lambda_{k\alpha} = 0 ,$$
$$\lambda_{\beta\beta} = \lambda\cos^2\beta + \lambda_z\sin^2\beta , \quad \lambda_{\beta\alpha} = 0 ,$$
$$\lambda_{\alpha\beta} = 0 , \quad \lambda_{\alpha\alpha} = \lambda ,$$

and use the identities $\lambda_1 = \lambda_{\alpha\alpha}$ and $\lambda_2 = \lambda_{\beta\beta}$, to obtain

$$k_1^2 = k_0^2\varepsilon\mu , \tag{1.35}$$

$$k_2^2 = k_0^2 \frac{\varepsilon\mu}{\cos^2\beta + \frac{\varepsilon}{\varepsilon_z}\sin^2\beta} , \tag{1.36}$$

where $\lambda = 1/\varepsilon$ and $\lambda_z = 1/\varepsilon_z$. Equation (1.35) is the dispersion relation for ordinary waves, while (1.36) is the dispersion relation for extraordinary waves. For $f = 0$ it follows that $\mathcal{D}_\beta^{(1)} = 0$ and $\mathcal{D}_\alpha^{(2)} = 0$, and further that $\mathcal{D}_\alpha^{(1)} = \mathcal{D}_\alpha$ and $\mathcal{D}_\beta^{(2)} = -\mathcal{D}_\beta$. The electric displacement is then given by

$$\boldsymbol{D}(\boldsymbol{r}) = \int_0^{2\pi} \int_0^{\pi} \left[\mathcal{D}_\alpha(\beta,\alpha)\boldsymbol{e}_\alpha \mathrm{e}^{\mathrm{j}\boldsymbol{k}_1(\beta,\alpha)\cdot\boldsymbol{r}} - \mathcal{D}_\beta(\beta,\alpha)\boldsymbol{e}_\beta \mathrm{e}^{\mathrm{j}\boldsymbol{k}_2(\beta,\alpha)\cdot\boldsymbol{r}} \right] \sin\beta \,\mathrm{d}\beta \,\mathrm{d}\alpha \,,$$
(1.37)

where $\boldsymbol{k}_1(\beta,\alpha) = k_1 \boldsymbol{e}_k(\beta,\alpha)$, $\boldsymbol{k}_2(\beta,\alpha) = k_2(\beta)\boldsymbol{e}_k(\beta,\alpha)$, and for notation simplification, the dependence of the spherical unit vectors $\boldsymbol{e}_\alpha$ and $\boldsymbol{e}_\beta$ on the spherical angles β and α is omitted. For $\varepsilon_{xy} = \varepsilon$, the integral representations for the electric and magnetic fields become

$$\boldsymbol{E}(\boldsymbol{r}) = \frac{1}{\varepsilon} \int_0^{2\pi} \int_0^{\pi} \left\{ \mathcal{D}_\alpha(\beta,\alpha)\boldsymbol{e}_\alpha \mathrm{e}^{\mathrm{j}\boldsymbol{k}_1(\beta,\alpha)\cdot\boldsymbol{r}} \right. \tag{1.38}$$

$$\left. - \varepsilon \left[\lambda_{k\beta}(\beta)\boldsymbol{e}_k + \lambda_{\beta\beta}(\beta)\boldsymbol{e}_\beta \right] \mathcal{D}_\beta(\beta,\alpha)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_2(\beta,\alpha)\cdot\boldsymbol{r}} \right\} \sin\beta \,\mathrm{d}\beta \,\mathrm{d}\alpha \,,$$

and

$$\boldsymbol{H}(\boldsymbol{r}) = -\frac{1}{\sqrt{\varepsilon\mu}} \int_0^{2\pi} \int_0^{\pi} \left[\mathcal{D}_\alpha(\beta,\alpha)\boldsymbol{e}_\beta \mathrm{e}^{\mathrm{j}\boldsymbol{k}_1(\beta,\alpha)\cdot\boldsymbol{r}} \right.$$

$$\left. + \sqrt{\varepsilon\lambda_{\beta\beta}(\beta)}\mathcal{D}_\beta(\beta,\alpha)\boldsymbol{e}_\alpha \mathrm{e}^{\mathrm{j}\boldsymbol{k}_2(\beta,\alpha)\cdot\boldsymbol{r}} \right] \sin\beta \,\mathrm{d}\beta \,\mathrm{d}\alpha \,, \tag{1.39}$$

respectively. For isotropic media, the only nonzero λ functions are $\lambda_{\beta\beta}$ and $\lambda_{\alpha\alpha}$, and we have $\lambda_{\beta\beta} = \lambda_{\alpha\alpha} = \lambda$. The two waves degenerate into one (ordinary) wave, i.e., $k_1 = k_2 = k$, and the dispersion relation is

$$k^2 = k_0^2 \varepsilon\mu \,.$$

Next we proceed to derive series representations for the electric and magnetic fields propagating in uniaxial anisotropic media. On the unit sphere, the tangential vector function $\mathcal{D}_\alpha(\beta,\alpha)\boldsymbol{e}_\alpha - \mathcal{D}_\beta(\beta,\alpha)\boldsymbol{e}_\beta$ can be expanded in terms of the vector spherical harmonics $\boldsymbol{m}_{mn}$ and $\boldsymbol{n}_{mn}$ as follows:

$$\mathcal{D}_\alpha(\beta,\alpha)\boldsymbol{e}_\alpha - \mathcal{D}_\beta(\beta,\alpha)\boldsymbol{e}_\beta = -\varepsilon \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \frac{1}{4\pi\mathrm{j}^{n+1}} \left[-\mathrm{j}c_{mn}\boldsymbol{m}_{mn}(\beta,\alpha) \right.$$

$$\left. + d_{mn}\boldsymbol{n}_{mn}(\beta,\alpha) \right] \,. \tag{1.40}$$

Because the system of vector spherical harmonics is orthogonal and complete in $L^2(\Omega)$, the series representation (1.40) is valid for any tangential vector field. Taking into account the expressions of the vector spherical harmonics (cf. (B.8) and (B.9)) we deduce that the expansions of $\mathcal{D}_\beta$ and $\mathcal{D}_\alpha$ are given by

$$-\mathcal{D}_\beta(\beta,\alpha) = -\varepsilon \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \left[m\pi_n^{|m|}(\beta)c_{mn} \right.$$

$$\left. + \tau_n^{|m|}(\beta)d_{mn} \right] \mathrm{e}^{\mathrm{j}m\alpha}$$

and

$$\mathcal{D}_\alpha(\beta,\alpha) = -\varepsilon \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \left[\mathrm{j}\tau_n^{|m|}(\beta)c_{mn} \right.$$

$$\left. + jm\pi_n^{|m|}(\beta)d_{mn} \right] \mathrm{e}^{\mathrm{j}m\alpha} \,,$$

respectively. Inserting the above expansions into (1.38) and (1.39), yields the series representations

$$\boldsymbol{E}(\boldsymbol{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} c_{mn}\boldsymbol{X}_{mn}^{\mathrm{e}}(\boldsymbol{r}) + d_{mn}\boldsymbol{Y}_{mn}^{\mathrm{e}}(\boldsymbol{r}) \,, \tag{1.41}$$

$$\boldsymbol{H}(\boldsymbol{r}) = -\mathrm{j}\sqrt{\frac{\varepsilon}{\mu}} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} c_{mn}\boldsymbol{X}_{mn}^{\mathrm{h}}(\boldsymbol{r}) + d_{mn}\boldsymbol{Y}_{mn}^{\mathrm{h}}(\boldsymbol{r}) \,, \tag{1.42}$$

where the new vector functions are defined as

$$\boldsymbol{X}_{mn}^{\mathrm{e}}(\boldsymbol{r}) = -\frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \int_0^{2\pi} \int_0^{\pi} \left\{ \mathrm{j}\tau_n^{|m|}(\beta)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_1(\beta,\alpha)\cdot\boldsymbol{r}}\boldsymbol{e}_\alpha \right.$$

$$\left. + \varepsilon\left[\lambda_{k\beta}(\beta)\boldsymbol{e}_k + \lambda_{\beta\beta}(\beta)\boldsymbol{e}_\beta\right] m\pi_n^{|m|}(\beta)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_2(\beta,\alpha)\cdot\boldsymbol{r}} \right\}$$

$$\times\mathrm{e}^{\mathrm{j}m\alpha} \sin\beta \, \mathrm{d}\beta \, \mathrm{d}\alpha \,, \tag{1.43}$$

$$\boldsymbol{Y}_{mn}^{\mathrm{e}}(\boldsymbol{r}) = -\frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \int_0^{2\pi} \int_0^{\pi} \left\{ jm\pi_n^{|m|}(\beta)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_1(\beta,\alpha)\cdot\boldsymbol{r}}\boldsymbol{e}_\alpha \right. \tag{1.44}$$

$$\left. + \varepsilon\left[\lambda_{k\beta}(\beta)\boldsymbol{e}_k + \lambda_{\beta\beta}(\beta)\boldsymbol{e}_\beta\right] \tau_n^{|m|}(\beta)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_2(\beta,\alpha)\cdot\boldsymbol{r}} \right\} \mathrm{e}^{\mathrm{j}m\alpha} \sin\beta \, \mathrm{d}\beta \, \mathrm{d}\alpha \,,$$

$$\boldsymbol{X}_{mn}^{\mathrm{h}}(\boldsymbol{r}) = -\frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \int_0^{2\pi} \int_0^{\pi} \left[\tau_n^{|m|}(\beta)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_1(\beta,\alpha)\cdot\boldsymbol{r}}\boldsymbol{e}_\beta \right. \tag{1.45}$$

$$\left. + \mathrm{j}\sqrt{\varepsilon\lambda_{\beta\beta}(\beta)}m\pi_n^{|m|}(\beta)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_2(\beta,\alpha)\cdot\boldsymbol{r}}\boldsymbol{e}_\alpha \right] \mathrm{e}^{\mathrm{j}m\alpha} \sin\beta \, \mathrm{d}\beta \, \mathrm{d}\alpha \,,$$

and

$$\boldsymbol{Y}_{mn}^{\mathrm{h}}(\boldsymbol{r}) = -\frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \int_0^{2\pi} \int_0^{\pi} \left[m\pi_n^{|m|}(\beta)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_1(\beta,\alpha)\cdot\boldsymbol{r}}\boldsymbol{e}_\beta \right.$$

$$\left. + \mathrm{j}\sqrt{\varepsilon\lambda_{\beta\beta}(\beta)}\tau_n^{|m|}(\beta)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_2(\beta,\alpha)\cdot\boldsymbol{r}}\boldsymbol{e}_\alpha \right] \mathrm{e}^{\mathrm{j}m\alpha} \sin\beta \, \mathrm{d}\beta \, \mathrm{d}\alpha \,. \tag{1.46}$$

In (1.38)–(1.39), the electromagnetic fields are expressed in terms of the unknown scalar functions $\mathcal{D}_\alpha$ and $\mathcal{D}_\beta$, while in (1.41) and (1.42), the electromagnetic fields are expressed in terms of the unknown expansion coefficients c_{mn} and d_{mn}. These unknowns will be determined from the boundary conditions for each specific scattering problem. The vector functions $\boldsymbol{X}_{mn}^{\mathrm{e,h}}$ and $\boldsymbol{Y}_{mn}^{\mathrm{e,h}}$ can be regarded as a generalization of the regular vector spherical wave functions $\boldsymbol{M}_{mn}^1$ and $\boldsymbol{N}_{mn}^1$. For isotropic media, we have $\varepsilon\lambda_{\beta\beta}=1$, $\lambda_{k\beta}=0$ and $k_1=k_2=k$, and we see that both systems of vector functions are equivalent:

$$
\begin{aligned}
\boldsymbol{X}_{mn}^{\mathrm{e}}(\boldsymbol{r}) &= \boldsymbol{Y}_{mn}^{\mathrm{h}}(\boldsymbol{r}) = \boldsymbol{M}_{mn}^1(k\boldsymbol{r})\,, \\
\boldsymbol{Y}_{mn}^{\mathrm{e}}(\boldsymbol{r}) &= \boldsymbol{X}_{mn}^{\mathrm{h}}(\boldsymbol{r}) = \boldsymbol{N}_{mn}^1(k\boldsymbol{r})\,.
\end{aligned}
\tag{1.47}
$$

As a result, we obtain the familiar expansions of the electromagnetic fields in terms of vector spherical wave functions of the interior wave equation:

$$
\boldsymbol{E}(\boldsymbol{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} c_{mn}\boldsymbol{M}_{mn}^1\left(k\boldsymbol{r}\right) + d_{mn}\boldsymbol{N}_{mn}^1(k\boldsymbol{r})\,,
$$

$$
\boldsymbol{H}(\boldsymbol{r}) = -\mathrm{j}\sqrt{\frac{\varepsilon}{\mu}}\sum_{n=1}^{\infty}\sum_{m=-n}^{n} c_{mn}\boldsymbol{N}_{mn}^1\left(k\boldsymbol{r}\right) + d_{mn}\boldsymbol{M}_{mn}^1(k\boldsymbol{r})\,.
$$

Although the derivation of $\boldsymbol{X}_{mn}^{\mathrm{e,h}}$ and $\boldsymbol{Y}_{mn}^{\mathrm{e,h}}$ differs from that of Kiselev et al. [119], the resulting systems of vector functions are identical except for a multiplicative constant. Accordingly to Kiselev et al. [119], this system of vector functions will be referred to as the system of vector quasi-spherical wave functions. In (1.43)–(1.46) the integration over α can be analytically performed by using the relations

$$
\begin{aligned}
\boldsymbol{e}_k &= \sin\beta\cos\alpha\boldsymbol{e}_x + \sin\beta\sin\alpha\boldsymbol{e}_y + \cos\beta\boldsymbol{e}_z\,, \\
\boldsymbol{e}_\beta &= \cos\beta\cos\alpha\boldsymbol{e}_x + \cos\beta\sin\alpha\boldsymbol{e}_y - \sin\beta\boldsymbol{e}_z\,, \\
\boldsymbol{e}_\alpha &= -\sin\alpha\boldsymbol{e}_x + \cos\alpha\boldsymbol{e}_y\,,
\end{aligned}
$$

and the standard integrals

$$
I_m(x,\varphi) = \int_0^{2\pi} \mathrm{e}^{\mathrm{j}x\cos(\alpha-\varphi)}e^{\mathrm{j}m\alpha}\,\mathrm{d}\alpha = 2\pi\mathrm{j}^m\mathrm{e}^{\mathrm{j}m\varphi}J_m(x)\,,
$$

$$
\begin{aligned}
I_m^{\mathrm{c}}(x,\varphi) = \int_0^{2\pi} \cos\alpha\mathrm{e}^{\mathrm{j}x\cos(\alpha-\varphi)}\mathrm{e}^{\mathrm{j}m\alpha}\,\mathrm{d}\alpha = \pi\Big[&\mathrm{j}^{m+1}\mathrm{e}^{\mathrm{j}(m+1)\varphi}J_{m+1}(x) \\
&+ \mathrm{j}^{m-1}\mathrm{e}^{\mathrm{j}(m-1)\varphi}J_{m-1}(x)\Big]\,,
\end{aligned}
$$

$$
\begin{aligned}
I_m^{\mathrm{s}}(x,\varphi) = \int_0^{2\pi} \sin\alpha\mathrm{e}^{\mathrm{j}x\cos(\alpha-\varphi)}\mathrm{e}^{\mathrm{j}m\alpha}\,\mathrm{d}\alpha = -\mathrm{j}\pi\Big[&\mathrm{j}^{m+1}\mathrm{e}^{\mathrm{j}(m+1)\varphi}J_{m+1}(x) \\
&- \mathrm{j}^{m-1}\mathrm{e}^{\mathrm{j}(m-1)\varphi}J_{m-1}(x)\Big]\,,
\end{aligned}
$$

where $(\boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z)$ are the Cartesian unit vectors and J_m is the cylindrical Bessel functions of order m. The expressions of the Cartesian components of the vector function $\boldsymbol{X}_{mn}^{\mathrm{e}}$ read as

$$X_{mn,x}^{\mathrm{e}}(\boldsymbol{r}) = -\frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \int_0^\pi \left\{ -\mathrm{j}\tau_n^{|m|}(\beta)I_m^{\mathrm{s}}(x_1,\varphi)\mathrm{e}^{\mathrm{j}y_1(r,\theta,\beta)} \right.$$

$$+\varepsilon\left[\lambda_{\beta\beta}(\beta)\cos\beta + \lambda_{k\beta}(\beta)\sin\beta\right]m\pi_n^{|m|}(\beta)$$

$$\left. \times I_m^{\mathrm{c}}(x_2,\varphi)\mathrm{e}^{\mathrm{j}y_2(r,\theta,\beta)} \right\} \sin\beta\,\mathrm{d}\beta \qquad (1.48)$$

$$X_{mn,y}^{\mathrm{e}}(\boldsymbol{r}) = -\frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \int_0^\pi \left\{ \mathrm{j}\tau_n^{|m|}(\beta)I_m^{\mathrm{c}}(x_1,\varphi)\mathrm{e}^{\mathrm{j}y_1(r,\theta,\beta)} \right.$$

$$+\varepsilon\left[\lambda_{\beta\beta}(\beta)\cos\beta + \lambda_{k\beta}(\beta)\sin\beta\right]m\pi_n^{|m|}(\beta)$$

$$\left. \times I_m^{\mathrm{s}}(x_2,\varphi)\mathrm{e}^{\mathrm{j}y_2(r,\theta,\beta)} \right\} \sin\beta\,\mathrm{d}\beta\,, \qquad (1.49)$$

$$X_{mn,z}^{\mathrm{e}}(\boldsymbol{r}) = -\frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \int_0^\pi \varepsilon\left[\lambda_{k\beta}(\beta)\cos\beta - \lambda_{\beta\beta}(\beta)\sin\beta\right]$$

$$\times m\pi_n^{|m|}(\beta)I_m(x_2,\varphi)\mathrm{e}^{\mathrm{j}y_2(r,\theta,\beta)} \sin\beta\,\mathrm{d}\beta\,, \qquad (1.50)$$

where $x_1(r,\theta,\beta) = k_1 r \sin\beta\sin\theta$, $x_2(r,\theta,\beta) = k_2(\beta)r\sin\beta\sin\theta$, $y_1(r,\theta,\beta) = k_1 r\cos\beta\cos\theta$ and $y_2(r,\theta,\beta) = k_2(\beta)r\cos\beta\cos\theta$, while the expressions of the Cartesian components of the vector functions $\boldsymbol{Y}_{mn}^{\mathrm{e}}$ are given by (1.48)–(1.50) with $m\pi_n^{|m|}$ and $\tau_n^{|m|}$ interchanged. Similarly, the Cartesian components of the vector function $\boldsymbol{X}_{mn}^{\mathrm{h}}$ are

$$X_{mn,x}^{\mathrm{h}}(\boldsymbol{r}) = -\frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \int_0^\pi \left[\tau_n^{|m|}(\beta)\cos\beta I_m^{\mathrm{c}}(x_1,\varphi)\mathrm{e}^{\mathrm{j}y_1(r,\theta,\beta)} \right.$$

$$\left. - \mathrm{j}\sqrt{\varepsilon\lambda_{\beta\beta}(\beta)}m\pi_n^{|m|}(\beta)I_m^{\mathrm{s}}(x_2,\varphi)\mathrm{e}^{\mathrm{j}y_2(r,\theta,\beta)} \right] \sin\beta\,\mathrm{d}\beta\,, \qquad (1.51)$$

$$X_{mn,y}^{\mathrm{h}}(\boldsymbol{r}) = -\frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \int_0^\pi \left[\tau_n^{|m|}(\beta)\cos\beta I_m^{\mathrm{s}}(x_1,\varphi)\mathrm{e}^{\mathrm{j}y_1(r,\theta,\beta)} \right.$$

$$\left. + \mathrm{j}\sqrt{\varepsilon\lambda_{\beta\beta}(\beta)}m\pi_n^{|m|}(\beta)I_m^{\mathrm{c}}(x_2,\varphi)\mathrm{e}^{\mathrm{j}y_2(r,\theta,\beta)} \right] \sin\beta\,\mathrm{d}\beta\,, \qquad (1.52)$$

$$X_{mn,z}^{\mathrm{h}}(\boldsymbol{r}) = \frac{1}{4\pi\mathrm{j}^{n+1}} \frac{1}{\sqrt{2n(n+1)}} \int_0^\pi \tau_n^{|m|}(\beta)I_m(x_1,\varphi)\mathrm{e}^{\mathrm{j}y_1(r,\theta,\beta)} \sin^2\beta\,\mathrm{d}\beta\,,$$

$$\qquad (1.53)$$

and as before, the components of the vector functions $\boldsymbol{Y}_{mn}^{\mathrm{h}}$ are given by (1.51)–(1.53) with $m\pi_n^{|m|}$ and $\tau_n^{|m|}$ interchanged.

In the above analysis, $\boldsymbol{X}_{mn}^{\mathrm{e,h}}$ and $\boldsymbol{Y}_{mn}^{\mathrm{e,h}}$ are expressed in the principal coordinate system, but in general, it is necessary to transform these vector functions from the principal coordinate system to the particle coordinate system through a rotation. The vector quasi-spherical wave functions can also be defined for biaxial media ($\varepsilon_x \neq \varepsilon_y \neq \varepsilon_z$) by considering the expansion of the tangential vector function $\mathcal{D}_\alpha(\beta, \alpha)\boldsymbol{v}_\alpha + \mathcal{D}_\beta(\beta, \alpha)\boldsymbol{v}_\beta$ in terms of vector spherical harmonics.

1.3.2 Chiral Media

For a source-free, isotropic, chiral medium, the Maxwell equations are given by (1.10), with the $\boldsymbol{K}$ matrix defined by (1.11). Following Bohren [16], the electromagnetic field is transformed to

$$\begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix} = \boldsymbol{A} \begin{bmatrix} \boldsymbol{L} \\ \boldsymbol{R} \end{bmatrix},$$

where $\boldsymbol{A}$ is a transformation matrix and

$$\boldsymbol{A} = \begin{bmatrix} 1 & -\mathrm{j}\sqrt{\frac{\mu}{\varepsilon}} \\ -\mathrm{j}\sqrt{\frac{\varepsilon}{\mu}} & 1 \end{bmatrix}.$$

The transformed fields $\boldsymbol{L}$ and $\boldsymbol{R}$ are the left- and right-handed circularly polarized waves, or simply the waves of left- and right-handed types. Explicitly, the electromagnetic field transformation is

$$\boldsymbol{E} = \boldsymbol{L} - \mathrm{j}\sqrt{\frac{\mu}{\varepsilon}}\boldsymbol{R},$$

$$\boldsymbol{H} = -\mathrm{j}\sqrt{\frac{\varepsilon}{\mu}}\boldsymbol{L} + \boldsymbol{R}$$

and note that this linear transformation diagonalizes the matrix $\boldsymbol{K}$,

$$\Lambda = \boldsymbol{A}^{-1}\boldsymbol{K}\boldsymbol{A} = \begin{bmatrix} \frac{k}{1-\beta k} & 0 \\ 0 & -\frac{k}{1+\beta k} \end{bmatrix}.$$

Defining the wave numbers

$$k_{\mathrm{L}} = \frac{k}{1 - \beta k},$$

$$k_{\mathrm{R}} = \frac{k}{1 + \beta k},$$

we see that the waves of left- and right-handed types satisfy the equations

$$\nabla \times \boldsymbol{L} = k_{\mathrm{L}} \boldsymbol{L}\,, \quad \nabla \cdot \boldsymbol{L} = 0 \tag{1.54}$$

and

$$\nabla \times \boldsymbol{R} = -k_{\mathrm{R}} \boldsymbol{R}\,, \quad \nabla \cdot \boldsymbol{R} = 0, \tag{1.55}$$

respectively.

For chiral media, we use the same technique as for anisotropic media and express the left- and right-handed circularly polarized waves as integrals over plane waves. For the Fourier transform corresponding to waves of left-handed type,

$$\boldsymbol{L}(\boldsymbol{r}) = \int \mathcal{L}\left(\boldsymbol{k}\right) \mathrm{e}^{\mathrm{j}\boldsymbol{k}\cdot\boldsymbol{r}} \, \mathrm{d}V\left(\boldsymbol{k}\right)\,,$$

the differential equations (1.54) yield

$$\mathcal{L}_\beta = -\mathrm{j}\frac{k_{\mathrm{L}}}{k}\mathcal{L}_\alpha\,,$$

$$\mathcal{L}_\alpha = \mathrm{j}\frac{k_{\mathrm{L}}}{k}\mathcal{L}_\beta\,,$$

and $\mathcal{L}_k = 0$. The above set of equations form a system of homogeneous equations and setting the determinant equal to zero, gives the dispersion relation for the waves of left-handed type

$$k^2 = k_{\mathrm{L}}^2\,.$$

Choosing $\mathcal{L}_\beta$ as an independent scalar function, we express $\boldsymbol{L}$ as

$$\boldsymbol{L}(\boldsymbol{r}) = \int_0^{2\pi} \int_0^{\pi} (\boldsymbol{e}_\beta + \mathrm{j}\boldsymbol{e}_\alpha)\,\mathcal{L}_\beta(\beta,\alpha)\mathrm{e}^{\mathrm{j}\boldsymbol{k}_{\mathrm{L}}(\beta,\alpha)\cdot\boldsymbol{r}} \sin\beta\,\mathrm{d}\beta\,\mathrm{d}\alpha\,, \tag{1.56}$$

where $\boldsymbol{k}_{\mathrm{L}}(\beta,\alpha) = k_{\mathrm{L}}\boldsymbol{e}_k(\beta,\alpha)$. The tangential field $(\boldsymbol{e}_\beta + \mathrm{j}\boldsymbol{e}_\alpha)\mathcal{L}_\beta$ is orthogonal to the vector spherical harmonics of right-handed type with respect to the scalar product in $L^2_{\mathrm{tan}}(\Omega)$ (cf. (B.16) and (B.17)), and as result, $(\boldsymbol{e}_\beta + \mathrm{j}\boldsymbol{e}_\alpha)\mathcal{L}_\beta$ possesses an expansion in terms of vector spherical harmonics of left-handed type (cf. (B.14))

$$(\boldsymbol{e}_\beta + \mathrm{j}\boldsymbol{e}_\alpha)\,\mathcal{L}_\beta(\beta,\alpha) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{1}{2\sqrt{2}\pi\mathrm{j}^n}c_{mn}\boldsymbol{l}_{mn}(\beta,\alpha) \tag{1.57}$$

$$= \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\frac{1}{4\pi\mathrm{j}^n}c_{mn}\left[\boldsymbol{m}_{mn}(\beta,\alpha) + \mathrm{j}\boldsymbol{n}_{mn}(\beta,\alpha)\right]\,.$$

Inserting (1.57) into (1.56), yields

$$\boldsymbol{L}(\boldsymbol{r}) = -\sum_{n=1}^{\infty} \sum_{m=-n}^{n} \frac{1}{4\pi \mathrm{j}^{n+1}} c_{mn} \int_0^{2\pi} \int_0^{\pi} [-\mathrm{j}\boldsymbol{m}_{mn}(\beta,\alpha)$$
$$+ \boldsymbol{n}_{mn}(\beta,\alpha)] \, \mathrm{e}^{\mathrm{j}\boldsymbol{k}_{\mathrm{L}}(\beta,\alpha)\cdot\boldsymbol{r}} \sin\beta \, \mathrm{d}\beta \, \mathrm{d}\alpha \,,$$

whence, using the integral representation for the vector spherical wave functions (cf. (B.26) and (B.27)), gives

$$\boldsymbol{L}(\boldsymbol{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} c_{mn} \boldsymbol{L}_{mn}(k_{\mathrm{L}}\boldsymbol{r})$$
$$= \sum_{n=1}^{\infty} \sum_{m=-n}^{n} c_{mn} \left[\boldsymbol{M}_{mn}^1(k_{\mathrm{L}}\boldsymbol{r}) + \boldsymbol{N}_{mn}^1(k_{\mathrm{L}}\boldsymbol{r}) \right] \,,$$

where the vector spherical wave functions of left-handed type $\boldsymbol{L}_{mn}$ are defined as

$$\boldsymbol{L}_{mn} = \boldsymbol{M}_{mn}^1 + \boldsymbol{N}_{mn}^1 \,. \tag{1.58}$$

For the waves of right-handed type we proceed analogously. We obtain the integral representation

$$\boldsymbol{R}(\boldsymbol{r}) = \int_0^{2\pi} \int_0^{\pi} (\boldsymbol{e}_\beta - \mathrm{j}\boldsymbol{e}_\alpha) \, \mathcal{R}_\beta(\beta,\alpha) \mathrm{e}^{\mathrm{j}\boldsymbol{k}_{\mathrm{R}}(\beta,\alpha)\cdot\boldsymbol{r}} \sin\beta \, \mathrm{d}\beta \, \mathrm{d}\alpha$$

with $\mathcal{R}_\beta$ being an independent scalar function, and the expansion

$$\boldsymbol{R}(\boldsymbol{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} d_{mn} \boldsymbol{R}_{mn}(k_{\mathrm{R}}\boldsymbol{r})$$
$$= \sum_{n=1}^{\infty} \sum_{m=-n}^{n} d_{mn} \left[\boldsymbol{M}_{mn}^1(k_{\mathrm{R}}\boldsymbol{r}) - \boldsymbol{N}_{mn}^1(k_{\mathrm{R}}\boldsymbol{r}) \right]$$

with the vector spherical wave functions of right-handed type $\boldsymbol{R}_{mn}$ being defined as

$$\boldsymbol{R}_{mn} = \boldsymbol{M}_{mn}^1 - \boldsymbol{N}_{mn}^1 \,. \tag{1.59}$$

In conclusion, the electric and magnetic fields propagating in isotropic, chiral media possess the expansions [16, 17, 135]

$$\boldsymbol{E}(\boldsymbol{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} c_{mn} \boldsymbol{L}_{mn}(k_{\mathrm{L}}\boldsymbol{r}) - \mathrm{j}\sqrt{\frac{\mu}{\varepsilon}} d_{mn} \boldsymbol{R}_{mn}(k_{\mathrm{R}}\boldsymbol{r}) \,,$$

$$\boldsymbol{H}(\boldsymbol{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} -\mathrm{j}\sqrt{\frac{\varepsilon}{\mu}} c_{mn} \boldsymbol{L}_{mn}(k_{\mathrm{L}}\boldsymbol{r}) + d_{mn} \boldsymbol{R}_{mn}(k_{\mathrm{R}}\boldsymbol{r}) \,.$$

An exhaustive treatment of electromagnetic wave propagation in isotropic, chiral media has been given by Lakhtakia et al. [136]. This analysis deals with the conservation of energy and momentum, properties of the infinite-medium Green's function and the mathematical expression of Huygens's principle.

1.4 Scattered Field

In this section we consider the basic properties of the scattered field as they are determined by energy conservation and by the propagation properties of the fields in source-free regions. The results are presented for electromagnetic scattering by dielectric particles, which is modeled by the transmission boundary-value problem. To formulate the transmission boundary-value problem we consider a bounded domain D_i (of class C^2) with boundary S and exterior D_s, and denote by $\boldsymbol{n}$ the unit normal vector to S directed into D_s (Fig. 1.8). The relative permittivity and relative permeability of the domain D_t are ε_t and μ_t, where t $=$ s, i, and the wave number in the domain D_t is $k_t = k_0\sqrt{\varepsilon_t\mu_t}$, where k_0 is the wave number in free space. The unbounded domain D_s is assumed to be lossless, i.e., $\varepsilon_s > 0$ and $\mu_s > 0$, and the external excitation is considered to be a vector plane wave

$$\boldsymbol{E}_e(\boldsymbol{r}) = \boldsymbol{E}_{e0}\mathrm{e}^{\mathrm{j}\boldsymbol{k}_e\cdot\boldsymbol{r}}, \quad \boldsymbol{H}_e(\boldsymbol{r}) = \sqrt{\frac{\varepsilon_s}{\mu_s}}\boldsymbol{e}_k \times \boldsymbol{E}_{e0}\mathrm{e}^{\mathrm{j}\boldsymbol{k}_e\cdot\boldsymbol{r}},$$

where $\boldsymbol{E}_{e0}$ is the complex amplitude vector and $\boldsymbol{e}_k$ is the unit vector in the direction of the wave vector $\boldsymbol{k}_e$. The transmission boundary-value problem has the following formulation.

Given $\boldsymbol{E}_e, \boldsymbol{H}_e$ as an entire solution to the Maxwell equations representing the external excitation, find the vector fields $\boldsymbol{E}_s, \boldsymbol{H}_s \in C^1(D_s) \cap C(\overline{D}_s)$ and $\boldsymbol{E}_i, \boldsymbol{H}_i \in C^1(D_i) \cap C(\overline{D}_i)$ satisfying the Maxwell equations

$$\nabla \times \boldsymbol{E}_t = \mathrm{j}k_0\mu_t\boldsymbol{H}_t, \quad \nabla \times \boldsymbol{H}_t = -\mathrm{j}k_0\varepsilon_t\boldsymbol{E}_t, \tag{1.60}$$
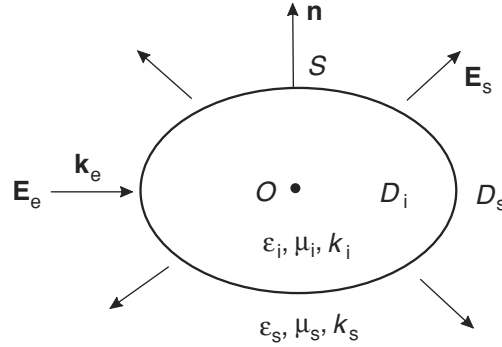
Fig. 1.8. The domain D_i with boundary S and exterior D_s

in D_t, $t = s, i$, and the two transmission conditions

$$\boldsymbol{n} \times \boldsymbol{E}_i - \boldsymbol{n} \times \boldsymbol{E}_s = \boldsymbol{n} \times \boldsymbol{E}_e \,,$$

$$\boldsymbol{n} \times \boldsymbol{H}_i - \boldsymbol{n} \times \boldsymbol{H}_s = \boldsymbol{n} \times \boldsymbol{H}_e \,, \tag{1.61}$$

on S. In addition, the scattered field $\boldsymbol{E}_s, \boldsymbol{H}_s$ must satisfy the Silver–Müller radiation condition

$$\frac{\boldsymbol{r}}{r} \times \sqrt{\mu_s} \boldsymbol{H}_s + \sqrt{\epsilon_s} \boldsymbol{E}_s = \mathrm{o}\left(\frac{1}{r}\right) \,, \quad as \quad r \to \infty \,, \tag{1.62}$$

uniformly for all directions $\boldsymbol{r}/r$.

It should be emphasized that for the assumed smoothness conditions, the transmission boundary-value problem possesses an unique solution [177].

Our presentation is focused on the analysis of the scattered field in the far-field region. We begin with a basic representation theorem for electromagnetic scattering and then introduce the primary quantities which define the single-scattering law: the far-field patterns and the amplitude matrix. Because the measurement of the amplitude matrix is a complicated experimental problem, we characterize the scattering process by other measurable quantities as for instance the optical cross-sections and the phase and extinction matrices.

In our analysis, we will frequently use the Green second vector theorem

$$\int_D \left[\boldsymbol{a} \cdot (\nabla \times \nabla \times \boldsymbol{b}) - \boldsymbol{b} \cdot (\nabla \times \nabla \times \boldsymbol{a}) \right] \mathrm{d}V$$

$$= \int_S \boldsymbol{n} \cdot \left[\boldsymbol{b} \times (\nabla \times \boldsymbol{a}) - \boldsymbol{a} \times (\nabla \times \boldsymbol{b}) \right] \mathrm{d}S \,,$$

where D is a bounded domain with boundary S and $\boldsymbol{n}$ is the outward unit normal vector to S.

1.4.1 Stratton–Chu Formulas

Representation theorems for electromagnetic fields have been given by Stratton and Chu [216]. If $\boldsymbol{E}_s$, $\boldsymbol{H}_s$ is a radiating solution to Maxwell's equations in D_s, then we have the Stratton–Chu formulas

$$\begin{pmatrix} \boldsymbol{E}_s(\boldsymbol{r}) \\ 0 \end{pmatrix} = \nabla \times \int_S \boldsymbol{e}_s(\boldsymbol{r}') \, g(k_s, \boldsymbol{r}, \boldsymbol{r}') \, \mathrm{d}S(\boldsymbol{r}') \tag{1.63}$$

$$+ \frac{\mathrm{j}}{k_0 \varepsilon_s} \nabla \times \nabla \times \int_S \boldsymbol{h}_s(\boldsymbol{r}') \, g(k_s, \boldsymbol{r}, \boldsymbol{r}') \, \mathrm{d}S(\boldsymbol{r}') \,, \quad \begin{pmatrix} \boldsymbol{r} \in D_s \\ \boldsymbol{r} \in D_i \end{pmatrix}$$

and

$$\begin{pmatrix} \boldsymbol{H}_{\mathrm{s}}(\boldsymbol{r}) \\ 0 \end{pmatrix} = \nabla \times \int_S \boldsymbol{h}_{\mathrm{s}}\left(\boldsymbol{r}'\right) g\left(k_{\mathrm{s}}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}')$$

$$- \frac{\mathrm{j}}{k_0 \mu_{\mathrm{s}}} \nabla \times \nabla \times \int_S \boldsymbol{e}_{\mathrm{s}}\left(\boldsymbol{r}'\right) g\left(k_{\mathrm{s}}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}'), \quad \begin{pmatrix} \boldsymbol{r} \in D_{\mathrm{s}} \\ \boldsymbol{r} \in D_{\mathrm{i}} \end{pmatrix},$$

where g is the Green function and the surface fields $\boldsymbol{e}_{\mathrm{s}}$ and $\boldsymbol{h}_{\mathrm{s}}$ are the tangential components of the electric and magnetic fields on the particle surface, i.e., $\boldsymbol{e}_{\mathrm{s}} = \boldsymbol{n} \times \boldsymbol{E}_{\mathrm{s}}$ and $\boldsymbol{h}_{\mathrm{s}} = \boldsymbol{n} \times \boldsymbol{H}_{\mathrm{s}}$, respectively. In the above equations we use a compact way of writing two formulas (for $\boldsymbol{r} \in D_{\mathrm{s}}$ and for $\boldsymbol{r} \in D_{\mathrm{i}}$) as a single equation.

A similar result holds for vector functions satisfying the Maxwell equations in bounded domains. With $\boldsymbol{E}_{\mathrm{i}}$, $\boldsymbol{H}_{\mathrm{i}}$ being a solution to Maxwell's equations in D_{i} we have

$$\begin{pmatrix} -\boldsymbol{E}_{\mathrm{i}}(\boldsymbol{r}) \\ 0 \end{pmatrix} = \nabla \times \int_S \boldsymbol{e}_{\mathrm{i}}\left(\boldsymbol{r}'\right) g\left(k_{\mathrm{i}}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}')$$

$$+ \frac{\mathrm{j}}{k_0 \varepsilon_{\mathrm{i}}} \nabla \times \nabla \times \int_S \boldsymbol{h}_{\mathrm{i}}\left(\boldsymbol{r}'\right) g\left(k_{\mathrm{i}}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}'), \quad \begin{pmatrix} \boldsymbol{r} \in D_{\mathrm{i}} \\ \boldsymbol{r} \in D_{\mathrm{s}} \end{pmatrix}$$

and

$$\begin{pmatrix} -\boldsymbol{H}_{\mathrm{i}}(\boldsymbol{r}) \\ 0 \end{pmatrix} = \nabla \times \int_S \boldsymbol{h}_{\mathrm{i}}\left(\boldsymbol{r}'\right) g\left(k_{\mathrm{i}}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}')$$

$$- \frac{\mathrm{j}}{k_0 \mu_{\mathrm{i}}} \nabla \times \nabla \times \int_S \boldsymbol{e}_{\mathrm{i}}\left(\boldsymbol{r}'\right) g\left(k_{\mathrm{i}}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}'), \quad \begin{pmatrix} \boldsymbol{r} \in D_{\mathrm{i}} \\ \boldsymbol{r} \in D_{\mathrm{s}} \end{pmatrix},$$

where $\boldsymbol{e}_{\mathrm{i}} = \boldsymbol{n} \times \boldsymbol{E}_{\mathrm{i}}$ and $\boldsymbol{h}_{\mathrm{i}} = \boldsymbol{n} \times \boldsymbol{H}_{\mathrm{i}}$.

A rigorous proof of these representation theorems on the assumptions $\boldsymbol{E}_{\mathrm{s}}$, $\boldsymbol{H}_{\mathrm{s}} \in C^1(D_{\mathrm{s}}) \cap C(\overline{D}_{\mathrm{s}})$ and $\boldsymbol{E}_{\mathrm{i}}$, $\boldsymbol{H}_{\mathrm{i}} \in C^1(D_{\mathrm{i}}) \cap C(\overline{D}_{\mathrm{i}})$ can be found in Colton and Kress [39]. An alternative proof can be given if we accept the validity of Green's second vector theorem for generalized functions such as the three-dimensional Dirac delta function $\delta(\boldsymbol{r} - \boldsymbol{r}')$. To prove the representation theorem for vector fields satisfying the Maxwell equations in bounded domains we use the Green second vector theorem for a divergence free vector field $\boldsymbol{a}$ ($\nabla \cdot \boldsymbol{a} = 0$). Using the vector identities $\nabla \times \nabla \times \boldsymbol{b} = -\Delta \boldsymbol{b} + \nabla \nabla \cdot \boldsymbol{b}$ and $\boldsymbol{a} \cdot (\nabla \nabla \cdot \boldsymbol{b}) = \nabla \cdot (\boldsymbol{a} \nabla \cdot \boldsymbol{b})$ for $\nabla \cdot \boldsymbol{a} = 0$, and the Gauss divergence theorem we see that

$$\int_D [\boldsymbol{a} \cdot \Delta \boldsymbol{b} + \boldsymbol{b} \cdot (\nabla \times \nabla \times \boldsymbol{a})] \, \mathrm{d}V = \int_S \{\boldsymbol{n} \cdot \boldsymbol{a} \, (\nabla \cdot \boldsymbol{b}) + \boldsymbol{n} \cdot [\boldsymbol{a} \times (\nabla \times \boldsymbol{b})$$

$$+ (\nabla \times \boldsymbol{a}) \times \boldsymbol{b}]\} \, \mathrm{d}S. \qquad (1.64)$$

In the above equations, the simplified notations $\nabla \nabla \cdot \boldsymbol{a}$ and $\boldsymbol{a} \nabla \cdot \boldsymbol{b}$ should be understood as $\nabla(\nabla \cdot \boldsymbol{a})$ and $\boldsymbol{a}(\nabla \cdot \boldsymbol{b})$, respectively. Next, we choose an

arbitrary constant unit vector $\boldsymbol{u}$ and apply Green's second vector theorem (1.64) to $\boldsymbol{a}(\boldsymbol{r}') = \boldsymbol{E}_\mathrm{i}(\boldsymbol{r}')$ and $\boldsymbol{b}(\boldsymbol{r}') = g(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r})\boldsymbol{u}$, for $\boldsymbol{r} \in D_\mathrm{i}$. Recalling that

$$\Delta' g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) + k_\mathrm{i}^2 g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) = -\delta\left(\boldsymbol{r}' - \boldsymbol{r}\right), \tag{1.65}$$

and $\nabla' \times \nabla' \times \mathbf{E}_\mathrm{i} = k_\mathrm{i}^2 \mathbf{E}_\mathrm{i}$, we see that the left-hand side of (1.64) is

$$\int_{D_\mathrm{i}} \left\{\boldsymbol{E}_\mathrm{i}\left(\boldsymbol{r}'\right) \cdot \Delta' g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) \boldsymbol{u} + g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) \boldsymbol{u} \cdot \left[\nabla' \times \nabla' \times \boldsymbol{E}_\mathrm{i}\left(\boldsymbol{r}'\right)\right]\right\}$$
$$\times \mathrm{d}V\left(\boldsymbol{r}'\right)$$
$$= -\int_{D_\mathrm{i}} \boldsymbol{u} \cdot \boldsymbol{E}_\mathrm{i}\left(\boldsymbol{r}'\right) \delta\left(\boldsymbol{r}' - \boldsymbol{r}\right) \mathrm{d}V\left(\boldsymbol{r}'\right) = -\boldsymbol{u} \cdot \boldsymbol{E}_\mathrm{i}(\boldsymbol{r}).$$

Taking into account that for $\boldsymbol{r}' \neq \boldsymbol{r}$,

$$\nabla' \times \nabla' \times g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) \boldsymbol{u} = k_\mathrm{i}^2 g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) \boldsymbol{u} + \nabla'\nabla' \cdot g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) \boldsymbol{u},$$

we rewrite the right-hand side of (1.64) as

$$\int_S \left\{\boldsymbol{n} \cdot \boldsymbol{E}_\mathrm{i}\left[\nabla' \cdot g\left(k_\mathrm{i}, \cdot\boldsymbol{r}\right) \boldsymbol{u}\right] + \boldsymbol{n} \cdot \left[\boldsymbol{E}_\mathrm{i} \times \left(\nabla' \times g\left(k_\mathrm{i}, \cdot\boldsymbol{r}\right) \boldsymbol{u}\right)\right.\right.$$
$$\left.+ \left(\nabla' \times \boldsymbol{E}_\mathrm{i}\right) \times g\left(k_\mathrm{i}, \cdot\boldsymbol{r}\right) \boldsymbol{u}\right]\right\} \mathrm{d}S$$
$$= \int_S \left\{\boldsymbol{n} \cdot \boldsymbol{E}_\mathrm{i}\left[\nabla' \cdot g\left(k_\mathrm{i}, \cdot\boldsymbol{r}\right) \boldsymbol{u}\right] + \boldsymbol{n} \cdot \left[\boldsymbol{E}_\mathrm{i} \times \left(\nabla' \times g\left(k_\mathrm{i}, \cdot\boldsymbol{r}\right) \boldsymbol{u}\right)\right]\right.$$
$$+ \frac{1}{k_\mathrm{i}^2} \boldsymbol{n} \cdot \left[\left(\nabla' \times \boldsymbol{E}_\mathrm{i}\right) \times \left(\nabla' \times \nabla' \times g\left(k_\mathrm{i}, \cdot\boldsymbol{r}\right) \boldsymbol{u}\right)\right.$$
$$\left.\left.- \left(\nabla' \times \boldsymbol{E}_\mathrm{i}\right) \times \nabla'\nabla' \cdot g\left(k_\mathrm{i}, \cdot\boldsymbol{r}\right) \boldsymbol{u}\right]\right\} \mathrm{d}S.$$

From Stokes theorem we have

$$\int_S \boldsymbol{n} \cdot \left\{\nabla' \times \left[\boldsymbol{H}_\mathrm{i}\nabla' \cdot g\left(k_\mathrm{i}, \cdot\boldsymbol{r}\right) \boldsymbol{u}\right]\right\} \mathrm{d}S = 0,$$

whence, using the vector identity $\nabla \times (\alpha\boldsymbol{b}) = \nabla\alpha \times \boldsymbol{b} + \alpha\nabla \times \boldsymbol{b}$ and the Maxwell equations, we obtain

$$\int_S \boldsymbol{n} \cdot \boldsymbol{E}_\mathrm{i}\left[\nabla' \cdot g\left(k_\mathrm{i}, \cdot, \boldsymbol{r}\right) \boldsymbol{u}\right] \mathrm{d}S$$
$$= \frac{1}{k_\mathrm{i}^2} \int_S \boldsymbol{n} \cdot \left[\left(\nabla' \times \boldsymbol{E}_\mathrm{i}\right) \times \nabla'\nabla' \cdot g\left(k_\mathrm{i}, \cdot, \boldsymbol{r}\right) \boldsymbol{u}\right] \mathrm{d}S.$$

Finally, using the vector identity $\boldsymbol{a} \cdot (\boldsymbol{b} \times \boldsymbol{c}) = (\boldsymbol{a} \times \boldsymbol{b}) \cdot \boldsymbol{c}$, the symmetry relation $\nabla'g(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}) = -\nabla g(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r})$, the Maxwell equations and the identities

$$\left[\nabla' \times g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) \boldsymbol{u}\right] \cdot \left[\boldsymbol{n}\left(\boldsymbol{r}'\right) \times \boldsymbol{E}_\mathrm{i}\left(\boldsymbol{r}'\right)\right]$$

$$= \left\{\nabla \times g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) \left[\boldsymbol{n}\left(\boldsymbol{r}'\right) \times \boldsymbol{E}_\mathrm{i}\left(\boldsymbol{r}'\right)\right]\right\} \cdot \boldsymbol{u}$$

and

$$\left[\nabla' \times \nabla' \times g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) \boldsymbol{u}\right] \cdot \left[\boldsymbol{n}\left(\boldsymbol{r}'\right) \times \boldsymbol{H}_\mathrm{i}\left(\boldsymbol{r}'\right)\right]$$

$$= \left\{\nabla \times \nabla \times g\left(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r}\right) \left[\boldsymbol{n}\left(\boldsymbol{r}'\right) \times \boldsymbol{H}_\mathrm{i}\left(\boldsymbol{r}'\right)\right]\right\} \cdot \boldsymbol{u}\,,$$

we arrive at

$$-\boldsymbol{u} \cdot \boldsymbol{E}_\mathrm{i}(\boldsymbol{r}) = \boldsymbol{u} \cdot \left\{\nabla \times \int_S \boldsymbol{n}\left(\boldsymbol{r}'\right) \times \boldsymbol{E}_\mathrm{i}\left(\boldsymbol{r}'\right) g\left(k_\mathrm{i}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}')\right.$$

$$\left. + \frac{\mathrm{j}}{k_0 \varepsilon_\mathrm{i}} \nabla \times \nabla \times \int_S \boldsymbol{n}\left(\boldsymbol{r}'\right) \times \boldsymbol{H}_\mathrm{i}\left(\boldsymbol{r}'\right) g\left(k_\mathrm{i}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}')\right\}\,.$$

Since $\boldsymbol{u}$ is arbitrary, we have established the Stratton–Chu formula for $\boldsymbol{r} \in D_\mathrm{i}$. If $\boldsymbol{r} \in D_\mathrm{s}$, we have

$$\int_{D_\mathrm{i}} \boldsymbol{u} \cdot \boldsymbol{E}_\mathrm{i}\left(\boldsymbol{r}'\right) \delta\left(\boldsymbol{r}' - \boldsymbol{r}\right) \mathrm{d}V\left(\boldsymbol{r}'\right) = 0\,,$$

and the proof follows in a similar manner. For radiating solutions to the Maxwell equations, we see that the proof is established if we can show that

$$\int_{S_\mathrm{R}} \left\{\boldsymbol{n} \cdot \left[\boldsymbol{E}_\mathrm{s} \times \left(\nabla' \times g\left(k_\mathrm{s}, \cdot, \boldsymbol{r}\right) \boldsymbol{u}\right)\right.\right.$$

$$\left.\left. + \frac{1}{k_\mathrm{s}^2} \left(\nabla' \times \boldsymbol{E}_\mathrm{s}\right) \times \left(\nabla' \times \nabla' \times g\left(k_\mathrm{s}, \cdot, \boldsymbol{r}\right) \boldsymbol{u}\right)\right]\right\} \mathrm{d}S \to 0\,,$$

as $R \to \infty$, where S_R is a spherical surface situated in the far-field region. To prove this assertion we use the Silver–Müller radiation condition and the general assumption $\mathrm{Im}\{k_\mathrm{s}\} \geq 0$.

Alternative representations for Stratton–Chu formulas involve the free space dyadic Green function $\overline{\boldsymbol{G}}$ instead of the fundamental solution g [228]. A dyad $\overline{\boldsymbol{D}}$ serves as a linear mapping from one vector to another vector, and in general, $\overline{\boldsymbol{D}}$ can be introduced as the dyadic product of two vectors: $\overline{\boldsymbol{D}} = \boldsymbol{a} \otimes \boldsymbol{b}$. The dot product of a dyad with a vector is another vector: $\overline{\boldsymbol{D}} \cdot \boldsymbol{c} = (\boldsymbol{a} \otimes \boldsymbol{b}) \cdot \boldsymbol{c} = \boldsymbol{a}(\boldsymbol{b} \cdot \boldsymbol{c})$ and $\boldsymbol{c} \cdot \overline{\boldsymbol{D}} = \boldsymbol{c} \cdot (\boldsymbol{a} \otimes \boldsymbol{b}) = (\boldsymbol{c} \cdot \boldsymbol{a})\boldsymbol{b}$, while the cross product of a dyad with a vector is another dyad: $\overline{\boldsymbol{D}} \times \boldsymbol{c} = (\boldsymbol{a} \otimes \boldsymbol{b}) \times \boldsymbol{c} = \boldsymbol{a} \otimes (\boldsymbol{b} \times \boldsymbol{c})$ and $\boldsymbol{c} \times \overline{\boldsymbol{D}} = \boldsymbol{c} \times (\boldsymbol{a} \otimes \boldsymbol{b}) = (\boldsymbol{c} \times \boldsymbol{a}) \otimes \boldsymbol{b}$. The free space dyadic Green function is defined as

$$\overline{\boldsymbol{G}}\left(k, \boldsymbol{r}, \boldsymbol{r}'\right) = \left(\overline{\boldsymbol{I}} + \frac{1}{k^2} \nabla \otimes \nabla\right) g\left(k, \boldsymbol{r}, \boldsymbol{r}'\right)\,,$$

where $\overline{\boldsymbol{I}}$ is the identity dyad ($\overline{\boldsymbol{D}} \cdot \overline{\boldsymbol{I}} = \overline{\boldsymbol{I}} \cdot \overline{\boldsymbol{D}} = \overline{\boldsymbol{D}}$). Multiplying the differential equation (1.65) by $\overline{\boldsymbol{I}}$ and using the identities

$$\nabla \times \nabla \times (\overline{\boldsymbol{I}} g) = \nabla \otimes \nabla g - \boldsymbol{I} \triangle g \,,$$

$$\nabla \times \nabla \times (\nabla \otimes \nabla g) = 0 \,,$$

gives the differential equation for the free space dyadic Green function

$$\nabla \times \nabla \times \overline{\boldsymbol{G}} (k, \boldsymbol{r}, \boldsymbol{r}') = k^2 \overline{\boldsymbol{G}} (k, \boldsymbol{r}, \boldsymbol{r}') + \delta (\boldsymbol{r} - \boldsymbol{r}') \overline{\boldsymbol{I}} \,. \qquad (1.66)$$

The Stratton–Chu formula for vector fields satisfying the Maxwell equations in bounded domains read as

$$\begin{pmatrix} -\boldsymbol{E}_\mathrm{i}(\boldsymbol{r}) \\ 0 \end{pmatrix} = \int_S \boldsymbol{e}_\mathrm{i} (\boldsymbol{r}') \cdot \left[\nabla' \times \overline{\boldsymbol{G}} (k_\mathrm{i}, \boldsymbol{r}, \boldsymbol{r}') \right] \mathrm{d}S(\boldsymbol{r}')$$

$$+ \mathrm{j} k_0 \mu_\mathrm{i} \int_S \boldsymbol{h}_\mathrm{i} (\boldsymbol{r}') \cdot \overline{\boldsymbol{G}} (k_\mathrm{i}, \boldsymbol{r}, \boldsymbol{r}') \, \mathrm{d}S(\boldsymbol{r}') \,, \quad \begin{pmatrix} \boldsymbol{r} \in D_\mathrm{i} \\ \boldsymbol{r} \in D_\mathrm{s} \end{pmatrix}$$

and this integral representation follows from the second vector-dyadic Green theorem [220]:

$$\int_D \left[\boldsymbol{a} \cdot (\nabla \times \nabla \times \overline{\boldsymbol{D}}) - (\nabla \times \nabla \times \boldsymbol{a}) \cdot \overline{\boldsymbol{D}} \right] \mathrm{d}V$$

$$= - \int_S \boldsymbol{n} \cdot \left[\boldsymbol{a} \times (\nabla \times \overline{\boldsymbol{D}}) + (\nabla \times \boldsymbol{a}) \times \overline{\boldsymbol{D}} \right] \mathrm{d}S \,,$$

applied to $\boldsymbol{a}(\boldsymbol{r}') = \boldsymbol{E}_\mathrm{i}(\boldsymbol{r}')$ and $\overline{\boldsymbol{D}}(\boldsymbol{r}') = \overline{\boldsymbol{G}}(k_\mathrm{i}, \boldsymbol{r}', \boldsymbol{r})$, the differential equation for the free space dyadic Green function, and the identity $\boldsymbol{a} \cdot (\boldsymbol{b} \times \overline{\boldsymbol{D}}) = (\boldsymbol{a} \times \boldsymbol{b}) \cdot \overline{\boldsymbol{D}}$. For radiating solutions to the Maxwell equations, we use the asymptotic behavior of the free space dyadic Green function in the far-field region

$$\frac{\boldsymbol{r}}{r} \times \left[\nabla \times \overline{\boldsymbol{G}} (k_\mathrm{s}, \boldsymbol{r}, \boldsymbol{r}') \right] + \mathrm{j} k_\mathrm{s} \overline{\boldsymbol{G}} (k_\mathrm{s}, \boldsymbol{r}, \boldsymbol{r}') = \mathrm{o} \left(\frac{1}{r} \right) \,, \quad \text{as} \quad r \to \infty \,,$$

to show that the integral over the spherical surface vanishes at infinity.

Remark. The Stratton–Chu formulas are surface-integral representations for the electromagnetic fields and are valid for homogeneous particles. For inhomogeneous particles, a volume-integral representation for the electric field can be derived. For this purpose, we consider the nonmagnetic domains D_s and D_i ($\mu_\mathrm{s} = \mu_\mathrm{i} = 1$), rewrite the Maxwell equations as

$$\nabla \times \boldsymbol{E}_\mathrm{t} = \mathrm{j} k_0 \boldsymbol{H}_\mathrm{t} \,, \quad \nabla \times \boldsymbol{H}_\mathrm{t} = -\mathrm{j} k_0 \varepsilon_\mathrm{t} \boldsymbol{E}_\mathrm{t} \quad \text{in} \quad D_\mathrm{t} \,, \quad \mathrm{t} = \mathrm{s}, \mathrm{i} \,,$$

and assume that the domain D_i is isotropic, linear and inhomogeneous, i.e., $\varepsilon_\mathrm{i} = \varepsilon_\mathrm{i}(\boldsymbol{r})$. The Maxwell *curl* equation for the magnetic field $\boldsymbol{H}_\mathrm{i}$ can be written as

$$\nabla \times \boldsymbol{H}_{\mathrm{i}} = -\mathrm{j}k_0\varepsilon_{\mathrm{s}}\boldsymbol{E}_{\mathrm{i}} - \mathrm{j}k_0\varepsilon_{\mathrm{s}}\left(\frac{\varepsilon_{\mathrm{i}}}{\varepsilon_{\mathrm{s}}} - 1\right)\boldsymbol{E}_{\mathrm{i}}$$

$$= -\mathrm{j}k_0\varepsilon_{\mathrm{s}}\boldsymbol{E}_{\mathrm{i}} - \frac{\mathrm{j}}{k_0}k_{\mathrm{s}}^2\left(m_{\mathrm{r}}^2 - 1\right)\boldsymbol{E}_{\mathrm{i}}\,,$$

where $m_{\mathrm{r}} = m_{\mathrm{r}}(\boldsymbol{r})$ is the relative refractive index and $k_{\mathrm{s}} = k_0\sqrt{\varepsilon_{\mathrm{s}}}$. Defining the total electric and magnetic fields everywhere in space by

$$\boldsymbol{E} = \begin{cases} \boldsymbol{E}_{\mathrm{s}} + \boldsymbol{E}_{\mathrm{e}} & \text{in} \quad D_{\mathrm{s}}\,, \\ \boldsymbol{E}_{\mathrm{i}} & \text{in} \quad D_{\mathrm{i}}\,, \end{cases}$$

and

$$\boldsymbol{H} = \begin{cases} \boldsymbol{H}_{\mathrm{s}} + \boldsymbol{H}_{\mathrm{e}} & \text{in} \quad D_{\mathrm{s}}\,, \\ \boldsymbol{H}_{\mathrm{i}} & \text{in} \quad D_{i}\,, \end{cases}$$

respectively, and the forcing function $\boldsymbol{J}$ by

$$\boldsymbol{J} = k_{\mathrm{s}}^2\left(m_{\mathrm{rt}}^2 - 1\right)\boldsymbol{E}\,,$$

where

$$m_{\mathrm{rt}} = \begin{cases} 1 & \text{in} \quad D_{\mathrm{s}}\,, \\ m_{\mathrm{r}} & \text{in} \quad D_{\mathrm{i}}\,, \end{cases}$$

we see that the total electric and magnetic fields satisfy the Maxwell *curl* equations,

$$\nabla \times \boldsymbol{E} = \mathrm{j}k_0\boldsymbol{H}\,, \quad \nabla \times \boldsymbol{H} = -\mathrm{j}k_0\varepsilon_{\mathrm{s}}\boldsymbol{E} - \frac{\mathrm{j}}{k_0}\boldsymbol{J} \quad \text{in} \quad D_{\mathrm{s}} \cup D_{\mathrm{i}}\,.$$

By taking the *curl* of the first equation we obtain an inhomogeneous differential equation for total electric field

$$\nabla \times \nabla \times \boldsymbol{E} - k_{\mathrm{s}}^2\boldsymbol{E} = \boldsymbol{J} \quad \text{in} \quad D_{\mathrm{s}} \cup D_{\mathrm{i}}\,. \tag{1.67}$$

Making use of the differential equation for the free space dyadic Green function (1.66) and the identity

$$\nabla \times \left[\overline{\boldsymbol{G}}\left(k_{\mathrm{s}}, \boldsymbol{r}, \boldsymbol{r}'\right) \cdot \boldsymbol{J}\left(\boldsymbol{r}'\right)\right] = \left[\nabla \times \overline{\boldsymbol{G}}\left(k_{\mathrm{s}}, \boldsymbol{r}, \boldsymbol{r}'\right)\right] \cdot \boldsymbol{J}\left(\boldsymbol{r}'\right)\,,$$

we derive

$$\nabla \times \nabla \times \left[\overline{\boldsymbol{G}}\left(k_{\mathrm{s}}, \boldsymbol{r}, \boldsymbol{r}'\right) \cdot \boldsymbol{J}\left(\boldsymbol{r}'\right)\right]$$
$$-k_{\mathrm{s}}^2\overline{\boldsymbol{G}}\left(k_{\mathrm{s}}, \boldsymbol{r}, \boldsymbol{r}'\right) \cdot \boldsymbol{J}\left(\boldsymbol{r}'\right) = \overline{\boldsymbol{I}} \cdot \boldsymbol{J}\left(\boldsymbol{r}'\right)\delta\left(\boldsymbol{r} - \boldsymbol{r}'\right)\,.$$

Integrating this equation over all $\boldsymbol{r}'$ and using the identity $\delta(\boldsymbol{r} - \boldsymbol{r}') = \delta(\boldsymbol{r}' - \boldsymbol{r})$, gives [131]

$$\left(\nabla \times \nabla \times \overline{\boldsymbol{I}} - k_{\mathrm{s}}^2\overline{\boldsymbol{I}}\right) \cdot \int_{\boldsymbol{R}^3} \overline{\boldsymbol{G}}\left(k_{\mathrm{s}}, \boldsymbol{r}, \boldsymbol{r}'\right) \cdot \boldsymbol{J}\left(\boldsymbol{r}'\right)\mathrm{d}V\left(\boldsymbol{r}'\right) = \boldsymbol{J}(\boldsymbol{r})\,. \tag{1.68}$$

Because (1.67) and (1.68) have the same right-hand side we deduce that

$$\boldsymbol{E}(\boldsymbol{r}) = \int_{\boldsymbol{R}^3} \overline{\boldsymbol{G}}\left(k_{\rm s}, \boldsymbol{r}, \boldsymbol{r}'\right) \cdot \boldsymbol{J}\left(\boldsymbol{r}'\right) \mathrm{d}V\left(\boldsymbol{r}'\right), \quad \boldsymbol{r} \in D_{\rm s} \cup D_{\rm i}$$

and, since $\boldsymbol{J} = 0$ in $D_{\rm s}$, we obtain

$$\boldsymbol{E}(\boldsymbol{r}) = \int_{D_{\rm i}} \overline{\boldsymbol{G}}\left(k_{\rm s}, \boldsymbol{r}, \boldsymbol{r}'\right) \cdot \boldsymbol{J}\left(\boldsymbol{r}'\right) \mathrm{d}V\left(\boldsymbol{r}'\right), \quad \boldsymbol{r} \in D_{\rm s} \cup D_{\rm i}\,.$$

This vector field is the particular solution to the differential equation (1.67) that depends on the forcing function. For $\boldsymbol{r} \in D_{\rm s}$, the particular solution satisfies the Silver–Müller radiation condition and gives the scattered field. The solution to the homogeneous equation or the complementary solution satisfies the equation

$$\nabla \times \nabla \times \boldsymbol{E}_{\rm e} - k_{\rm s}^2 \boldsymbol{E}_{\rm e} = 0 \quad \text{in} \quad D_{\rm s} \cup D_{\rm i}\,.$$

and describes the field that would exist in the absence of the scattering object, i.e., the incident field. Thus, the complete solution to (1.67) can be written as

$$\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}_{\rm e}(\boldsymbol{r}) + \int_{D_{\rm i}} \overline{\boldsymbol{G}}\left(k_{\rm s}, \boldsymbol{r}, \boldsymbol{r}'\right) \cdot \boldsymbol{J}\left(\boldsymbol{r}'\right) \mathrm{d}V\left(\boldsymbol{r}'\right)$$

$$= \boldsymbol{E}_{\rm e}(\boldsymbol{r}) + k_{\rm s}^2 \int_{D_{\rm i}} \overline{\boldsymbol{G}}\left(k_{\rm s}, \boldsymbol{r}, \boldsymbol{r}'\right) \cdot \left[m_{\rm r}^2\left(\boldsymbol{r}'\right) - 1\right] \boldsymbol{E}\left(\boldsymbol{r}'\right) \mathrm{d}V\left(\boldsymbol{r}'\right),$$

$$\boldsymbol{r} \in D_{\rm s} \cup D_{\rm i}\,.$$

We note that for a nontrivial magnetic permeability of the particle, a volume-surface integral equation has been derived by Volakis [245], and a "pure" volume-integral equation has been given by Volakis et al. [246].

1.4.2 Far-Field Pattern and Amplitude Matrix

Application of Stratton–Chu representation theorem to the vector fields $\boldsymbol{E}_{\rm s}$ and $\boldsymbol{E}_{\rm e}$ in the domain $D_{\rm s}$ together with the boundary conditions $\boldsymbol{e}_{\rm s} + \boldsymbol{e}_{\rm e} = \boldsymbol{e}_{\rm i}$ and $\boldsymbol{h}_{\rm s} + \boldsymbol{h}_{\rm e} = \boldsymbol{h}_{\rm i}$, yield

$$\boldsymbol{E}_{\rm s}(\boldsymbol{r}) = \nabla \times \int_S \boldsymbol{e}_{\rm i}\left(\boldsymbol{r}'\right) g\left(k_{\rm s}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}')$$

$$+ \frac{\mathrm{j}}{k_0 \varepsilon_{\rm s}} \nabla \times \nabla \times \int_S \boldsymbol{h}_{\rm i}\left(\boldsymbol{r}'\right) g\left(k_{\rm s}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}'), \quad \boldsymbol{r} \in D_{\rm s}\,,$$

where $\boldsymbol{E}_{\rm s}, \boldsymbol{H}_{\rm s}$ and $\boldsymbol{E}_{\rm i}, \boldsymbol{H}_{\rm i}$ solve the transmission boundary-value problem. The above equation is known as the Huygens principle and it expresses the field in the domain $D_{\rm s}$ in terms of the surface fields on the surface S (see, for

example, [229]). Application of Stratton–Chu representation theorem in the domain D_i gives the (general) null-field equation or the extinction theorem:

$$\boldsymbol{E}_\mathrm{e}(\boldsymbol{r}) + \nabla \times \int_S \boldsymbol{e}_\mathrm{i}\left(\boldsymbol{r}'\right) g\left(k_\mathrm{s}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}')$$

$$+ \frac{\mathrm{j}}{k_0 \varepsilon_\mathrm{s}} \nabla \times \nabla \times \int_S \boldsymbol{h}_\mathrm{i}\left(\boldsymbol{r}'\right) g\left(k_\mathrm{s}, \boldsymbol{r}, \boldsymbol{r}'\right) \mathrm{d}S(\boldsymbol{r}') = 0\,, \quad \boldsymbol{r} \in D_\mathrm{i}\,,$$

which shows that the radiation of the surface fields into D_i extinguishes the incident wave [229]. In the null-field method, the extinction theorem is used to derive a set of integral equations for the surface fields, while the Huygens principle is employed to compute the scattered field.

Every radiating solution $\boldsymbol{E}_\mathrm{s}, \boldsymbol{H}_\mathrm{s}$ to the Maxwell equations has the asymptotic form

$$\boldsymbol{E}_\mathrm{s}(\boldsymbol{r}) = \frac{\mathrm{e}^{\mathrm{j}k_\mathrm{s}r}}{r} \left\{ \boldsymbol{E}_{\mathrm{s}\infty}(\boldsymbol{e}_r) + \mathrm{O}\left(\frac{1}{r}\right) \right\}\,, \quad r \to \infty\,,$$

$$\boldsymbol{H}_\mathrm{s}(\boldsymbol{r}) = \frac{\mathrm{e}^{\mathrm{j}k_\mathrm{s}r}}{r} \left\{ \boldsymbol{H}_{\mathrm{s}\infty}(\boldsymbol{e}_r) + \mathrm{O}\left(\frac{1}{r}\right) \right\}\,, \quad r \to \infty\,,$$

uniformly for all directions $\boldsymbol{e}_r = \boldsymbol{r}/r$. The vector fields $\boldsymbol{E}_{\mathrm{s}\infty}$ and $\boldsymbol{H}_{\mathrm{s}\infty}$ defined on the unit sphere are the electric and magnetic far-field patterns, respectively, and satisfy the relations:

$$\boldsymbol{H}_{\mathrm{s}\infty} = \sqrt{\frac{\varepsilon_\mathrm{s}}{\mu_\mathrm{s}}} \boldsymbol{e}_r \times \boldsymbol{E}_{\mathrm{s}\infty}\,,$$

$$\boldsymbol{e}_r \cdot \boldsymbol{E}_{\mathrm{s}\infty} = \boldsymbol{e}_r \cdot \boldsymbol{H}_{\mathrm{s}\infty} = 0\,.$$

Because $\boldsymbol{E}_{\mathrm{s}\infty}$ also depends on the incident direction $\boldsymbol{e}_k$, $\boldsymbol{E}_{\mathrm{s}\infty}$ is known as the scattering amplitude from the direction $\boldsymbol{e}_k$ into the direction $\boldsymbol{e}_r$ [229]. Using the Huygens principle and the asymptotic expressions

$$\nabla \times \left[\boldsymbol{a}\left(\boldsymbol{r}'\right) \frac{\mathrm{e}^{\mathrm{j}k_\mathrm{s}|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r} - \boldsymbol{r}'|} \right] = \mathrm{j}k_\mathrm{s} \frac{\mathrm{e}^{\mathrm{j}k_\mathrm{s}r}}{r} \left\{ \mathrm{e}^{-\mathrm{j}k_\mathrm{s}\boldsymbol{e}_r \cdot \boldsymbol{r}'} \boldsymbol{e}_r \times \boldsymbol{a}\left(\boldsymbol{r}'\right) + \mathrm{O}\left(\frac{a}{r}\right) \right\}\,,$$

$$\nabla \times \nabla \times \left[\boldsymbol{a}\left(\boldsymbol{r}'\right) \frac{\mathrm{e}^{\mathrm{j}k_\mathrm{s}|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r} - \boldsymbol{r}'|} \right] = k_\mathrm{s}^2 \frac{\mathrm{e}^{\mathrm{j}k_\mathrm{s}r}}{r}$$

$$\times \left\{ \mathrm{e}^{-\mathrm{j}k_\mathrm{s}\boldsymbol{e}_r \cdot \boldsymbol{r}'} \boldsymbol{e}_r \times \left[\boldsymbol{a}\left(\boldsymbol{r}'\right) \times \boldsymbol{e}_r \right] + \mathrm{O}\left(\frac{a}{r}\right) \right\}\,,$$

as $r \to \infty$, we obtain the following integral representations for the far-field patterns [40]

$$\boldsymbol{E}_{\mathrm{s}\infty}(\boldsymbol{e}_r) = \frac{\mathrm{j}k_\mathrm{s}}{4\pi} \int_S \left\{ \boldsymbol{e}_r \times \boldsymbol{e}_\mathrm{s}(\boldsymbol{r}') \right.$$

$$\left. + \sqrt{\frac{\mu_\mathrm{s}}{\varepsilon_\mathrm{s}}} \boldsymbol{e}_r \times \left[\boldsymbol{h}_\mathrm{s}\left(\boldsymbol{r}'\right) \times \boldsymbol{e}_r \right] \right\} \mathrm{e}^{-\mathrm{j}k_\mathrm{s}\boldsymbol{e}_r \cdot \boldsymbol{r}'} \mathrm{d}S\left(\boldsymbol{r}'\right)\,, \quad (1.69)$$

$$\boldsymbol{H}_{s\infty}(\boldsymbol{e}_r) = \frac{jk_s}{4\pi} \int_S \left\{ \boldsymbol{e}_r \times \boldsymbol{h}_s(\boldsymbol{r}') \right.$$

$$\left. - \sqrt{\frac{\varepsilon_s}{\mu_s}} \boldsymbol{e}_r \times [\boldsymbol{e}_s(\boldsymbol{r}') \times \boldsymbol{e}_r] \right\} e^{-jk_s \boldsymbol{e}_r \cdot \boldsymbol{r}'} dS(\boldsymbol{r}') . \quad (1.70)$$

The quantity $\sigma_d = |\boldsymbol{E}_{s\infty}|^2$ is called the differential scattering cross-section and describes the angular distribution of the scattered light. The differential scattering cross-section depends on the polarization state of the incident field and on the incident and scattering directions. The quantities $\sigma_{dp} = |E_{s\infty,\theta}|^2$ and $\sigma_{ds} = |E_{s\infty,\varphi}|^2$ are referred to as the differential scattering cross-sections for parallel and perpendicular polarizations, respectively. The differential scattering cross-section has the dimension of area, and a dimensionless quantity is the normalized differential scattering cross-section $\sigma_{dn} = \sigma_d/\pi a_c^2$, where a_c is a characteristic dimension of the particle.

To introduce the concepts of tensor scattering amplitude and amplitude matrix it is necessary to choose an orthonormal unit system for polarization description. In Sect. 1.2 we chose a global coordinate system and used the vertical and horizontal polarization unit vectors $\boldsymbol{e}_\alpha$ and $\boldsymbol{e}_\beta$, to describe the polarization state of the incident wave (Fig. 1.9a). For the scattered wave we can proceed analogously by considering the vertical and horizontal polarization unit vectors $\boldsymbol{e}_\varphi$ and $\boldsymbol{e}_\theta$. Essentially, $(\boldsymbol{e}_k, \boldsymbol{e}_\beta, \boldsymbol{e}_\alpha)$ are the spherical unit vectors of $\boldsymbol{k}_e$, while $(\boldsymbol{e}_r, \boldsymbol{e}_\theta, \boldsymbol{e}_\varphi)$ are the spherical unit vectors of $\boldsymbol{k}_s$ in
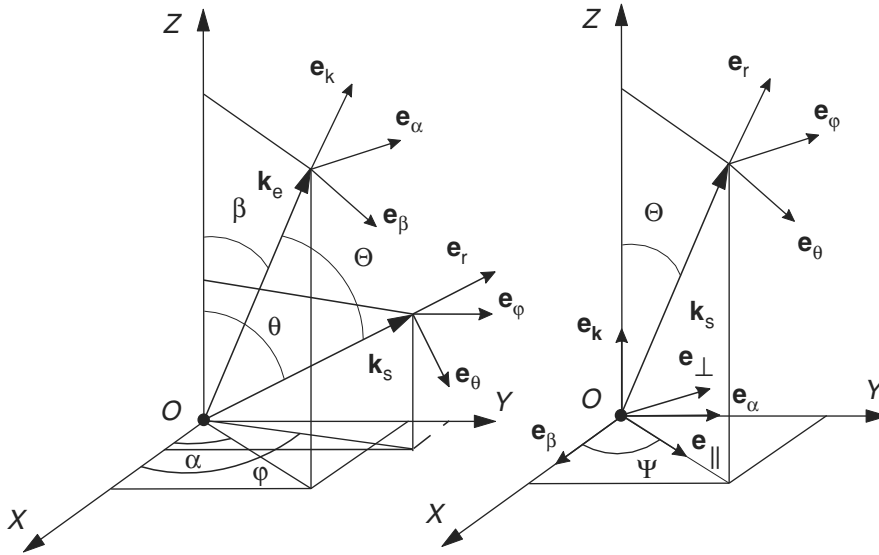

Fig. 1.9. Reference frames: (**a**) global coordinate system and (**b**) beam coordinate system

the global coordinate system. A second choice is the system based on the scattering plane. In this case we consider the beam coordinate system with the Z-axis directed along the incidence direction, and define the Stokes vectors with respect to the scattering plane, that is, the plane through the direction of incidence and scattering (Fig. 1.9b). For the scattered wave, the polarization description is in terms of the vertical and horizontal polarization unit vectors $\boldsymbol{e}_\varphi$ and $\boldsymbol{e}_\theta$, while for the incident wave, the polarization description is in terms of the unit vectors $\boldsymbol{e}_\perp = \boldsymbol{e}_\varphi$ and $\boldsymbol{e}_\parallel = \boldsymbol{e}_\perp \times \boldsymbol{e}_k$. The advantage of this system is that the scattering amplitude can take simple forms for particles with symmetry, and the disadvantage is that $\boldsymbol{e}_\perp$ and $\boldsymbol{e}_\parallel$ depend on the scattering direction. Furthermore, any change in the direction of light incidence also changes the orientation of the particle with respect to the reference frame. In our analysis we will use a fixed global coordinate system to specify both the direction of propagation and the states of polarization of the incident and scattered waves and the particle orientation (see also, [169, 228]).

The tensor scattering amplitude or the scattering dyad is given by [169]

$$\boldsymbol{E}_{\mathrm{s}\infty}(\boldsymbol{e}_r) = \overline{\boldsymbol{A}}\left(\boldsymbol{e}_r, \boldsymbol{e}_k\right) \cdot \boldsymbol{E}_{\mathrm{e}0}\,, \tag{1.71}$$

and since $\boldsymbol{e}_r \cdot \boldsymbol{E}_{\mathrm{s}\infty} = 0$, it follows that:

$$\boldsymbol{e}_r \cdot \overline{\boldsymbol{A}}\left(\boldsymbol{e}_r, \boldsymbol{e}_k\right) = 0\,. \tag{1.72}$$

Because the incident wave is a transverse wave, $\boldsymbol{e}_k \cdot \boldsymbol{E}_{\mathrm{e}0} = 0$, the dot product $\overline{\boldsymbol{A}}(\boldsymbol{e}_r, \boldsymbol{e}_k) \cdot \boldsymbol{e}_k$ is not defined by (1.71), and to complete the definition, we take

$$\overline{\boldsymbol{A}}\left(\boldsymbol{e}_r, \boldsymbol{e}_k\right) \cdot \boldsymbol{e}_k = 0\,. \tag{1.73}$$

Although the scattering dyad describes the scattering of a vector plane wave, it can be used to describe the scattering of any incident field, because any regular solution to the Maxwell equations can be expressed as an integral over vector plane waves. As a consequence of (1.72) and (1.73), only four components of the scattering dyad are independent and it is convenient to introduce the 2×2 amplitude matrix $\boldsymbol{S}$ to describe the transformation of the transverse components of the incident wave into the transverse components of the scattered wave in the far-field region. The amplitude matrix is given by [17, 169, 228]

$$\begin{bmatrix} E_{\mathrm{s}\infty,\theta}(\boldsymbol{e}_r) \\ E_{\mathrm{s}\infty,\varphi}(\boldsymbol{e}_r) \end{bmatrix} = \boldsymbol{S}\left(\boldsymbol{e}_r, \boldsymbol{e}_k\right) \begin{bmatrix} E_{\mathrm{e}0,\beta} \\ E_{\mathrm{e}0,\alpha} \end{bmatrix}\,, \tag{1.74}$$

where $E_{\mathrm{e}0,\beta}$ and $E_{\mathrm{e}0,\alpha}$ do not depend on the incident direction. Essentially, the amplitude matrix is a generalization of the scattering amplitudes including polarization effects. The amplitude matrix provides a complete description of the far-field patterns and it depends on the incident and scattering directions as well on the size, optical properties and orientation of the particle. The elements of the amplitude matrix

$$\mathbf{S} = \begin{bmatrix} S_{\theta\beta} & S_{\theta\alpha} \\ S_{\varphi\beta} & S_{\varphi\alpha} \end{bmatrix}$$

are expressed in terms of the scattering dyad as follows:

$$\begin{aligned} S_{\theta\beta} &= \boldsymbol{e}_\theta \cdot \overline{\boldsymbol{A}} \cdot \boldsymbol{e}_\beta \,, \\ S_{\theta\alpha} &= \boldsymbol{e}_\theta \cdot \overline{\boldsymbol{A}} \cdot \boldsymbol{e}_\alpha \,, \\ S_{\varphi\beta} &= \boldsymbol{e}_\varphi \cdot \overline{\boldsymbol{A}} \cdot \boldsymbol{e}_\beta \,, \\ S_{\varphi\alpha} &= \boldsymbol{e}_\varphi \cdot \overline{\boldsymbol{A}} \cdot \boldsymbol{e}_\alpha \,. \end{aligned} \tag{1.75}$$

1.4.3 Phase and Extinction Matrices

As in optics the electric and magnetics fields cannot directly be measured because of their high frequency oscillations, other measurable quantities describing the change of the polarization state upon scattering have to be defined. The transformation of the polarization characteristic of the incident light into that of the scattered light is given by the phase matrix. The coherency phase matrix $\boldsymbol{Z}_{\mathrm{c}}$ relates the coherency vectors of the incident and scattered fields

$$\boldsymbol{J}_{\mathrm{s}}\left(r\boldsymbol{e}_r\right) = \frac{1}{r^2} \boldsymbol{Z}_{\mathrm{c}}\left(\boldsymbol{e}_r, \boldsymbol{e}_k\right) \boldsymbol{J}_{\mathrm{e}} \,,$$

where the coherency vector of the incident field $\boldsymbol{J}_{\mathrm{e}}$ is given by (1.19) and the coherency vector of the scattered field $\boldsymbol{J}_{\mathrm{s}}$ is defined as

$$\boldsymbol{J}_{\mathrm{s}}\left(r\boldsymbol{e}_r\right) = \frac{1}{2r^2} \sqrt{\frac{\varepsilon_{\mathrm{s}}}{\mu_{\mathrm{s}}}} \begin{bmatrix} E_{\mathrm{s}\infty,\theta}\left(\boldsymbol{e}_r\right) E_{\mathrm{s}\infty,\theta}^*\left(\boldsymbol{e}_r\right) \\ E_{\mathrm{s}\infty,\theta}\left(\boldsymbol{e}_r\right) E_{\mathrm{s}\infty,\varphi}^*\left(\boldsymbol{e}_r\right) \\ E_{\mathrm{s}\infty,\varphi}\left(\boldsymbol{e}_r\right) E_{\mathrm{s}\infty,\theta}^*\left(\boldsymbol{e}_r\right) \\ E_{\mathrm{s}\infty,\varphi}\left(\boldsymbol{e}_r\right) E_{\mathrm{s}\infty,\varphi}^*\left(\boldsymbol{e}_r\right) \end{bmatrix} \,.$$

Explicitly, the coherency phase matrix is given by

$$\boldsymbol{Z}_{\mathrm{c}} = \begin{bmatrix} |S_{\theta\beta}|^2 & S_{\theta\beta}S_{\theta\alpha}^* & S_{\theta\alpha}S_{\theta\beta}^* & |S_{\theta\alpha}|^2 \\ S_{\theta\beta}S_{\varphi\beta}^* & S_{\theta\beta}S_{\varphi\alpha}^* & S_{\theta\alpha}S_{\varphi\beta}^* & S_{\theta\alpha}S_{\varphi\alpha}^* \\ S_{\varphi\beta}S_{\theta\beta}^* & S_{\varphi\beta}S_{\theta\alpha}^* & S_{\varphi\alpha}S_{\theta\beta}^* & S_{\varphi\alpha}S_{\theta\alpha}^* \\ |S_{\varphi\beta}|^2 & S_{\varphi\beta}S_{\varphi\alpha}^* & S_{\varphi\alpha}S_{\varphi\beta}^* & |S_{\varphi\alpha}|^2 \end{bmatrix} \,.$$

The phase matrix $\boldsymbol{Z}$ describes the transformation of the Stokes vector of the incident field into that of the scattered field

$$\boldsymbol{I}_{\mathrm{s}}\left(r\boldsymbol{e}_r\right) = \frac{1}{r^2} \boldsymbol{Z}\left(\boldsymbol{e}_r, \boldsymbol{e}_k\right) \boldsymbol{I}_{\mathrm{e}} \tag{1.76}$$

and we have

$$\boldsymbol{Z}\left(\boldsymbol{e}_r, \boldsymbol{e}_k\right) = \boldsymbol{D}\boldsymbol{Z}_{\mathrm{c}}\left(\boldsymbol{e}_r, \boldsymbol{e}_k\right) \boldsymbol{D}^{-1} \,,$$

where the transformation matrix $\boldsymbol{D}$ is given by (1.21), the Stokes vector of the incident field $\boldsymbol{I}_e$ is given by (1.20) and the Stokes vector of the scattered field $\boldsymbol{I}_s$ is defined as

$$\boldsymbol{I}_s\left(r\boldsymbol{e}_r\right) = \frac{1}{r^2}\begin{bmatrix} I_s\left(\boldsymbol{e}_r\right) \\ Q_s\left(\boldsymbol{e}_r\right) \\ U_s\left(\boldsymbol{e}_r\right) \\ V_s\left(\boldsymbol{e}_r\right) \end{bmatrix} = \boldsymbol{D}\boldsymbol{J}_s\left(r\boldsymbol{e}_r\right)$$

$$= \frac{1}{2r^2}\sqrt{\frac{\varepsilon_s}{\mu_s}}\begin{bmatrix} \left|E_{s\infty,\theta}\left(\boldsymbol{e}_r\right)\right|^2 + \left|E_{s\infty,\varphi}\left(\boldsymbol{e}_r\right)\right|^2 \\ \left|E_{s\infty,\theta}\left(\boldsymbol{e}_r\right)\right|^2 - \left|E_{s\infty,\varphi}\left(\boldsymbol{e}_r\right)\right|^2 \\ -E_{s\infty,\varphi}\left(\boldsymbol{e}_r\right)E_{s\infty,\theta}^*\left(\boldsymbol{e}_r\right) - E_{s\infty,\theta}\left(\boldsymbol{e}_r\right)E_{s\infty,\varphi}^*\left(\boldsymbol{e}_r\right) \\ j\left[E_{s\infty,\varphi}\left(\boldsymbol{e}_r\right)E_{s\infty,\theta}^*\left(\boldsymbol{e}_r\right) - E_{s\infty,\theta}\left(\boldsymbol{e}_r\right)E_{s\infty,\varphi}^*\left(\boldsymbol{e}_r\right)\right] \end{bmatrix}.$$

Explicit formulas for the elements of the phase matrix are:

$$Z_{11} = \frac{1}{2}\left(\left|S_{\theta\beta}\right|^2 + \left|S_{\theta\alpha}\right|^2 + \left|S_{\varphi\beta}\right|^2 + \left|S_{\varphi\alpha}\right|^2\right),$$

$$Z_{12} = \frac{1}{2}\left(\left|S_{\theta\beta}\right|^2 - \left|S_{\theta\alpha}\right|^2 + \left|S_{\varphi\beta}\right|^2 - \left|S_{\varphi\alpha}\right|^2\right),$$

$$Z_{13} = -\mathrm{Re}\left\{S_{\theta\beta}S_{\theta\alpha}^* + S_{\varphi\alpha}S_{\varphi\beta}^*\right\},$$

$$Z_{14} = -\mathrm{Im}\left\{S_{\theta\beta}S_{\theta\alpha}^* - S_{\varphi\alpha}S_{\varphi\beta}^*\right\},$$

$$Z_{21} = \frac{1}{2}\left(\left|S_{\theta\beta}\right|^2 + \left|S_{\theta\alpha}\right|^2 - \left|S_{\varphi\beta}\right|^2 - \left|S_{\varphi\alpha}\right|^2\right),$$

$$Z_{22} = \frac{1}{2}\left(\left|S_{\theta\beta}\right|^2 - \left|S_{\theta\alpha}\right|^2 - \left|S_{\varphi\beta}\right|^2 + \left|S_{\varphi\alpha}\right|^2\right),$$

$$Z_{23} = -\mathrm{Re}\left\{S_{\theta\beta}S_{\theta\alpha}^* - S_{\varphi\alpha}S_{\varphi\beta}^*\right\},$$

$$Z_{24} = -\mathrm{Im}\left\{S_{\theta\beta}S_{\theta\alpha}^* + S_{\varphi\alpha}S_{\varphi\beta}^*\right\},$$

$$Z_{31} = -\mathrm{Re}\left\{S_{\theta\beta}S_{\varphi\beta}^* + S_{\varphi\alpha}S_{\theta\alpha}^*\right\},$$

$$Z_{32} = -\mathrm{Re}\left\{S_{\theta\beta}S_{\varphi\beta}^* - S_{\varphi\alpha}S_{\theta\alpha}^*\right\},$$

$$Z_{33} = \mathrm{Re}\left\{S_{\theta\beta}S_{\varphi\alpha}^* + S_{\theta\alpha}S_{\varphi\beta}^*\right\},$$

$$Z_{34} = \mathrm{Im}\left\{S_{\theta\beta}S_{\varphi\alpha}^* + S_{\varphi\beta}S_{\theta\alpha}^*\right\},$$

$$Z_{41} = -\mathrm{Im}\left\{S_{\varphi\beta}S_{\theta\beta}^* + S_{\varphi\alpha}S_{\theta\alpha}^*\right\},$$

$$Z_{42} = -\mathrm{Im}\left\{S_{\varphi\beta}S_{\theta\beta}^* - S_{\varphi\alpha}S_{\theta\alpha}^*\right\},$$

$$Z_{43} = \mathrm{Im}\left\{S_{\varphi\alpha}S_{\theta\beta}^* - S_{\theta\alpha}S_{\varphi\beta}^*\right\},$$

$$Z_{44} = \mathrm{Re}\left\{S_{\varphi\alpha}S_{\theta\beta}^* - S_{\theta\alpha}S_{\varphi\beta}^*\right\}. \tag{1.77}$$

The above phase matrix is also known as the pure phase matrix, because its elements follow directly from the corresponding amplitude matrix that transforms the two electric field components [100]. The phase matrix of a particle in a fixed orientation may contain sixteen nonvanishing elements. Because only phase differences occur in the expressions of Z_{ij}, $i, j = 1, 2, 3, 4$, the phase matrix elements are essentially determined by no more than seven real numbers: the four moduli $|S_{pq}|$ and the three differences in phase between the S_{pq}, where $p = \theta$, φ and $q = \beta$, α. Consequently, only seven phase matrix elements are independent and there are nine linear relations among the sixteen elements. These linear dependent relations show that a pure phase matrix has a certain internal structure. Several linear and quadratic inequalities for the phase matrix elements have been reported by exploiting the internal structure of the pure phase matrix, and the most important inequalities are $Z_{11} \geq 0$ and $|Z_{ij}| \leq Z_{11}$ for $i, j = 1, 2, 3, 4$ [102–104]. In principle, all scalar and matrix properties of pure phase matrices can be used for theoretical purposes or to test whether an experimentally or numerically determined matrix can be a pure phase matrix.

Equation (1.76) shows that electromagnetic scattering produces light with polarization characteristics different from those of the incident light. If the incident beam is unpolarized, $\boldsymbol{I}_e = [I_e, 0, 0, 0]^T$, the Stokes vector of the scattered field has at least one nonvanishing component other than intensity, $\boldsymbol{I}_s = [Z_{11}I_e, Z_{21}I_e, Z_{31}I_e, Z_{41}I_e]^T$. When the incident beam is linearly polarized, $\boldsymbol{I}_e = [I_e, Q_e, U_e, 0]^T$, the scattered light may become elliptically polarized since V_s may be nonzero. However, if the incident beam is fully polarized ($P_e = 1$), then the scattered light is also fully polarized ($P_s = 1$) [104].

As mentioned before, a scattering particle can change the state of polarization of the incident beam after it passes the particle. This phenomenon is called dichroism and is a consequence of the different values of attenuation rates for different polarization components of the incident light. A complete description of the extinction process requires the introduction of the so-called extinction matrix. In order to derive the expression of the extinction matrix we consider the case of the forward-scattering direction, $\boldsymbol{e}_r = \boldsymbol{e}_k$, and define the coherency vector of the total field $\boldsymbol{E} = \boldsymbol{E}_s + \boldsymbol{E}_e$ by

$$\boldsymbol{J}(r\boldsymbol{e}_k) = \frac{1}{2}\sqrt{\frac{\varepsilon_s}{\mu_s}} \begin{bmatrix} E_\beta(r\boldsymbol{e}_k) E_\beta^*(r\boldsymbol{e}_k) \\ E_\beta(r\boldsymbol{e}_k) E_\alpha^*(r\boldsymbol{e}_k) \\ E_\alpha(r\boldsymbol{e}_k) E_\beta^*(r\boldsymbol{e}_k) \\ E_\alpha(r\boldsymbol{e}_k) E_\alpha^*(r\boldsymbol{e}_k) \end{bmatrix}.$$

Using the decomposition

$$E_p(\boldsymbol{r})E_q^*(\boldsymbol{r}) = E_{e0,p}E_{e0,q}^* + E_{e0,p}e^{j\boldsymbol{k}_e \cdot \boldsymbol{r}} E_{s,q}^*(\boldsymbol{r})$$
$$+ E_{s,p}(\boldsymbol{r})E_{e0,q}^* e^{-j\boldsymbol{k}_e \cdot \boldsymbol{r}} + E_{s,p}(\boldsymbol{r})E_{s,q}^*(\boldsymbol{r}),$$

where p and q stand for β and α, we approximate the integral of the generic term $E_p E_q^*$ in the far-field region and over a small solid angle $\Delta\Omega$ around the
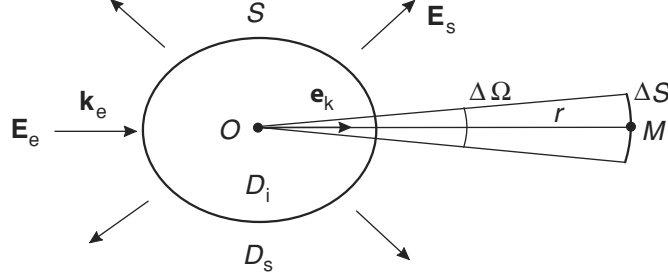
Fig. 1.10. Elementary surface ΔS in the far-field region

direction $\boldsymbol{e}_k$ by

$$\int_{\Delta\Omega} E_p(\boldsymbol{r})E_q^*(\boldsymbol{r})r^2\,\mathrm{d}\Omega\,(\boldsymbol{e}_r) \approx E_p\,(r\boldsymbol{e}_k)\,E_q^*\,(r\boldsymbol{e}_k)\,\Delta S\,,$$

where $\Delta S = r^2\Delta\Omega$ (Fig. 1.10). On the other hand, using the far-field representation for the scattered field

$$E_{\mathrm{s},p}(\boldsymbol{r}) = \frac{\mathrm{e}^{\mathrm{j}k_\mathrm{s}r}}{r}\left\{E_{\mathrm{s}\infty,p}(\boldsymbol{e}_r) + \mathrm{O}\left(\frac{1}{r}\right)\right\}$$

and the asymptotic expression of the plane wave $\exp(\mathrm{j}\boldsymbol{k}_\mathrm{e}\cdot\boldsymbol{r})$ (cf. (B.7)) we approximate the integrals of each term composing $E_p E_q^*$ as follows:

$$\int_{\Delta\Omega} E_{\mathrm{e}0,p}E_{\mathrm{e}0,q}^*r^2\,\mathrm{d}\Omega\,(\boldsymbol{e}_r) \approx E_{\mathrm{e}0,p}E_{\mathrm{e}0,q}^*\Delta S\,,$$

$$\int_{\Delta\Omega} E_{\mathrm{e}0,p}\mathrm{e}^{\mathrm{j}\boldsymbol{k}_\mathrm{e}\cdot\boldsymbol{r}} E_{\mathrm{s},q}^*(\boldsymbol{r})r^2\,\mathrm{d}\Omega\,(\boldsymbol{e}_r) \approx -\frac{2\pi\mathrm{j}}{k_\mathrm{s}}E_{\mathrm{e}0,p}E_{\mathrm{s}\infty,q}^*\,(\boldsymbol{e}_k)\,,$$

$$\int_{\Delta\Omega} E_{\mathrm{s},p}(\boldsymbol{r})E_{\mathrm{e}0,q}^*\mathrm{e}^{-\mathrm{j}\boldsymbol{k}_\mathrm{e}\cdot\boldsymbol{r}}r^2\,\mathrm{d}\Omega\,(\boldsymbol{e}_r) \approx \frac{2\pi\mathrm{j}}{k_\mathrm{s}}E_{\mathrm{s}\infty,p}\,(\boldsymbol{e}_k)\,E_{\mathrm{e}0,q}^*\,,$$

$$\int_{\Delta\Omega} E_{\mathrm{s},p}(\boldsymbol{r})E_{\mathrm{s},q}^*(\boldsymbol{r})r^2\,\mathrm{d}\Omega\,(\boldsymbol{e}_r) \approx E_{\mathrm{s}\infty,p}\,(\boldsymbol{e}_k)\,E_{\mathrm{s}\infty,q}^*\,(\boldsymbol{e}_k)\,\frac{\Delta S}{r^2}\,.$$

Neglecting the term proportional to r^{-2}, we see that

$$E_p\,(r\boldsymbol{e}_k)\,E_q^*\,(r\boldsymbol{e}_k)\,\Delta S \approx E_{\mathrm{e}0,p}E_{\mathrm{e}0,q}^*\Delta S$$

$$-\frac{2\pi\mathrm{j}}{k_\mathrm{s}}\left[E_{\mathrm{e}0,p}E_{\mathrm{s}\infty,q}^*\,(\boldsymbol{e}_k) - E_{\mathrm{s}\infty,p}\,(\boldsymbol{e}_k)\,E_{\mathrm{e}0,q}^*\right]$$

and the above relation gives

$$\boldsymbol{J}\,(r\boldsymbol{e}_k)\,\Delta S \approx \boldsymbol{J}_\mathrm{e}\Delta S - \boldsymbol{K}_\mathrm{c}\,(\boldsymbol{e}_k)\,\boldsymbol{J}_\mathrm{e}\,,$$

where the coherency extinction matrix $\boldsymbol{K}_\mathrm{c}$ is defined as

$$\boldsymbol{K}_\mathrm{c} = \frac{2\pi\mathrm{j}}{k_\mathrm{s}} \begin{bmatrix} S_{\theta\beta}^* - S_{\theta\beta} & S_{\theta\alpha}^* & -S_{\theta\alpha} & 0 \\ S_{\varphi\beta}^* & S_{\varphi\alpha}^* - S_{\theta\beta} & 0 & -S_{\theta\alpha} \\ -S_{\varphi\beta} & 0 & S_{\theta\beta}^* - S_{\varphi\alpha} & S_{\theta\alpha}^* \\ 0 & -S_{\varphi\beta} & S_{\varphi\beta}^* & S_{\varphi\alpha}^* - S_{\varphi\alpha} \end{bmatrix}.$$

For the Stokes parameters we have

$$\boldsymbol{I}\left(r\boldsymbol{e}_k\right)\Delta S \approx \boldsymbol{I}_\mathrm{e}\Delta S - \boldsymbol{K}\left(\boldsymbol{e}_k\right)\boldsymbol{I}_e \tag{1.78}$$

with the extinction matrix $\boldsymbol{K}$ being defined as

$$\boldsymbol{K}\left(\boldsymbol{e}_k\right) = \boldsymbol{D}\boldsymbol{K}_\mathrm{c}\left(\boldsymbol{e}_k\right)\boldsymbol{D}^{-1}.$$

The explicit formulas for the elements of the extinction matrix are

$$K_{ii} = \frac{2\pi}{k_\mathrm{s}}\mathrm{Im}\left\{S_{\theta\beta} + S_{\varphi\alpha}\right\}, \quad i = 1, 2, 3, 4,$$

$$K_{12} = K_{21} = \frac{2\pi}{k_\mathrm{s}}\mathrm{Im}\left\{S_{\theta\beta} - S_{\varphi\alpha}\right\},$$

$$K_{13} = K_{31} = -\frac{2\pi}{k_\mathrm{s}}\mathrm{Im}\left\{S_{\theta\alpha} + S_{\varphi\beta}\right\},$$

$$K_{14} = K_{41} = \frac{2\pi}{k_\mathrm{s}}\mathrm{Re}\left\{S_{\varphi\beta} - S_{\theta\alpha}\right\},$$

$$K_{23} = -K_{32} = \frac{2\pi}{k_\mathrm{s}}\mathrm{Im}\left\{S_{\varphi\beta} - S_{\theta\alpha}\right\},$$

$$K_{24} = -K_{42} = -\frac{2\pi}{k_\mathrm{s}}\mathrm{Re}\left\{S_{\theta\alpha} + S_{\varphi\beta}\right\},$$

$$K_{34} = -K_{43} = \frac{2\pi}{k_\mathrm{s}}\mathrm{Re}\left\{S_{\varphi\alpha} - S_{\theta\beta}\right\}. \tag{1.79}$$

The elements of the extinction matrix have the dimension of area and only seven components are independent. Equation (1.78) is an interpretation of the so-called optical theorem which will be discussed in the next section. This relation shows that the particle changes not only the total electromagnetic power received by a detector in the forward scattering direction, but also its state of polarization.

1.4.4 Extinction, Scattering and Absorption Cross-Sections

Scattering and absorption of light changes the characteristics of the incident beam after it passes the particle. Let us assume that the particle is placed in a beam of electromagnetic radiation and a detector located in the far-field region measures the radiation in the forward scattering direction ($\boldsymbol{e}_r = \boldsymbol{e}_k$). Let W

be the electromagnetic power received by the detector downstream from the particle, and W_0 the electromagnetic power received by the detector if the particle is removed. Evidently, $W_0 > W$ and we say that the presence of the particle has resulted in extinction of the incident beam. For a nonabsorbing medium, the electromagnetic power removed from the incident beam $W_0 - W$ is accounted for by absorption in the particle and scattering by the particle.

We now consider extinction from a computational point of view. In order to simplify the notations we will use the conventional expressions of the Poynting vectors and the electromagnetic powers in terms of the transformed fields introduced in Sect. 1.1 (we will omit the multiplicative factor $1/\sqrt{\varepsilon_0 \mu_0}$). The time-averaged Poynting vector $\langle \boldsymbol{S} \rangle$ can be written as [17]

$$\langle \boldsymbol{S} \rangle = \frac{1}{2} \mathrm{Re} \left\{ \boldsymbol{E} \times \boldsymbol{H}^* \right\} = \langle \boldsymbol{S}_{\mathrm{inc}} \rangle + \langle \boldsymbol{S}_{\mathrm{scat}} \rangle + \langle \boldsymbol{S}_{\mathrm{ext}} \rangle \, ,$$

where $\boldsymbol{E} = \boldsymbol{E}_{\mathrm{s}} + \boldsymbol{E}_{\mathrm{e}}$ and $\boldsymbol{H} = \boldsymbol{H}_{\mathrm{s}} + \boldsymbol{H}_{\mathrm{e}}$ are the total electric and magnetic fields,

$$\langle \boldsymbol{S}_{\mathrm{inc}} \rangle = \frac{1}{2} \mathrm{Re} \left\{ \boldsymbol{E}_{\mathrm{e}} \times \boldsymbol{H}_{\mathrm{e}}^* \right\}$$

is the Poynting vector associated with the external excitation,

$$\langle \boldsymbol{S}_{\mathrm{scat}} \rangle = \frac{1}{2} \mathrm{Re} \left\{ \boldsymbol{E}_{\mathrm{s}} \times \boldsymbol{H}_{\mathrm{s}}^* \right\}$$

is the Poynting vector corresponding to the scattered field and

$$\langle \boldsymbol{S}_{\mathrm{ext}} \rangle = \frac{1}{2} \mathrm{Re} \left\{ \boldsymbol{E}_{\mathrm{e}} \times \boldsymbol{H}_{\mathrm{s}}^* + \boldsymbol{E}_{\mathrm{s}} \times \boldsymbol{H}_{\mathrm{e}}^* \right\}$$

is the Poynting vector caused by the interaction between the scattered and incident fields.

Taking into account the boundary conditions $\boldsymbol{n} \times \boldsymbol{E}_{\mathrm{i}} = \boldsymbol{n} \times \boldsymbol{E}$ and $\boldsymbol{n} \times \boldsymbol{H}_{\mathrm{i}} = \boldsymbol{n} \times \boldsymbol{H}$ on S, we express the time-averaged power absorbed by the particle as

$$W_{\mathrm{abs}} = -\frac{1}{2} \int_S \boldsymbol{n} \cdot \mathrm{Re} \left\{ \boldsymbol{E}_{\mathrm{i}} \times \boldsymbol{H}_{\mathrm{i}}^* \right\} \mathrm{d}S$$

$$= -\frac{1}{2} \int_S \boldsymbol{n} \cdot \mathrm{Re} \left\{ \boldsymbol{E} \times \boldsymbol{H}^* \right\} \mathrm{d}S \, .$$

With S_{c} being an auxiliary surface enclosing S (Fig. 1.11), we apply the Green second vector theorem to the vector fields $\boldsymbol{E}$ and $\boldsymbol{E}^*$ in the domain D bounded by S and S_{c}. We obtain

$$\int_S \boldsymbol{n} \cdot \left(\boldsymbol{E} \times \boldsymbol{H}^* + \boldsymbol{E}^* \times \boldsymbol{H} \right) \mathrm{d}S = \int_{S_{\mathrm{c}}} \boldsymbol{n} \cdot \left(\boldsymbol{E} \times \boldsymbol{H}^* + \boldsymbol{E}^* \times \boldsymbol{H} \right) \mathrm{d}S \, ,$$

and further

$$\int_S \boldsymbol{n} \cdot \mathrm{Re} \left\{ \boldsymbol{E} \times \boldsymbol{H}^* \right\} \mathrm{d}S = \int_{S_{\mathrm{c}}} \boldsymbol{n} \cdot \mathrm{Re} \left\{ \boldsymbol{E} \times \boldsymbol{H}^* \right\} \mathrm{d}S \, .$$
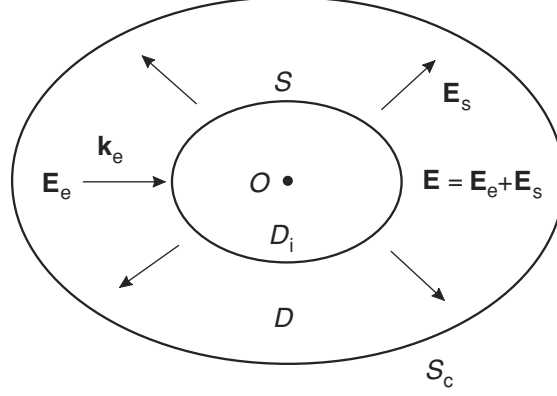
Fig. 1.11. Auxiliary surface S_c

The time-averaged power absorbed by the particle then becomes

$$W_\mathrm{abs} = -\frac{1}{2}\int_{S_\mathrm{c}} \boldsymbol{n}\cdot\mathrm{Re}\left\{\boldsymbol{E}\times\boldsymbol{H}^*\right\}\mathrm{d}S = -\int_{S_\mathrm{c}} \boldsymbol{n}\cdot\langle\boldsymbol{S}\rangle\,\mathrm{d}S$$

$$= W_\mathrm{inc} - W_\mathrm{scat} + W_\mathrm{ext}\,,$$

where

$$W_\mathrm{inc} = -\int_{S_\mathrm{c}} \boldsymbol{n}\cdot\langle\boldsymbol{S}_\mathrm{inc}\rangle\,\mathrm{d}S = -\frac{1}{2}\int_{S_\mathrm{c}} \boldsymbol{n}\cdot\mathrm{Re}\left\{\boldsymbol{E}_\mathrm{e}\times\boldsymbol{H}_\mathrm{e}^*\right\}\mathrm{d}S\,, \qquad (1.80)$$

$$W_\mathrm{scat} = \int_{S_\mathrm{c}} \boldsymbol{n}\cdot\langle\boldsymbol{S}_\mathrm{scat}\rangle\,\mathrm{d}S = \frac{1}{2}\int_{S_\mathrm{c}} \boldsymbol{n}\cdot\mathrm{Re}\left\{\boldsymbol{E}_\mathrm{s}\times\boldsymbol{H}_\mathrm{s}^*\right\}\mathrm{d}S\,, \qquad (1.81)$$

$$W_\mathrm{ext} = -\int_{S_\mathrm{c}} \boldsymbol{n}\cdot\langle\boldsymbol{S}_\mathrm{ext}\rangle\,\mathrm{d}S = -\frac{1}{2}\int_{S_\mathrm{c}} \boldsymbol{n}\cdot\mathrm{Re}\left\{\boldsymbol{E}_\mathrm{e}\times\boldsymbol{H}_\mathrm{s}^* + \boldsymbol{E}_\mathrm{s}\times\boldsymbol{H}_\mathrm{e}^*\right\}\mathrm{d}S\,.$$

$$(1.82)$$

The divergence theorem applied to the excitation field in the domain D_c bounded by S_c gives

$$\int_{D_\mathrm{c}} \nabla\cdot(\boldsymbol{E}_\mathrm{e}\times\boldsymbol{H}_\mathrm{e}^*)\,\mathrm{d}V = \int_{S_\mathrm{c}} \boldsymbol{n}\cdot(\boldsymbol{E}_\mathrm{e}\times\boldsymbol{H}_\mathrm{e}^*)\,\mathrm{d}S\,,$$

whence, using

$$\nabla\cdot(\boldsymbol{E}_\mathrm{e}\times\boldsymbol{H}_\mathrm{e}^*) = jk_0\left(\mu_\mathrm{s}\left|\boldsymbol{H}_\mathrm{e}\right|^2 - \varepsilon_\mathrm{s}\left|\boldsymbol{E}_\mathrm{e}\right|^2\right)\,,$$

and

$$\mathrm{Re}\left\{\nabla\cdot(\boldsymbol{E}_\mathrm{e}\times\boldsymbol{H}_\mathrm{e}^*)\right\} = 0\,,$$

yield

$$W_\mathrm{inc} = 0\,.$$

Thus, W_{ext} is the sum of the electromagnetic scattering power and the electromagnetic absorption power

$$W_{\mathrm{ext}} = W_{\mathrm{scat}} + W_{\mathrm{abs}}\,.$$

For a plane wave incidence, the extinction and scattering cross-sections are given by

$$C_{\mathrm{ext}} = \frac{W_{\mathrm{ext}}}{\frac{1}{2}\sqrt{\frac{\varepsilon_{\mathrm{s}}}{\mu_{\mathrm{s}}}}\,|\boldsymbol{E}_{\mathrm{e0}}|^2}\,, \tag{1.83}$$

$$C_{\mathrm{scat}} = \frac{W_{\mathrm{scat}}}{\frac{1}{2}\sqrt{\frac{\varepsilon_{\mathrm{s}}}{\mu_{\mathrm{s}}}}\,|\boldsymbol{E}_{\mathrm{e0}}|^2}\,, \tag{1.84}$$

the absorption cross-section is

$$C_{\mathrm{abs}} = C_{\mathrm{ext}} - C_{\mathrm{scat}} \geq 0\,,$$

while the single-scattering albedo is

$$\omega = \frac{C_{\mathrm{scat}}}{C_{\mathrm{ext}}} \leq 1\,.$$

Essentially, C_{scat} and C_{abs} represent the electromagnetic powers removed from the incident wave as a result of scattering and absorption of the incident radiation, while C_{ext} gives the total electromagnetic power removed from the incident wave by the combined effect of scattering and absorption. The optical cross-sections have the dimension of area and depend on the direction and polarization state of the incident wave as well on the size, optical properties and orientation of the particle. The efficiencies (or efficiency factors) for extinction, scattering and absorption are defined as

$$Q_{\mathrm{ext}} = \frac{C_{\mathrm{ext}}}{G}\,, \quad Q_{\mathrm{scat}} = \frac{C_{\mathrm{scat}}}{G}\,, \quad Q_{\mathrm{abs}} = \frac{C_{\mathrm{abs}}}{G}\,,$$

where G is the particle cross-sectional area projected onto a plane perpendicular to the incident beam. In view of the definition of the normalized differential scattering cross-section, we set $G = \pi a_{\mathrm{c}}^2$, where a_{c} is the area-equivalent-circle radius. From the point of view of geometrical optics we expect that the extinction efficiency of all particles would be identically equal to unity. In fact, there are many particles which can scatter and absorb more light than is geometrically incident upon them [17].

The scattering cross-section is the integral of the differential scattering cross-section over the unit sphere. To prove this assertion, we express C_{scat} as

$$C_{\mathrm{scat}} = \frac{1}{|\boldsymbol{E}_{\mathrm{e0}}|^2}\sqrt{\frac{\mu_{\mathrm{s}}}{\varepsilon_{\mathrm{s}}}}\int_{S_c}\boldsymbol{e}_r\cdot\mathrm{Re}\left\{\boldsymbol{E}_{\mathrm{s}}\times\boldsymbol{H}_{\mathrm{s}}^*\right\}\mathrm{d}S\,,$$

where S_c is a spherical surface situated at infinity and use the far-field representation

$$\boldsymbol{e}_r \cdot (\boldsymbol{E}_\mathrm{s} \times \boldsymbol{H}_\mathrm{s}^*) = \frac{1}{r^2} \sqrt{\frac{\varepsilon_\mathrm{s}}{\mu_\mathrm{s}}} \left[|\boldsymbol{E}_{\mathrm{s}\infty}|^2 + \mathrm{O}\left(\frac{1}{r}\right) \right], \quad r \to \infty$$

to obtain

$$C_\mathrm{scat} = \frac{1}{|\boldsymbol{E}_{\mathrm{e}0}|^2} \int_\Omega |\boldsymbol{E}_{\mathrm{s}\infty}|^2 \, \mathrm{d}\Omega. \qquad (1.85)$$

The scattering cross-section can be expressed in terms of the elements of the phase matrix and the Stokes parameters of the incident wave. Taking into account the expressions of I_e and I_s, and using (1.76) we obtain

$$\begin{aligned}
C_\mathrm{scat} &= \frac{1}{I_\mathrm{e}} \int_\Omega I_\mathrm{s}(\boldsymbol{e}_r) \, \mathrm{d}\Omega(\boldsymbol{e}_r) \\
&= \frac{1}{I_\mathrm{e}} \int_\Omega [Z_{11}(\boldsymbol{e}_r, \boldsymbol{e}_k) I_\mathrm{e} + Z_{12}(\boldsymbol{e}_r, \boldsymbol{e}_k) Q_\mathrm{e} \\
&\quad + Z_{13}(\boldsymbol{e}_r, \boldsymbol{e}_k) U_\mathrm{e} + Z_{14}(\boldsymbol{e}_r, \boldsymbol{e}_k) V_\mathrm{e}] \, \mathrm{d}\Omega(\boldsymbol{e}_r). \qquad (1.86)
\end{aligned}$$

The phase function is related to the differential scattering cross-section by the relation

$$p(\boldsymbol{e}_r, \boldsymbol{e}_k) = \frac{4\pi}{C_\mathrm{scat} |\boldsymbol{E}_{\mathrm{e}0}|^2} |\boldsymbol{E}_{\mathrm{s}\infty}(\boldsymbol{e}_r)|^2$$

and in view of (1.85) we see that p is dimensionless and normalized, i.e.,

$$\frac{1}{4\pi} \int_\Omega p \, \mathrm{d}\Omega = 1.$$

The mean direction of propagation of the scattered field is defined as

$$\boldsymbol{g} = \frac{1}{C_\mathrm{scat} |\boldsymbol{E}_{\mathrm{e}0}|^2} \int_\Omega |\boldsymbol{E}_{\mathrm{s}\infty}(\boldsymbol{e}_r)|^2 \boldsymbol{e}_r \, \mathrm{d}\Omega(\boldsymbol{e}_r) \qquad (1.87)$$

and obviously

$$\begin{aligned}
\boldsymbol{g} &= \frac{1}{C_\mathrm{scat} I_\mathrm{e}} \int_\Omega I_\mathrm{s}(\boldsymbol{e}_r) \boldsymbol{e}_r \, \mathrm{d}\Omega(\boldsymbol{e}_r) \\
&= \frac{1}{C_\mathrm{scat} I_\mathrm{e}} \int_\Omega [Z_{11}(\boldsymbol{e}_r, \boldsymbol{e}_k) I_\mathrm{e} + Z_{12}(\boldsymbol{e}_r, \boldsymbol{e}_k) Q_\mathrm{e} \\
&\quad + Z_{13}(\boldsymbol{e}_r, \boldsymbol{e}_k) U_\mathrm{e} + Z_{14}(\boldsymbol{e}_r, \boldsymbol{e}_k) V_\mathrm{e}] \boldsymbol{e}_r \, \mathrm{d}\Omega(\boldsymbol{e}_r).
\end{aligned}$$

The asymmetry parameter $\langle \cos \Theta \rangle$ is the dot product between the vector $\boldsymbol{g}$ and the incident direction $\boldsymbol{e}_k$ [17, 169],

$$\langle \cos \Theta \rangle = \boldsymbol{g} \cdot \boldsymbol{e}_k = \frac{1}{C_{\text{scat}} \left| \boldsymbol{E}_{\text{e0}} \right|^2} \int_\Omega \left| \boldsymbol{E}_{\text{s}\infty} \left(\boldsymbol{e}_r \right) \right|^2 \boldsymbol{e}_r \cdot \boldsymbol{e}_k \, \mathrm{d}\Omega \left(\boldsymbol{e}_r \right)$$

$$= \frac{1}{4\pi} \int_\Omega p \left(\boldsymbol{e}_r, \boldsymbol{e}_k \right) \cos \Theta \, \mathrm{d}\Omega \left(\boldsymbol{e}_r \right) ,$$

where $\cos \Theta = \boldsymbol{e}_r \cdot \boldsymbol{e}_k$, and it is apparent that the asymmetry parameter is the average cosine of the scattering angle Θ. If the particle scatters more light toward the forward direction ($\Theta = 0$), $\langle \cos \Theta \rangle$ is positive and $\langle \cos \Theta \rangle$ is negative if the scattering is directed more toward the backscattering direction ($\Theta = 180°$). If the scattering is symmetric about a scattering angle of $90°$, $\langle \cos \Theta \rangle$ vanishes.

1.4.5 Optical Theorem

The expression of extinction has been derived by integrating the Poynting vector over an auxiliary surface around the particle. This derivation emphasized the conservation of energy aspect of extinction: extinction is the combined effect of absorption and scattering. A second derivation emphasizes the interference aspect of extinction: extinction is a result of the interference between the incident and forward scattered light [17]. Applying Green's second vector theorem to the vector fields $\boldsymbol{E}_\text{s}$ and $\boldsymbol{E}_\text{e}^*$ in the domain D bounded by S and S_c, we obtain

$$\int_S \boldsymbol{n} \cdot \left(\boldsymbol{E}_\text{s} \times \boldsymbol{H}_\text{e}^* + \boldsymbol{E}_\text{e}^* \times \boldsymbol{H}_\text{s} \right) \mathrm{d}S = \int_{S_\text{c}} \boldsymbol{n} \cdot \left(\boldsymbol{E}_\text{s} \times \boldsymbol{H}_\text{e}^* + \boldsymbol{E}_\text{e}^* \times \boldsymbol{H}_\text{s} \right) \mathrm{d}S$$

and further

$$\int_S \boldsymbol{n} \cdot \operatorname{Re} \left\{ \boldsymbol{E}_\text{s} \times \boldsymbol{H}_\text{e}^* + \boldsymbol{E}_\text{e}^* \times \boldsymbol{H}_\text{s} \right\} \mathrm{d}S = \int_{S_\text{c}} \boldsymbol{n} \cdot \operatorname{Re} \left\{ \boldsymbol{E}_\text{s} \times \boldsymbol{H}_\text{e}^* + \boldsymbol{E}_\text{e}^* \times \boldsymbol{H}_\text{s} \right\} \mathrm{d}S .$$

This result together with (1.82) and the identity $\operatorname{Re}\{\boldsymbol{E}_\text{e} \times \boldsymbol{H}_\text{s}^*\} = \operatorname{Re}\{\boldsymbol{E}_\text{e}^* \times \boldsymbol{H}_\text{s}\}$ give

$$W_{\text{ext}} = -\frac{1}{2} \int_S \boldsymbol{n} \cdot \operatorname{Re} \left\{ \boldsymbol{E}_\text{s} \times \boldsymbol{H}_\text{e}^* + \boldsymbol{E}_\text{e}^* \times \boldsymbol{H}_\text{s} \right\} \mathrm{d}S ,$$

whence, using the explicit expressions for $\boldsymbol{E}_\text{e}$ and $\boldsymbol{H}_\text{e}$, we derive

$$W_{\text{ext}} = \frac{1}{2} \operatorname{Re} \left\{ \int_S \left[\boldsymbol{E}_{\text{e0}}^* \cdot \boldsymbol{h}_\text{s} \left(\boldsymbol{r}' \right) \right. \right.$$
$$\left. \left. - \sqrt{\frac{\varepsilon_\text{s}}{\mu_\text{s}}} \left(\boldsymbol{e}_k \times \boldsymbol{E}_{\text{e0}}^* \right) \cdot \boldsymbol{e}_\text{s} \left(\boldsymbol{r}' \right) \right] \mathrm{e}^{-\mathrm{j}\boldsymbol{k}_\text{e} \cdot \boldsymbol{r}'} \mathrm{d}S \left(\boldsymbol{r}' \right) \right\} .$$

In the integral representation for the electric far-field pattern (cf. (1.69)) we set $\boldsymbol{e}_r = \boldsymbol{e}_k$, take the dot product between $\boldsymbol{E}_{\text{s}\infty}(\boldsymbol{e}_k)$ and $\boldsymbol{E}_{\text{e0}}^*$, and obtain

$$\boldsymbol{E}_{\text{e0}}^* \cdot \boldsymbol{E}_{\text{s}\infty}\left(\boldsymbol{e}_k\right) = \frac{\text{j}k_{\text{s}}}{4\pi} \sqrt{\frac{\mu_{\text{s}}}{\varepsilon_{\text{s}}}} \int_S \left\{ \boldsymbol{E}_{\text{e0}}^* \cdot \boldsymbol{h}_{\text{s}}\left(\boldsymbol{r}'\right) \right.$$

$$\left. - \sqrt{\frac{\varepsilon_{\text{s}}}{\mu_{\text{s}}}}\left(\boldsymbol{e}_k \times \boldsymbol{E}_{\text{e0}}^*\right) \cdot \boldsymbol{e}_{\text{s}}\left(\boldsymbol{r}'\right) \right\} \text{e}^{-\text{j}\boldsymbol{k}_{\text{e}}\cdot\boldsymbol{r}'} \, \text{d}S\left(\boldsymbol{r}'\right) .$$

The last two relations imply that

$$W_{\text{ext}} = \frac{1}{2}\text{Re}\left\{ \sqrt{\frac{\varepsilon_{\text{s}}}{\mu_{\text{s}}}} \frac{4\pi}{\text{j}k_{\text{s}}} \boldsymbol{E}_{\text{e0}}^* \cdot \boldsymbol{E}_{\text{s}\infty}\left(\boldsymbol{e}_k\right) \right\}$$

and further that

$$C_{\text{ext}} = \frac{4\pi}{k_{\text{s}}\left|\boldsymbol{E}_{\text{e0}}\right|^2}\text{Im}\left\{ \boldsymbol{E}_{\text{e0}}^* \cdot \boldsymbol{E}_{\text{s}\infty}\left(\boldsymbol{e}_k\right) \right\} . \tag{1.88}$$

The above relation is a representation of the optical theorem, and since the extinction cross-section is in terms of the scattering amplitude in the forward direction, the optical theorem is also known as the extinction theorem or the forward scattering theorem. This fundamental relation can be used to compute the extinction cross-section when the imaginary part of the scattering amplitude in the forward direction is known accurately. In view of (1.88) and (1.74), and taking into account the explicit expressions of the elements of the extinction matrix we see that

$$C_{\text{ext}} = \frac{1}{I_{\text{e}}}\left[K_{11}\left(\boldsymbol{e}_k\right)I_{\text{e}} + K_{12}\left(\boldsymbol{e}_k\right)Q_{\text{e}} + K_{13}\left(\boldsymbol{e}_k\right)U_{\text{e}} + K_{14}\left(\boldsymbol{e}_k\right)V_{\text{e}} \right] . \tag{1.89}$$

1.4.6 Reciprocity

The tensor scattering amplitude satisfies a useful symmetry property which is referred to as reciprocity. As a consequence, reciprocity relations for the amplitude, phase and extinction matrices can be derived. Reciprocity is a manifestation of the symmetry of the scattering process with respect to an inversion of time and holds for particles in arbitrary orientations [169]. In order to derive this property we use the following result: if $\boldsymbol{E}_1$, $\boldsymbol{H}_1$ and $\boldsymbol{E}_2$, $\boldsymbol{H}_2$ are the total fields generated by the incident fields $\boldsymbol{E}_{\text{e1}}$, $\boldsymbol{H}_{\text{e1}}$ and $\boldsymbol{E}_{\text{e2}}$, $\boldsymbol{H}_{\text{e2}}$, respectively, we have

$$\int_S \boldsymbol{n} \cdot \left(\boldsymbol{E}_2 \times \boldsymbol{H}_1 - \boldsymbol{E}_1 \times \boldsymbol{H}_2\right) \text{d}S = \int_{S_{\text{c}}} \boldsymbol{n} \cdot \left(\boldsymbol{E}_2 \times \boldsymbol{H}_1 - \boldsymbol{E}_1 \times \boldsymbol{H}_2\right) \text{d}S ,$$

where as before, S_{c} is an auxiliary surface enclosing S. Since $\boldsymbol{E}_1$ and $\boldsymbol{E}_2$ are source free in the domain bounded by S and S_{c}, the above equation follows immediately from Green second vector theorem. Further, applying Green's second vector theorem to the internal fields $\boldsymbol{E}_{\text{i1}}$ and $\boldsymbol{E}_{\text{i2}}$ in the domain D_{i}, and taking into account the boundary conditions $\boldsymbol{n} \times \boldsymbol{E}_{\text{i1,2}} = \boldsymbol{n} \times \boldsymbol{E}_{1,2}$ and $\boldsymbol{n} \times \boldsymbol{H}_{\text{i1,2}} = \boldsymbol{n} \times \boldsymbol{H}_{1,2}$ on S, yields

$$\int_S \boldsymbol{n} \cdot (\boldsymbol{E}_2 \times \boldsymbol{H}_1 - \boldsymbol{E}_1 \times \boldsymbol{H}_2) \, \mathrm{d}S = 0 \,,$$

whence

$$\int_{S_{\mathrm{c}}} \boldsymbol{n} \cdot (\boldsymbol{E}_2 \times \boldsymbol{H}_1 - \boldsymbol{E}_1 \times \boldsymbol{H}_2) \, \mathrm{d}S = 0 \,, \tag{1.90}$$

follows. We take the surface S_{c} as a large sphere of outward unit normal vector $\boldsymbol{e}_r$, consider the limit when the radius R becomes infinite, and write the integrand in (1.90) as

$$\boldsymbol{E}_2 \times \boldsymbol{H}_1 - \boldsymbol{E}_1 \times \boldsymbol{H}_2$$

$$= \boldsymbol{E}_{\mathrm{e}2} \times \boldsymbol{H}_{\mathrm{e}1} - \boldsymbol{E}_{\mathrm{e}1} \times \boldsymbol{H}_{\mathrm{e}2} + \boldsymbol{E}_{\mathrm{s}2} \times \boldsymbol{H}_{\mathrm{s}1} - \boldsymbol{E}_{\mathrm{s}1} \times \boldsymbol{H}_{\mathrm{s}2}$$

$$+ \boldsymbol{E}_{\mathrm{s}2} \times \boldsymbol{H}_{\mathrm{e}1} - \boldsymbol{E}_{\mathrm{e}1} \times \boldsymbol{H}_{\mathrm{s}2} + \boldsymbol{E}_{\mathrm{e}2} \times \boldsymbol{H}_{\mathrm{s}1} - \boldsymbol{E}_{\mathrm{s}1} \times \boldsymbol{H}_{\mathrm{e}2} \,.$$

The Green second vector theorem applied to the incident fields $\boldsymbol{E}_{\mathrm{e}1}$ and $\boldsymbol{E}_{\mathrm{e}2}$ in any bounded domain shows that the vector plane wave terms do not contribute to the integral. Furthermore, using the far-field representation

$$\boldsymbol{E}_{\mathrm{s}2} \times \boldsymbol{H}_{\mathrm{s}1} - \boldsymbol{E}_{\mathrm{s}1} \times \boldsymbol{H}_{\mathrm{s}2}$$

$$= \frac{\mathrm{e}^{2jk_{\mathrm{s}}r}}{r^2} \left\{ \boldsymbol{E}_{\mathrm{s}\infty 2} \times \boldsymbol{H}_{\mathrm{s}\infty 1} - \boldsymbol{E}_{\mathrm{s}\infty 1} \times \boldsymbol{H}_{\mathrm{s}\infty 2} + \mathrm{O}\left(\frac{1}{r}\right) \right\} \,,$$

and taking into account the transversality of the far-field patterns

$$\boldsymbol{E}_{\mathrm{s}\infty 2} \times \boldsymbol{H}_{\mathrm{s}\infty 1} - \boldsymbol{E}_{\mathrm{s}\infty 1} \times \boldsymbol{H}_{\mathrm{s}\infty 2} = 0 \,,$$

we see that the integral over the scattered wave terms also vanishes. Thus, (1.90) implies that

$$\int_{S_{\mathrm{c}}} \boldsymbol{e}_r \cdot (\boldsymbol{E}_{\mathrm{s}2} \times \boldsymbol{H}_{\mathrm{e}1} - \boldsymbol{E}_{\mathrm{e}1} \times \boldsymbol{H}_{\mathrm{s}2}) \, \mathrm{d}S = \int_{S_{\mathrm{c}}} \boldsymbol{e}_r \cdot (\boldsymbol{E}_{\mathrm{s}1} \times \boldsymbol{H}_{\mathrm{e}2} - \boldsymbol{E}_{\mathrm{e}2} \times \boldsymbol{H}_{\mathrm{s}1}) \, \mathrm{d}S \,. \tag{1.91}$$

For plane wave incidence,

$$\boldsymbol{E}_{\mathrm{e}u}(\boldsymbol{r}) = \boldsymbol{E}_{\mathrm{e}0u} \exp\left(j\boldsymbol{k}_{\mathrm{e}u} \cdot \boldsymbol{r}\right) \,, \quad \boldsymbol{k}_{\mathrm{e}u} = k_{\mathrm{s}}\boldsymbol{e}_{ku} \,, \quad u = 1, 2 \,,$$

the integrands in (1.91) contain the term $\exp(jk_{\mathrm{s}}R\boldsymbol{e}_{k1,2} \cdot \boldsymbol{e}_r)$. Since R is large, the stationary point method can be used to compute the integrals accordingly to the basic result

$$\frac{kR}{2\pi j} \int_0^{2\pi} \int_0^{\pi} g\left(\theta, \varphi\right) \mathrm{e}^{jkRf(\theta,\varphi)} \mathrm{d}\theta \, \mathrm{d}\varphi = \frac{1}{\sqrt{f_{\theta\theta} f_{\varphi\varphi} - f_{\theta\varphi}^2}} g\left(\theta_{\mathrm{st}}, \varphi_{\mathrm{st}}\right) \mathrm{e}^{jkRf(\theta_{\mathrm{st}},\varphi_{\mathrm{st}})} \,, \tag{1.92}$$

where $(\theta_{st}, \varphi_{st})$ is the stationary point of f, $f_{\theta\theta} = \partial^2 f/\partial\theta^2$, $f_{\varphi\varphi} = \partial^2 f/\partial\varphi^2$ and $f_{\theta\varphi} = \partial^2 f/\partial\theta\partial\varphi$. The integrals in (1.91) are then given by

$$\int_{S_c} \boldsymbol{e}_r \cdot (\boldsymbol{E}_{s2} \times \boldsymbol{H}_{e1} - \boldsymbol{E}_{e1} \times \boldsymbol{H}_{s2})\, \mathrm{d}S$$

$$= -4\pi\mathrm{j}\frac{R}{k_s}\sqrt{\frac{\varepsilon_s}{\mu_s}}\boldsymbol{E}_{s\infty2}(-\boldsymbol{e}_{k1}) \cdot \boldsymbol{E}_{e01}\mathrm{e}^{-\mathrm{j}k_s R},$$

$$\int_{S_c} \boldsymbol{e}_r \cdot (\boldsymbol{E}_{s1} \times \boldsymbol{H}_{e2} - \boldsymbol{E}_{e2} \times \boldsymbol{H}_{s1})\, \mathrm{d}S$$

$$= -4\pi\mathrm{j}\frac{R}{k_s}\sqrt{\frac{\varepsilon_s}{\mu_s}}\boldsymbol{E}_{s\infty1}(-\boldsymbol{e}_{k2}) \cdot \boldsymbol{E}_{e02}\mathrm{e}^{-\mathrm{j}k_s R},$$

and we deduce the reciprocity relation for the far-field pattern (Fig. 1.12):

$$\boldsymbol{E}_{s\infty2}(-\boldsymbol{e}_{k1}) \cdot \boldsymbol{E}_{e01} = \boldsymbol{E}_{s\infty1}(-\boldsymbol{e}_{k2}) \cdot \boldsymbol{E}_{e02}.$$

The above relation gives

$$\boldsymbol{E}_{e01} \cdot \overline{\boldsymbol{A}}(-\boldsymbol{e}_{k1}, \boldsymbol{e}_{k2}) \cdot \boldsymbol{E}_{e02} = \boldsymbol{E}_{e02} \cdot \overline{\boldsymbol{A}}(-\boldsymbol{e}_{k2}, \boldsymbol{e}_{k1}) \cdot \boldsymbol{E}_{e01}$$

and since $\boldsymbol{a} \cdot \overline{\boldsymbol{D}} \cdot \boldsymbol{b} = \boldsymbol{b} \cdot \overline{\boldsymbol{D}}^{\mathrm{T}} \cdot \boldsymbol{a}$, and $\boldsymbol{E}_{e01}$ and $\boldsymbol{E}_{e02}$ are arbitrary transverse vectors, the following constraint on the tensor scattering amplitude:

$$\overline{\boldsymbol{A}}(-\boldsymbol{e}_{k2}, -\boldsymbol{e}_{k1}) = \overline{\boldsymbol{A}}^{\mathrm{T}}(\boldsymbol{e}_{k1}, \boldsymbol{e}_{k2})$$

follows. This is the reciprocity relation for the tensor scattering amplitude which relates scattering from the direction $-\boldsymbol{e}_{k1}$ into $-\boldsymbol{e}_{k2}$ to scattering from $\boldsymbol{e}_{k2}$ to $\boldsymbol{e}_{k1}$. Taking into account the representation of the amplitude matrix elements in terms of the tensor scattering amplitude and the fact that for
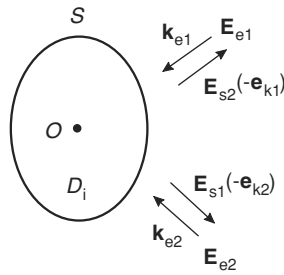

Fig. 1.12. Illustration of the reciprocity relation

$e'_k = -e_k$ we have $e'_\beta = e_\beta$ and $e'_\alpha = -e_\alpha$, we obtain the reciprocity relation for the amplitude matrix:

$$S\left(-e_{k2}, -e_{k1}\right) = \begin{bmatrix} S_{\theta\beta}\left(e_{k1}, e_{k2}\right) & -S_{\varphi\beta}\left(e_{k1}, e_{k2}\right) \\ -S_{\theta\alpha}\left(e_{k1}, e_{k2}\right) & S_{\varphi\alpha}\left(e_{k1}, e_{k2}\right) \end{bmatrix}.$$

If we choose $e_{k1} = -e_{k2} = -e_k$, we obtain

$$S_{\varphi\beta}\left(-e_k, e_k\right) = -S_{\theta\alpha}\left(-e_k, e_k\right),$$

which is a representation of the backscattering theorem [169].

From the reciprocity relation for the amplitude matrix we easily derive the reciprocity relation for the phase and extinction matrices:

$$Z\left(-e_k, -e_r\right) = QZ^{\mathrm{T}}\left(e_r, e_k\right)Q$$

and

$$K\left(-e_k\right) = QK^{\mathrm{T}}\left(e_k\right)Q,$$

respectively, where $Q = \mathrm{diag}[1, 1, -1, 1]$.

The reciprocity relations can be used in practice for testing the results of theoretical computations and laboratory measurements. It should be remarked that reciprocity relations give also rise to symmetry relations for the dyadic Green functions [229].

1.5 Transition Matrix

The transition matrix relates the expansion coefficients of the incident and scattered fields. The existence of the transition matrix is "postulated" by the T-Matrix Ansatz and is a consequence of the series expansions of the incident and scattered fields and the linearity of the Maxwell equations. Historically, the transition matrix has been introduced within the null-field method formalism (see [253, 256]), and for this reason, the null-field method has often been referred to as the T-matrix method. However, the null-field method is only one among many methods that can be used to compute the transition matrix. The transition matrix can also be derived in the framework of the method of moments [88], the separation of variables method [208], the discrete dipole approximation [151] and the point matching method [181]. Rother et al. [205] found a general relation between the surface Green function and the transition matrix for the exterior Maxwell problem, which in principle, allows to compute the transition matrix with the finite-difference technique.

In this section we review the general properties of the transition matrix such as unitarity and symmetry and discuss analytical procedures for averaging scattering characteristics over particle orientations. These procedures

relying on the rotation transformation rule for vector spherical wave functions are of general use because an explicit expression of the transition matrix is not required. In order to simplify our analysis we consider a vector plane wave of unit amplitude

$$\boldsymbol{E}_{\mathrm{e}}(\boldsymbol{r}) = \boldsymbol{e}_{\mathrm{pol}}\mathrm{e}^{\mathrm{j}\boldsymbol{k}_{\mathrm{e}}\cdot\boldsymbol{r}}, \quad \boldsymbol{H}_{\mathrm{e}}(\boldsymbol{r}) = \sqrt{\frac{\varepsilon_{\mathrm{s}}}{\mu_{\mathrm{s}}}}\boldsymbol{e}_k \times \boldsymbol{e}_{\mathrm{pol}}\mathrm{e}^{\mathrm{j}\boldsymbol{k}_{\mathrm{e}}\cdot\boldsymbol{r}},$$

where $\boldsymbol{e}_{\mathrm{pol}} \cdot \boldsymbol{e}_k = 0$ and $|\boldsymbol{e}_{\mathrm{pol}}| = 1$.

1.5.1 Definition

Everywhere outside the (smallest) sphere circumscribing the particle it is appropriate to expand the scattered field in terms of radiating vector spherical wave functions

$$\boldsymbol{E}_{\mathrm{s}}(\boldsymbol{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} f_{mn}\boldsymbol{M}_{mn}^{3}\left(k_{\mathrm{s}}\boldsymbol{r}\right) + g_{mn}\boldsymbol{N}_{mn}^{3}\left(k_{\mathrm{s}}\boldsymbol{r}\right) \tag{1.93}$$

and the incident field in terms of regular vector spherical wave functions

$$\boldsymbol{E}_{\mathrm{e}}(\boldsymbol{r}) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} a_{mn}\boldsymbol{M}_{mn}^{1}\left(k_{\mathrm{s}}\boldsymbol{r}\right) + b_{mn}\boldsymbol{N}_{mn}^{1}\left(k_{\mathrm{s}}\boldsymbol{r}\right) . \tag{1.94}$$

Within the vector spherical wave formalism, the scattering problem is solved by determining f_{mn} and g_{mn} as functions of a_{mn} and b_{mn}. Due to the linearity relations of the Maxwell equations and the constitutive relations, the relation between the scattered and incident field coefficients must be linear. This relation is given by the so-called transition matrix $\boldsymbol{T}$ as follows [256]

$$\begin{bmatrix} f_{mn} \\ g_{mn} \end{bmatrix} = \boldsymbol{T} \begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix} = \begin{bmatrix} \boldsymbol{T}^{11} & \boldsymbol{T}^{12} \\ \boldsymbol{T}^{21} & \boldsymbol{T}^{22} \end{bmatrix} \begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix} . \tag{1.95}$$

Essentially, the transition matrix depends on the physical and geometrical characteristics of the particle and is independent on the propagation direction and polarization states of the incident and scattered field.

If the transition matrix is known, the scattering characteristics (introduced in Sect. 1.4) can be readily computed. Taking into account the asymptotic behavior of the vector spherical wave functions we see that the far-field pattern can be expressed in terms of the elements of the transition matrix by the relation

$$\begin{aligned} \boldsymbol{E}_{\mathrm{s}\infty}\left(\boldsymbol{e}_r\right) &= \frac{1}{k_{\mathrm{s}}}\sum_{n,m}(-\mathrm{j})^{n+1}\left[f_{mn}\boldsymbol{m}_{mn}(\boldsymbol{e}_r) + \mathrm{j}g_{mn}\boldsymbol{n}_{mn}(\boldsymbol{e}_r)\right] \\ &= \frac{1}{k_{\mathrm{s}}}\sum_{n,m}\sum_{n_1,m_1}(-\mathrm{j})^{n+1} \\ &\quad \times \left[\left(T_{mn,m_1n_1}^{11}a_{m_1n_1} + T_{mn,m_1n_1}^{12}b_{m_1n_1}\right)\boldsymbol{m}_{mn}(\boldsymbol{e}_r) \right. \\ &\quad \left. + \mathrm{j}\left(T_{mn,m_1n_1}^{21}a_{m_1n_1} + T_{mn,m_1n_1}^{22}b_{m_1n_1}\right)\boldsymbol{n}_{mn}(\boldsymbol{e}_r)\right] . \tag{1.96} \end{aligned}$$

To derive the expressions of the tensor scattering amplitude and amplitude matrix, we consider the scattering and incident directions $\boldsymbol{e}_r$ and $\boldsymbol{e}_k$, and express the vector spherical harmonics as

$$\boldsymbol{x}_{mn}(\boldsymbol{e}_r) = x_{mn,\theta}\left(\boldsymbol{e}_r\right)\boldsymbol{e}_\theta + x_{mn,\varphi}\left(\boldsymbol{e}_r\right)\boldsymbol{e}_\varphi\,,$$

$$\boldsymbol{x}_{mn}(\boldsymbol{e}_k) = x_{mn,\beta}\left(\boldsymbol{e}_k\right)\boldsymbol{e}_\beta + x_{mn,\alpha}\left(\boldsymbol{e}_k\right)\boldsymbol{e}_\alpha\,,$$

where $\boldsymbol{x}_{mn}$ stands for $\boldsymbol{m}_{mn}$ and $\boldsymbol{n}_{mn}$. Recalling the expressions of the incident field coefficients for a plane wave excitation (cf. (1.26))

$$a_{mn} = 4\mathrm{j}^n\boldsymbol{e}_{\mathrm{pol}}\cdot\boldsymbol{m}^*_{mn}\left(\boldsymbol{e}_k\right)\,,$$

$$b_{mn} = -4\mathrm{j}^{n+1}\boldsymbol{e}_{\mathrm{pol}}\cdot\boldsymbol{n}^*_{mn}\left(\boldsymbol{e}_k\right)\,,$$

and using the definition of the tensor scattering amplitude (cf. (1.71)), we obtain

$$\overline{\boldsymbol{A}}\left(\boldsymbol{e}_r,\boldsymbol{e}_k\right) = \frac{4}{k_{\mathrm{s}}}\sum_{n,m}\sum_{n_1,m_1}(-\mathrm{j})^{n+1}\,\mathrm{j}^{n_1}\left\{\left[T^{11}_{mn,m_1n_1}\boldsymbol{m}_{mn}\left(\boldsymbol{e}_r\right)\right.\right.$$

$$\left.+jT^{21}_{mn,m_1n_1}\boldsymbol{n}_{mn}\left(\boldsymbol{e}_r\right)\right]\otimes\boldsymbol{m}^*_{m_1n_1}\left(\boldsymbol{e}_k\right)+\left[-\mathrm{j}T^{12}_{mn,m_1n_1}\boldsymbol{m}_{mn}\left(\boldsymbol{e}_r\right)\right.$$

$$\left.\left.+T^{22}_{mn,m_1n_1}\boldsymbol{n}_{mn}\left(\boldsymbol{e}_r\right)\right]\otimes\boldsymbol{n}^*_{m_1n_1}\left(\boldsymbol{e}_k\right)\right\}\,.$$

In view of (1.75), the elements of the amplitude matrix are given by

$$S_{pq}\left(\boldsymbol{e}_r,\boldsymbol{e}_k\right) = \frac{4}{k_{\mathrm{s}}}\sum_{n,m}\sum_{n_1,m_1}(-\mathrm{j})^{n+1}\,\mathrm{j}^{n_1}\left\{\left[T^{11}_{mn,m_1n_1}m^*_{m_1n_1,q}\left(\boldsymbol{e}_k\right)\right.\right.$$

$$\left.-jT^{12}_{mn,m_1n_1}n^*_{m_1n_1,q}\left(\boldsymbol{e}_k\right)\right]m_{mn,p}\left(\boldsymbol{e}_r\right)$$

$$+\mathrm{j}\left[T^{21}_{mn,m_1n_1}m^*_{m_1n_1,q}\left(\boldsymbol{e}_k\right)\right.\,,$$

$$\left.\left.-jT^{22}_{mn,m_1n_1}n^*_{m_1n_1,q}\left(\boldsymbol{e}_k\right)\right]n_{mn,p}\left(\boldsymbol{e}_r\right)\right\} \tag{1.97}$$

for $p = \theta,\varphi$ and $q = \beta,\alpha$. For a vector plane wave linearly polarized in the β-direction, $a_{mn} = 4\mathrm{j}^n m^*_{mn,\beta}$ and $b_{mn} = -4\mathrm{j}^{n+1}n^*_{mn,\beta}$, and $S_{\theta\beta} = E_{\mathrm{s}\infty,\theta}$ and $S_{\varphi\beta} = E_{\mathrm{s}\infty,\varphi}$. Analogously, for a vector plane wave linearly polarized in the α-direction, $a_{mn} = 4\mathrm{j}^n m^*_{mn,\alpha}$ and $b_{mn} = -4\mathrm{j}^{n+1}n^*_{mn,\alpha}$, and $S_{\theta\alpha} = E_{\mathrm{s}\infty,\theta}$ and $S_{\varphi\alpha} = E_{\mathrm{s}\infty,\varphi}$. In practical computer calculations, this technique, relying on the computation of the far-field patterns for parallel and perpendicular polarizations, can be used to determine the elements of the amplitude matrix.

For our further analysis, it is more convenient to express the above equations in matrix form. Defining the vectors

$$\boldsymbol{s} = \begin{bmatrix} f_{mn} \\ g_{mn} \end{bmatrix}\,,\quad \boldsymbol{e} = \begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix}$$

and the "augmented" vector of spherical harmonics

$$
\boldsymbol{v}\left(\boldsymbol{e}_r\right) = \begin{bmatrix} (-\mathrm{j})^n \, \boldsymbol{m}_{mn}\left(\boldsymbol{e}_r\right) \\ \mathrm{j}\left(-\mathrm{j}\right)^n \, \boldsymbol{n}_{mn}\left(\boldsymbol{e}_r\right) \end{bmatrix}
$$

we see that

$$
\boldsymbol{E}_{\mathrm{s}\infty}\left(\boldsymbol{e}_r\right) = -\frac{\mathrm{j}}{k_{\mathrm{s}}}\boldsymbol{v}^{\mathrm{T}}\left(\boldsymbol{e}_r\right)\boldsymbol{s} = -\frac{\mathrm{j}}{k_{\mathrm{s}}}\boldsymbol{v}^{\mathrm{T}}\left(\boldsymbol{e}_r\right)\boldsymbol{T}\boldsymbol{e} = -\frac{\mathrm{j}}{k_{\mathrm{s}}}\boldsymbol{e}^{\mathrm{T}}\boldsymbol{T}^{\mathrm{T}}\boldsymbol{v}\left(\boldsymbol{e}_r\right) , \qquad (1.98)
$$

and, since $\boldsymbol{e} = 4\boldsymbol{e}_{\mathrm{pol}}\cdot\boldsymbol{v}^*(\boldsymbol{e}_k)$, we obtain

$$
S_{pq}\left(\boldsymbol{e}_r, \boldsymbol{e}_k\right) = -\frac{4\mathrm{j}}{k_{\mathrm{s}}}\boldsymbol{v}_p^{\mathrm{T}}\left(\boldsymbol{e}_r\right)\boldsymbol{T}\boldsymbol{v}_q^*\left(\boldsymbol{e}_k\right) = -\frac{4\mathrm{j}}{k_{\mathrm{s}}}\boldsymbol{v}_q^{\dagger}\left(\boldsymbol{e}_k\right)\boldsymbol{T}^{\mathrm{T}}\boldsymbol{v}_p\left(\boldsymbol{e}_r\right) . \qquad (1.99)
$$

The superscript † means complex conjugate transpose, and

$$
\boldsymbol{v}_p\left(\cdot\right) = \begin{bmatrix} (-\mathrm{j})^n \, m_{mn,p}\left(\cdot\right) \\ \mathrm{j}\left(-\mathrm{j}\right)^n \, n_{mn,p}\left(\cdot\right) \end{bmatrix} ,
$$

where $p = \theta, \varphi$ for the $\boldsymbol{e}_r$-dependency and $p = \beta, \alpha$ for the $\boldsymbol{e}_k$-dependency.

The extinction and scattering cross-sections can be expressed in terms of the expansion coefficients a_{mn}, b_{mn}, f_{mn} and g_{mn}. Denoting by S_{c} the circumscribing sphere of outward unit normal vector $\boldsymbol{e}_r$ and radius R, and using the definition of the extinction cross-section (cf. (1.82) and (1.83) with $|\boldsymbol{E}_{\mathrm{e}0}| = 1$), yields

$$
\begin{aligned}
C_{\mathrm{ext}} &= -\sqrt{\frac{\mu_{\mathrm{s}}}{\varepsilon_{\mathrm{s}}}} \int_{S_c} \boldsymbol{e}_r \cdot \mathrm{Re}\left\{\boldsymbol{E}_{\mathrm{e}} \times \boldsymbol{H}_{\mathrm{s}}^* + \boldsymbol{E}_{\mathrm{s}} \times \boldsymbol{H}_{\mathrm{e}}^*\right\} \mathrm{d}S \\
&= -\mathrm{Re}\left\{\mathrm{j} \sum_{n,m} \sum_{n_1,m_1} \int_{S_c} \left\{\left(f_{mn}a_{m_1 n_1}^* + g_{mn}b_{m_1 n_1}^*\right)\right.\right. \\
&\quad \times \left[\left(\boldsymbol{e}_r \times \boldsymbol{M}_{mn}^3\right) \cdot \boldsymbol{N}_{m_1 n_1}^{1*} + \left(\boldsymbol{e}_r \times \boldsymbol{N}_{mn}^3\right) \cdot \boldsymbol{M}_{m_1 n_1}^{1*}\right] \\
&\quad + \left(f_{mn}b_{m_1 n_1}^* + g_{mn}a_{m_1 n_1}^*\right) \\
&\quad \left.\left. \times \left[\left(\boldsymbol{e}_r \times \boldsymbol{M}_{mn}^3\right) \cdot \boldsymbol{M}_{m_1 n_1}^{1*} + \left(\boldsymbol{e}_r \times \boldsymbol{N}_{mn}^3\right) \cdot \boldsymbol{N}_{m_1 n_1}^{1*}\right]\right\} \mathrm{d}S\right\} .
\end{aligned}
$$

Taking into account the orthogonality relations of the vector spherical wave functions on a spherical surface (cf. (B.18) and (B.19)) we obtain

$$
\begin{aligned}
C_{\mathrm{ext}} &= -\mathrm{Re}\left\{\frac{\mathrm{j}\pi R}{k_{\mathrm{s}}} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left(f_{mn}a_{mn}^* + g_{mn}b_{mn}^*\right)\right. \\
&\quad \left. \times \left\{h_n^{(1)}(k_{\mathrm{s}}R)\left[k_{\mathrm{s}}R\mathrm{j}_n(k_{\mathrm{s}}R)\right]' - \mathrm{j}_n(k_{\mathrm{s}}R)\left[k_{\mathrm{s}}Rh_n^{(1)}(k_{\mathrm{s}}R)\right]'\right\}\right\} ,
\end{aligned}
$$

whence, using the Wronskian relation

$$
h_n^{(1)}(k_{\mathrm{s}}R)\left[k_{\mathrm{s}}R\mathrm{j}_n(k_{\mathrm{s}}R)\right]' - \mathrm{j}_n(k_{\mathrm{s}}R)\left[k_{\mathrm{s}}Rh_n^{(1)}(k_{\mathrm{s}}R)\right]' = -\frac{\mathrm{j}}{k_{\mathrm{s}}R} ,
$$

we end up with

$$C_{\text{ext}} = -\frac{\pi}{k_{\text{s}}^2} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \text{Re}\left\{f_{mn}a_{mn}^* + g_{mn}b_{mn}^*\right\} . \qquad (1.100)$$

For the scattering cross-section, the expansion of the far-field pattern in terms of vector spherical harmonics (cf. (1.96)) and the orthogonality relations of the vector spherical harmonics (cf. (B.12) and (B.13)), yields

$$C_{\text{scat}} = \frac{\pi}{k_{\text{s}}^2} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} |f_{mn}|^2 + |g_{mn}|^2 . \qquad (1.101)$$

Thus, the extinction cross-section is given by the expansion coefficients of the incident and scattered field, while the scattering cross-section is determined by the expansion coefficients of the scattered field.

1.5.2 Unitarity and Symmetry

It is of interest to investigate general constraints of the transition matrix such as unitarity and symmetry. These properties can be established by applying the principle of conservation of energy to nonabsorbing particles ($\varepsilon_{\text{i}} > 0$ and $\mu_{\text{i}} > 0$). We begin our analysis by defining the $\mathcal{S}$ matrix in terms of the $\boldsymbol{T}$ matrix by the relation

$$\mathcal{S} = \boldsymbol{I} + 2\boldsymbol{T} ,$$

where $\boldsymbol{I}$ is the identity matrix. In the literature, the $\mathcal{S}$ matrix is also known as the scattering matrix but in our analysis we avoid this term because the scattering matrix will have another significance.

First we consider the unitarity property. Application of the divergence theorem to the total fields $\boldsymbol{E} = \boldsymbol{E}_{\text{s}} + \boldsymbol{E}_{\text{e}}$ and $\boldsymbol{H} = \boldsymbol{H}_{\text{s}} + \boldsymbol{H}_{\text{e}}$ in the domain D bounded by the surface S and a spherical surface S_{c} situated in the far-field region, yields

$$\int_D \nabla\cdot(\boldsymbol{E}\times\boldsymbol{H}^*)\,\mathrm{d}V = -\int_S \boldsymbol{n}\cdot(\boldsymbol{E}\times\boldsymbol{H}^*)\,\mathrm{d}S + \int_{S_{\text{c}}} \boldsymbol{e}_r\cdot(\boldsymbol{E}\times\boldsymbol{H}^*)\,\mathrm{d}S. \quad (1.102)$$

We consider the real part of the above equation and since the bounded domain D is assumed to be lossless ($\varepsilon_{\text{s}} > 0$ and $\mu_{\text{s}} > 0$) it follows that:

$$\text{Re}\left\{\nabla\cdot(\boldsymbol{E}\times\boldsymbol{H}^*)\right\} = \text{Re}\left\{jk_0\mu_{\text{s}}|\boldsymbol{H}|^2 - \mathrm{j}k_0\varepsilon_{\text{s}}|\boldsymbol{E}|^2\right\} = 0 \quad \text{in} \quad D. \quad (1.103)$$

On the other hand, taking into account the boundary conditions $\boldsymbol{n}\times\boldsymbol{E}_{\text{i}} = \boldsymbol{n}\times\boldsymbol{E}$ and $\boldsymbol{n}\times\boldsymbol{H}_{\text{i}} = \boldsymbol{n}\times\boldsymbol{H}$ on S, we have

$$\int_S \boldsymbol{n}\cdot(\boldsymbol{E}\times\boldsymbol{H}^*)\,\mathrm{d}S = \int_S \boldsymbol{n}\cdot(\boldsymbol{E}_{\text{i}}\times\boldsymbol{H}_{\text{i}}^*)\,\mathrm{d}S = \int_{D_{\text{i}}} \nabla\cdot(\boldsymbol{E}_{\text{i}}\times\boldsymbol{H}_{\text{i}}^*)\,\mathrm{d}V$$

and since for nonabsorbing particles

$$\mathrm{Re}\left\{\nabla \cdot (\boldsymbol{E}_\mathrm{i} \times \boldsymbol{H}_\mathrm{i}^*)\right\} = \mathrm{Re}\left\{\mathrm{j}k_0\mu_\mathrm{i}\left|\boldsymbol{H}_\mathrm{i}\right|^2 - \mathrm{j}k_0\varepsilon_\mathrm{i}\left|\boldsymbol{E}_\mathrm{i}\right|^2\right\} = 0 \quad \text{in} \quad D_\mathrm{i},$$

we obtain

$$\int_S \boldsymbol{n} \cdot \mathrm{Re}\left\{\boldsymbol{E} \times \boldsymbol{H}^*\right\} \mathrm{d}S = 0. \tag{1.104}$$

Combining (1.102), (1.103) and (1.104) we deduce that

$$\int_{S_c} \boldsymbol{e}_r \cdot \mathrm{Re}\left\{\boldsymbol{E} \times \boldsymbol{H}^*\right\} \mathrm{d}S = 0. \tag{1.105}$$

We next seek to find a series representation for the total electric field. For this purpose, we use the decomposition

$$\begin{pmatrix} \boldsymbol{M}_{mn}^1 \\ \boldsymbol{N}_{mn}^1 \end{pmatrix} = \frac{1}{2}\left[\begin{pmatrix} \boldsymbol{M}_{mn}^3 \\ \boldsymbol{N}_{mn}^3 \end{pmatrix} + \begin{pmatrix} \boldsymbol{M}_{mn}^2 \\ \boldsymbol{N}_{mn}^2 \end{pmatrix}\right],$$

where the vector spherical wave functions $\boldsymbol{M}_{mn}^2$ and $\boldsymbol{N}_{mn}^2$ have the same expressions as the vector spherical wave functions $\boldsymbol{M}_{mn}^3$ and $\boldsymbol{N}_{mn}^3$, but with the spherical Hankel functions of the second kind $h_n^{(2)}$ in place of the spherical Hankel functions of the first kind $h_n^{(1)}$. It should be remarked that for real arguments x, $h_n^{(2)}(x) = [h_n^{(1)}(x)]^*$. In the far-field region

$$\boldsymbol{M}_{mn}^2(k\boldsymbol{r}) = \frac{\mathrm{e}^{-\mathrm{j}kr}}{kr}\left\{\mathrm{j}^{n+1}\boldsymbol{m}_{mn}(\theta,\varphi) + \mathrm{O}\left(\frac{1}{r}\right)\right\},$$

$$\boldsymbol{N}_{mn}^2(k\boldsymbol{r}) = \frac{\mathrm{e}^{-\mathrm{j}kr}}{kr}\left\{\mathrm{j}^n\boldsymbol{n}_{mn}(\theta,\varphi) + \mathrm{O}\left(\frac{1}{r}\right)\right\},$$

as $r \to \infty$, and we see that $\boldsymbol{M}_{mn}^2$ and $\boldsymbol{N}_{mn}^2$ behave as incoming transverse vector spherical waves.

The expansion of the incident field then becomes

$$\boldsymbol{E}_e = \sum_{n,m} a_{mn}\boldsymbol{M}_{mn}^1 + b_{mn}\boldsymbol{N}_{mn}^1$$

$$= \frac{1}{2}\sum_{n,m} a_{mn}\boldsymbol{M}_{mn}^3 + b_{mn}\boldsymbol{N}_{mn}^3 + \frac{1}{2}\sum_{n,m} a_{mn}\boldsymbol{M}_{mn}^2 + b_{mn}\boldsymbol{N}_{mn}^2,$$

whence

$$\boldsymbol{E} = \sum_{n,m}\left(f_{mn} + \frac{1}{2}a_{mn}\right)\boldsymbol{M}_{mn}^3 + \left(g_{mn} + \frac{1}{2}b_{mn}\right)\boldsymbol{N}_{mn}^3$$

$$+ \frac{1}{2}\sum_{n,m} a_{mn}\boldsymbol{M}_{mn}^2 + b_{mn}\boldsymbol{N}_{mn}^2,$$

follows. Setting

$$c_{mn} = 2f_{mn} + a_{mn} \, ,$$

$$d_{mn} = 2g_{mn} + b_{mn} \, ,$$

and using the $\boldsymbol{T}$-matrix equation, yields

$$\begin{bmatrix} c_{mn} \\ d_{mn} \end{bmatrix} = \mathcal{S} \begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix} = (\boldsymbol{I} + 2\boldsymbol{T}) \begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix} \, .$$

The coefficients a_{mn} and b_{mn} are determined by the incoming field. Since in the far-field region $\boldsymbol{M}_{mn}^2$ and $\boldsymbol{N}_{mn}^2$ become incoming vector spherical waves, we see that the $\mathcal{S}$ matrix determines how an incoming vector spherical wave is scattered into the same one.

In the far-field region, the total electric field

$$\boldsymbol{E} = \frac{1}{2} \sum_{n,m} c_{mn} \boldsymbol{M}_{mn}^3 + d_{mn} \boldsymbol{N}_{mn}^3 + \frac{1}{2} \sum_{n,m} a_{mn} \boldsymbol{M}_{mn}^2 + b_{mn} \boldsymbol{N}_{mn}^2$$

can be expressed as a superposition of outgoing and incoming transverse spherical waves

$$\boldsymbol{E}(\boldsymbol{r}) = \frac{\mathrm{e}^{\mathrm{j}k_\mathrm{s}r}}{r} \left\{ \boldsymbol{E}_\infty^{(1)}(\boldsymbol{e}_r) + \mathrm{O}\left(\frac{1}{r}\right) \right\} + \frac{\mathrm{e}^{-\mathrm{j}k_\mathrm{s}r}}{r} \left\{ \boldsymbol{E}_\infty^{(2)}(\boldsymbol{e}_r) + \mathrm{O}\left(\frac{1}{r}\right) \right\} \, ,$$

$$r \to \infty \tag{1.106}$$

with

$$\boldsymbol{E}_\infty^{(1)}(\boldsymbol{e}_r) = \frac{1}{2k_\mathrm{s}} \sum_{n,m} (-\mathrm{j})^{n+1} \left[c_{mn} \boldsymbol{m}_{mn}(\boldsymbol{e}_r) + \mathrm{j}d_{mn} \boldsymbol{n}_{mn}(\boldsymbol{e}_r) \right] \, ,$$

$$\boldsymbol{E}_\infty^{(2)}(\boldsymbol{e}_r) = \frac{1}{2k_\mathrm{s}} \sum_{n,m} \mathrm{j}^{n+1} \left[a_{mn} \boldsymbol{m}_{mn}(\boldsymbol{e}_r) - \mathrm{j}b_{mn} \boldsymbol{n}_{mn}(\boldsymbol{e}_r) \right] \, .$$

For the total magnetic field we proceed analogously and obtain

$$\boldsymbol{H}(\boldsymbol{r}) = \frac{\mathrm{e}^{\mathrm{j}k_\mathrm{s}r}}{r} \left\{ \boldsymbol{H}_\infty^{(1)}(\boldsymbol{e}_r) + \mathrm{O}\left(\frac{1}{r}\right) \right\} + \frac{\mathrm{e}^{-\mathrm{j}k_\mathrm{s}r}}{r} \left\{ \boldsymbol{H}_\infty^{(2)}(\boldsymbol{e}_r) + \mathrm{O}\left(\frac{1}{r}\right) \right\}$$

$$r \to \infty$$

with

$$\boldsymbol{H}_\infty^{(1)} = \sqrt{\frac{\varepsilon_\mathrm{s}}{\mu_\mathrm{s}}} \boldsymbol{e}_r \times \boldsymbol{E}_\infty^{(1)} \, ,$$

$$\boldsymbol{H}_\infty^{(2)} = -\sqrt{\frac{\varepsilon_\mathrm{s}}{\mu_\mathrm{s}}} \boldsymbol{e}_r \times \boldsymbol{E}_\infty^{(2)} \, .$$

Thus

$$\text{Re}\left\{\boldsymbol{e}_r \cdot (\boldsymbol{E} \times \boldsymbol{H}^*)\right\} = \frac{1}{r^2}\sqrt{\frac{\varepsilon_\text{s}}{\mu_\text{s}}}\left\{\left|\boldsymbol{E}_\infty^{(1)}\right|^2 - \left|\boldsymbol{E}_\infty^{(2)}\right|^2 + \text{O}\left(\frac{1}{r}\right)\right\}, \quad r \to \infty$$

and (1.105) yields

$$\int_\Omega \left(\left|\boldsymbol{E}_\infty^{(1)}\right|^2 - \left|\boldsymbol{E}_\infty^{(2)}\right|^2\right)\text{d}\Omega = 0. \tag{1.107}$$

The orthogonality relations of the vector spherical harmonics on the unit sphere give

$$\int_\Omega \left|\boldsymbol{E}_\infty^{(1)}\right|^2 \text{d}\Omega = \frac{\pi}{4k_\text{s}^2}[a_{mn}^*, b_{mn}^*]\,\mathcal{S}^\dagger\mathcal{S}\begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix},$$

$$\int_\Omega \left|\boldsymbol{E}_\infty^{(2)}\right|^2 \text{d}\Omega = \frac{\pi}{4k_\text{s}^2}[a_{mn}^*, b_{mn}^*]\begin{bmatrix} a_{mn} \\ b_{mn} \end{bmatrix} \tag{1.108}$$

and since the incident field is arbitrarily, (1.107) and (1.108) implies that [217, 228, 256]

$$\mathcal{S}^\dagger\mathcal{S} = \boldsymbol{I}. \tag{1.109}$$

The above relation is the unitary condition for nonabsorbing particles. In terms of the transition matrix, this condition is

$$\boldsymbol{T}^\dagger\boldsymbol{T} = -\frac{1}{2}\left(\boldsymbol{T} + \boldsymbol{T}^\dagger\right),$$

or explicitly

$$\sum_{k=1}^{2}\sum_{n'=1}^{\infty}\sum_{m'=-n'}^{n'} T_{m'n',mn}^{ki*}T_{m'n',m_1n_1}^{kj} = -\frac{1}{2}\left(T_{m_1n_1,mn}^{ji*} + T_{mn,m_1n_1}^{ij}\right). \tag{1.110}$$

For absorbing particles, the integral in (1.107) is negative. Consequently, the equality in (1.110) transforms into an inequality which is equivalent to the contractivity of the $\mathcal{S}$ matrix [169]. Taking the trace of (1.110), Mishchenko et al. [169] derived an equality (inequality) between the $\boldsymbol{T}$-matrix elements of an axisymmetric particle provided that the z-axis of the particle coordinate system is directed along the axis of symmetry.

To obtain the symmetry relation we proceed as in the derivation of the reciprocity relation for the tensor scattering amplitude, i.e., we consider the electromagnetic fields $\boldsymbol{E}_u$, $\boldsymbol{H}_u$ generated by the incident fields $\boldsymbol{E}_{\text{e}u}$, $\boldsymbol{H}_{\text{e}u}$, with $u = 1, 2$. The starting point is the integral (cf. (1.90))

$$\int_{S_\text{c}} \boldsymbol{e}_r \cdot (\boldsymbol{E}_2 \times \boldsymbol{H}_1 - \boldsymbol{E}_1 \times \boldsymbol{H}_2)\,\text{d}S = 0$$

over a spherical surface S_c situated in the far-field region. Then, using the asymptotic form (cf. (1.106))

$$\boldsymbol{E}_u(\boldsymbol{r}) = \frac{\mathrm{e}^{\mathrm{j}k_\mathrm{s}r}}{r} \left\{ \boldsymbol{E}_{u\infty}^{(1)}(\boldsymbol{e}_r) + \mathrm{O}\left(\frac{1}{r}\right) \right\} + \frac{\mathrm{e}^{-\mathrm{j}k_\mathrm{s}r}}{r} \left\{ \boldsymbol{E}_{u\infty}^{(2)}(\boldsymbol{e}_r) + \mathrm{O}\left(\frac{1}{r}\right) \right\},$$

$$r \to \infty$$

for $u = 1, 2$, we obtain

$$\int_\Omega \left(\boldsymbol{e}_r \times \boldsymbol{E}_{2\infty}^{(1)} \right) \cdot \left(\boldsymbol{e}_r \times \boldsymbol{E}_{1\infty}^{(2)} \right) \mathrm{d}\Omega = \int_\Omega \left(\boldsymbol{e}_r \times \boldsymbol{E}_{1\infty}^{(1)} \right) \cdot \left(\boldsymbol{e}_r \times \boldsymbol{E}_{2\infty}^{(2)} \right) \mathrm{d}\Omega.$$
(1.111)

Taking into account the vector spherical harmonic expansions of the far-field patterns $\boldsymbol{E}_{u\infty}^{(1)}$ and $\boldsymbol{E}_{u\infty}^{(2)}$, $u = 1, 2$, and the relations $\boldsymbol{e}_r \times \boldsymbol{m}_{mn} = \boldsymbol{n}_{mn}$ and $\boldsymbol{e}_r \times \boldsymbol{n}_{mn} = -\boldsymbol{m}_{mn}$, we see that

$$\int_\Omega \left(\boldsymbol{e}_r \times \boldsymbol{E}_{2\infty}^{(1)} \right) \cdot \left(\boldsymbol{e}_r \times \boldsymbol{E}_{1\infty}^{(2)} \right) \mathrm{d}\Omega = \frac{\pi}{4k_\mathrm{s}^2} \left[a_{1,m_1n_1}, b_{1,m_1n_1} \right] \begin{bmatrix} c_{2,-m_1n_1} \\ d_{2,-m_1n_1} \end{bmatrix},$$

$$\int_\Omega \left(\boldsymbol{e}_r \times \boldsymbol{E}_{1\infty}^{(1)} \right) \cdot \left(\boldsymbol{e}_r \times \boldsymbol{E}_{2\infty}^{(2)} \right) \mathrm{d}\Omega = \frac{\pi}{4k_\mathrm{s}^2} \left[c_{1,mn}, d_{1,mn} \right] \begin{bmatrix} a_{2,-mn} \\ b_{2,-mn} \end{bmatrix},$$

where $a_{u,mn}$, $b_{u,mn}$ are the expansion coefficients of the far-field pattern $\boldsymbol{E}_{u\infty}^{(2)}$, while $c_{u,mn}$, $d_{u,mn}$ are the expansion coefficients of the far-field pattern $\boldsymbol{E}_{u\infty}^{(1)}$. Consequently, (1.111) can be written in matrix form as

$$\left[a_{1,m_1n_1}, b_{1,m_1n_1} \right] \begin{bmatrix} \mathcal{S}_{-m_1n_1,-mn}^{11} & \mathcal{S}_{-m_1n_1,-mn}^{12} \\ \mathcal{S}_{-m_1n_1,-mn}^{21} & \mathcal{S}_{-m_1n_1,-mn}^{22} \end{bmatrix} \begin{bmatrix} a_{2,-mn} \\ b_{2,-mn} \end{bmatrix}$$

$$= \left[a_{1,m_1n_1}, b_{1,m_1n_1} \right] \begin{bmatrix} \mathcal{S}_{mn,m_1n_1}^{11} & \mathcal{S}_{mn,m_1n_1}^{21} \\ \mathcal{S}_{mn,m_1n_1}^{12} & \mathcal{S}_{mn,m_1n_1}^{22} \end{bmatrix} \begin{bmatrix} a_{2,-mn} \\ b_{2,mn} \end{bmatrix}$$

and since the above equation holds true for any incident field, we find that

$$\mathcal{S}_{mn,m_1n_1}^{ij} = \mathcal{S}_{-m_1n_1,-mn}^{ji}$$

and further that

$$T_{mn,m_1n_1}^{ij} = T_{-m_1n_1,-mn}^{ji} \tag{1.112}$$

for $i, j = 1, 2$. This relation reflects the symmetry property of the transition matrix and is of basic importance in practical computer calculations. We note that the symmetry relation (1.112) can be obtained directly from the reciprocity relation for the tensor scattering amplitude

$$\overline{\boldsymbol{A}}\left(\theta_1, \varphi_1; \theta_2, \varphi_2\right) = \overline{\boldsymbol{A}}^\mathrm{T}\left(\pi - \theta_2, \pi + \varphi_2; \pi - \theta_1, \pi + \varphi_1\right)$$

and the identities

$$\boldsymbol{m}_{mn}\left(\pi-\theta,\pi+\varphi\right)=(-1)^{n}\boldsymbol{m}_{mn}\left(\theta,\varphi\right)\ ,$$

$$\boldsymbol{n}_{mn}\left(\pi-\theta,\pi+\varphi\right)=(-1)^{n+1}\boldsymbol{n}_{mn}\left(\theta,\varphi\right)\ ,$$

and

$$\boldsymbol{m}_{-mn}\left(\theta,\varphi\right)=\boldsymbol{m}_{mn}^{*}\left(\theta,\varphi\right)\ ,$$

$$\boldsymbol{n}_{-mn}\left(\theta,\varphi\right)=\boldsymbol{n}_{mn}^{*}\left(\theta,\varphi\right)\ .$$

Additional properties of the transition matrix for particles with specific symmetries will be discussed in the next chapter. The "exact" infinite transition matrix satisfies the unitarity and symmetry conditions (1.110) and (1.112), respectively. However, in practical computer calculations, the truncated transition matrix may not satisfies these conditions and we can test the unitarity and symmetry conditions to get a rough idea regarding the convergence to be expected in the solution computation.

Remark. In the above analysis, the incident field is a vector plane wave whose source is situated at infinity. Other incident fields than vector plane waves can be considered, but we shall assume that the source of the incident field lies outside the circumscribing sphere S_{c}. In this case, the incident field is regular everywhere inside the circumscribing sphere, and both expansions (1.93) and (1.94) are valid on S_{c}. The $\boldsymbol{T}$-matrix equation holds true at finite distances from the particle (not only in the far-field region), and therefore, the transition matrix is also known as the "nonasymptotic vector-spherical-wave transition matrix". The properties of the transition matrix (unitarity and symmetry) can also be established by considering the energy flow through a finite sphere S_{c} [238]. If we now let the source of the incident field recede to infinity, we can let the surface S_{c} follow, i.e., we can consider the case of an arbitrary large sphere and this brings us to the precedent analysis.

1.5.3 Randomly Oriented Particles

In the following analysis we consider scattering by an ensemble of randomly oriented, identical particles. Random particle orientation means that the orientation distribution of the particles is uniform. As a consequence of random particle orientation, the scattering medium is macroscopically isotropic, i.e., the scattering characteristics are independent of the incident and scattering directions $\boldsymbol{e}_{k}$ and $\boldsymbol{e}_{r}$, and depend only on the angle between the unit vectors $\boldsymbol{e}_{k}$ and $\boldsymbol{e}_{r}$. For this type of scattering problem, it is convenient to direct the Z-axis of the global coordinate system along the incident direction and to choose the XZ-plane as the scattering plane (Fig. 1.13).
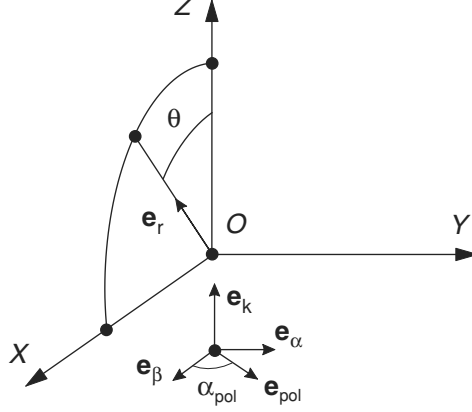
Fig. 1.13. The Z-axis of the global coordinate system is along the incident direction and the XZ-plane is the scattering plane

General Considerations

The phase matrix of a volume element containing randomly oriented particles can be written as

$$\boldsymbol{Z}\left(\boldsymbol{e}_r, \boldsymbol{e}_k\right) = \boldsymbol{Z}\left(\theta, \varphi = 0, \beta = 0, \alpha = 0\right),$$

where, in general, θ and φ are the polar angles of the scattering direction $\boldsymbol{e}_r$, and β and α are the polar angles of the incident direction $\boldsymbol{e}_k$. The phase matrix $\boldsymbol{Z}(\theta, 0, 0, 0)$ is known as the scattering matrix $\boldsymbol{F}$ and relates the Stokes parameters of the incident and scattered fields defined with respect to the scattering plane. Taking into account that for an incident direction (β, α), the backscattering direction is $(\pi - \beta, \alpha + \pi)$, the complete definition of the scattering matrix is [169]

$$\boldsymbol{F}(\theta) = \begin{cases} \boldsymbol{Z}(\theta, 0, 0, 0), & \theta \in [0, \pi), \\ \boldsymbol{Z}\left(\pi, \pi, 0, 0\right), & \theta = \pi. \end{cases}$$

The scattering matrix of a volume element containing randomly oriented particles has the following structure:

$$\boldsymbol{F}(\theta) = \begin{bmatrix} F_{11}(\theta) & F_{12}(\theta) & F_{13}(\theta) & F_{14}(\theta) \\ F_{12}(\theta) & F_{22}(\theta) & F_{23}(\theta) & F_{24}(\theta) \\ -F_{13}(\theta) & -F_{23}(\theta) & F_{33}(\theta) & F_{34}(\theta) \\ F_{14}(\theta) & F_{24}(\theta) & -F_{34}(\theta) & F_{44}(\theta) \end{bmatrix}. \tag{1.113}$$

If each particle has a plane of symmetry or, equivalently, the particles and their mirror-symmetric particles are present in equal numbers, the scattering

medium is called macroscopically isotropic and mirror-symmetric. Note that rotationally symmetric particles are obviously mirror-symmetric with respect to the plane through the axis of symmetry. Because of symmetry, the scattering matrix of a macroscopically isotropic and mirror-symmetric scattering medium has the following block-diagonal structure [103, 169]:

$$
\boldsymbol{F}(\theta) = \begin{bmatrix} F_{11}(\theta) & F_{12}(\theta) & 0 & 0 \\ F_{12}(\theta) & F_{22}(\theta) & 0 & 0 \\ 0 & 0 & F_{33}(\theta) & F_{34}(\theta) \\ 0 & 0 & -F_{34}(\theta) & F_{44}(\theta) \end{bmatrix} . \tag{1.114}
$$

The phase matrix can be related to the scattering matrix by using the rotation transformation rule (1.22), and this procedure involves two rotations as shown in Fig. 1.14. Taking into account that the scattering matrix relates the Stokes vectors of the incident and scattered fields specified relative to the scattering plane, $\boldsymbol{I}'_{\mathrm{s}} = (1/r^2)\boldsymbol{F}(\Theta)\boldsymbol{I}'_{\mathrm{e}}$, and using the transformation rule of the Stokes vectors under coordinate rotations $\boldsymbol{I}'_{\mathrm{e}} = \boldsymbol{L}(\sigma_1)\boldsymbol{I}_{\mathrm{e}}$ and $\boldsymbol{I}_{\mathrm{s}} = \boldsymbol{L}(-\sigma_2)\boldsymbol{I}'_{\mathrm{s}}$, we obtain

$$
\boldsymbol{Z}\left(\theta, \varphi, \beta, \alpha\right) = \boldsymbol{L}\left(-\sigma_2\right) \boldsymbol{F}\left(\Theta\right) \boldsymbol{L}\left(\sigma_1\right) ,
$$

where

$$
\cos\Theta = \boldsymbol{e}_k \cdot \boldsymbol{e}_r = \cos\beta\cos\theta + \sin\beta\sin\theta\cos\left(\varphi - \alpha\right) ,
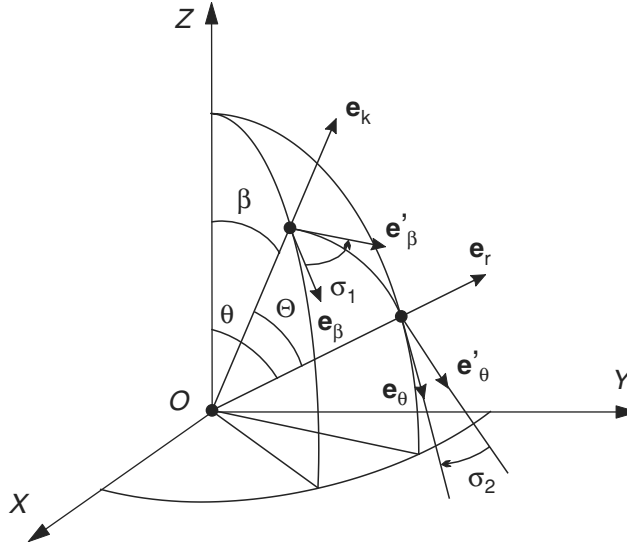$$

Fig. 1.14. Incident and scattering directions $\boldsymbol{e}_k$ and $\boldsymbol{e}_r$. The scattering matrix relates the Stokes vectors of the incident and scattered fields specified relative to the scattering plane

$$\cos \sigma_1 = \boldsymbol{e}'_\alpha \cdot \boldsymbol{e}_\alpha = -\frac{\sin \beta \cos \theta - \cos \beta \sin \theta \cos (\varphi - \alpha)}{\sin \Theta} \,,$$

$$\cos \sigma_2 = \boldsymbol{e}'_\varphi \cdot \boldsymbol{e}_\varphi = \frac{\cos \beta \sin \theta - \sin \beta \cos \theta \cos (\varphi - \alpha)}{\sin \Theta} \,.$$

For an ensemble of randomly positioned particles, the waves scattered by different particles are random in phase, and the Stokes parameters of these incoherent waves add up. Therefore, the scattering matrix for the ensemble is the sum of the scattering matrices of the individual particles:

$$\boldsymbol{F} = N \langle \boldsymbol{F} \rangle \,,$$

where N is number of particles and $\langle \boldsymbol{F} \rangle$ denotes the ensemble-average scattering matrix per particle. Similar relations hold for the extinction matrix and optical cross-sections. Because the particles are identical, the ensemble-average of a scattering quantity X is the orientation-averaged quantity

$$\langle X \rangle = \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} X \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) \sin\beta_{\mathrm{p}} \, \mathrm{d}\beta_{\mathrm{p}} \, \mathrm{d}\alpha_{\mathrm{p}} \, \mathrm{d}\gamma_{\mathrm{p}} \,,$$

where α_{p}, β_{p} and γ_{p} are the particle orientation angles.

In the following analysis, the $\boldsymbol{T}$ matrix formulation is used to derive efficient analytical techniques for computing $\langle X \rangle$. These methods work much faster than the standard approaches based on the numerical averaging of results computed for many discrete orientations of the particle. We begin with the derivation of the rotation transformation rule for the transition matrix and then compute the orientation-averaged transition matrix, optical cross-sections and extinction matrix. An analytical procedure for computing the orientation-averaged scattering matrix will conclude our analysis.

Rotation Transformation of the Transition Matrix

To derive the rotation transformation rule for the transition matrix we assume that the orientation of the particle coordinate system $Oxyz$ with respect to the global coordinate system $OXYZ$ is specified by the Euler angles α_{p}, β_{p} and γ_{p}.

In the particle coordinate system, the expansions of the incident and scattered field are given by

$$\boldsymbol{E}_{\mathrm{e}} \left(r, \theta, \varphi \right) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} a_{mn} \boldsymbol{M}_{mn}^1 \left(k_{\mathrm{s}} r, \theta, \varphi \right) + b_{mn} \boldsymbol{N}_{mn}^1 \left(k_{\mathrm{s}} r, \theta, \varphi \right) \,,$$

$$\boldsymbol{E}_{\mathrm{s}} \left(r, \theta, \varphi \right) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} f_{mn} \boldsymbol{M}_{mn}^3 \left(k_{\mathrm{s}} r, \theta, \varphi \right) + g_{mn} \boldsymbol{N}_{mn}^3 \left(k_{\mathrm{s}} r, \theta, \varphi \right) \,,$$

while in the global coordinate system, these expansions take the form

$$\boldsymbol{E}_{\mathrm{e}}\left(r, \Phi, \Psi\right) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \widetilde{a}_{mn} \boldsymbol{M}_{mn}^{1}\left(k_{\mathrm{s}}r, \Phi, \Psi\right) + \widetilde{b}_{mn} \boldsymbol{N}_{mn}^{1}\left(k_{\mathrm{s}}r, \Phi, \Psi\right),$$

$$\boldsymbol{E}_{\mathrm{s}}\left(r, \Phi, \Psi\right) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \widetilde{f}_{mn} \boldsymbol{M}_{mn}^{3}\left(r, \Phi, \Psi\right) + \widetilde{g}_{mn} \boldsymbol{N}_{mn}^{3}\left(k_{\mathrm{s}}r, \Phi, \Psi\right).$$

Assuming the $\boldsymbol{T}$-matrix equations $\boldsymbol{s} = \boldsymbol{T}\boldsymbol{e}$ and $\widetilde{\boldsymbol{s}} = \widetilde{\boldsymbol{T}}\widetilde{\boldsymbol{e}}$, our task is to express the transition matrix in the global coordinate system $\widetilde{\boldsymbol{T}}$ in terms of the transition matrix in the particle coordinate system $\boldsymbol{T}$. Defining the "augmented" vectors of spherical wave functions in each coordinate system

$$\boldsymbol{w}_{1,3}\left(k_{\mathrm{s}}r, \theta, \varphi\right) = \begin{bmatrix} \boldsymbol{M}_{mn}^{1,3}\left(k_{\mathrm{s}}r, \theta, \varphi\right) \\ \boldsymbol{N}_{mn}^{1,3}\left(k_{\mathrm{s}}r, \theta, \varphi\right) \end{bmatrix}$$

and

$$\widetilde{\boldsymbol{w}}_{1,3}\left(k_{\mathrm{s}}r, \Phi, \Psi\right) = \begin{bmatrix} \boldsymbol{M}_{mn}^{1,3}\left(k_{\mathrm{s}}r, \Phi, \Psi\right) \\ \boldsymbol{N}_{mn}^{1,3}\left(k_{\mathrm{s}}r, \Phi, \Psi\right) \end{bmatrix},$$

and using the rotation addition theorem for vector spherical wave functions, we obtain

$$\boldsymbol{E}_{\mathrm{e}} = \boldsymbol{e}^{\mathrm{T}}\boldsymbol{w}_{1} = \widetilde{\boldsymbol{e}}^{\mathrm{T}}\widetilde{\boldsymbol{w}}_{1} = \widetilde{\boldsymbol{e}}^{\mathrm{T}}\mathcal{R}\left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}}\right)\boldsymbol{w}_{1},$$

$$\boldsymbol{E}_{\mathrm{s}} = \widetilde{\boldsymbol{s}}^{\mathrm{T}}\widetilde{\boldsymbol{w}}_{3} = \boldsymbol{s}^{\mathrm{T}}\boldsymbol{w}_{3} = \boldsymbol{s}^{\mathrm{T}}\mathcal{R}\left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}}\right)\widetilde{\boldsymbol{w}}_{3}.$$

Consequently

$$\boldsymbol{e} = \mathcal{R}^{\mathrm{T}}\left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}}\right)\widetilde{\boldsymbol{e}},$$

$$\widetilde{\boldsymbol{s}} = \mathcal{R}^{\mathrm{T}}\left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}}\right)\boldsymbol{s},$$

and therefore,

$$\widetilde{\boldsymbol{T}}\left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}}\right) = \mathcal{R}^{\mathrm{T}}\left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}}\right)\boldsymbol{T}\mathcal{R}^{\mathrm{T}}\left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}}\right). \tag{1.115}$$

The explicit expression of the matrix elements is [169, 228, 233]

$$\widetilde{T}_{mn,m_1 n_1}^{ij}\left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}}\right) = \sum_{m'=-n}^{n} \sum_{m_1'=-n_1}^{n_1} D_{m'm}^{n}\left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}}\right) T_{m'n,m_1' n_1}^{ij}$$

$$\times D_{m_1 m_1'}^{n_1}\left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}}\right) \tag{1.116}$$

for $i, j = 1, 2$.

Because the elements of the amplitude matrix can be expressed in terms of the elements of the transition matrix, the above relation can be used to express the elements of the amplitude matrix as functions of the particle orientation angles α_{p}, β_{p} and γ_{p}. The properties of the Wigner D-functions can then be used to compute the integrals over the particle orientation angles.

Orientation-Averaged Transition Matrix

The elements of the orientation-averaged transition matrix with respect to the global coordinate system are given by

$$\left\langle \widetilde{T}^{ij}_{mn,m_1 n_1} \right\rangle = \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} \widetilde{T}^{ij}_{mn,m_1 n_1} (\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}}) \sin\beta_{\mathrm{p}} \, \mathrm{d}\beta_{\mathrm{p}} \, \mathrm{d}\alpha_{\mathrm{p}} \, \mathrm{d}\gamma_{\mathrm{p}}$$

$$= \frac{1}{8\pi^2} \sum_{m'=-n}^{n} \sum_{m'_1=-n_1}^{n_1} T^{ij}_{m'n,m'_1 n_1} \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} D^n_{m'm} (-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}})$$

$$\times D^{n_1}_{m_1 m'_1} (\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}}) \sin\beta_{\mathrm{p}} \, \mathrm{d}\beta_{\mathrm{p}} \, \mathrm{d}\alpha_{\mathrm{p}} \, \mathrm{d}\gamma_{\mathrm{p}} \,. \tag{1.117}$$

Using the definition of the Wigner D-functions (cf. (B.34)), the symmetry relation of the Wigner d-functions $d^n_{m'm}(-\beta_{\mathrm{p}}) = d^n_{mm'}(\beta_{\mathrm{p}})$, and integrating over α_{p} and γ_{p}, yields

$$\left\langle \widetilde{T}^{ij}_{mn,m_1 n_1} \right\rangle = \frac{1}{2} \sum_{m'=-n}^{n} \sum_{m'_1=-n_1}^{n_1} \Delta_{m'm} \Delta_{m_1 m'_1} \delta_{m'm'_1} \delta_{mm_1}$$

$$\times T^{ij}_{m'n,m'_1 n_1} \int_0^{\pi} d^n_{mm'} (\beta_{\mathrm{p}}) \, d^{n_1}_{m_1 m'_1} (\beta_{\mathrm{p}}) \sin\beta_{\mathrm{p}} \, \mathrm{d}\beta_{\mathrm{p}} \,,$$

where $\Delta_{mm'}$ is given by (B.36). Taking into account the identities: $\Delta_{m'm} = \Delta_{mm'}$ and $(\Delta_{mm'})^2 = 1$, and using the orthogonality property of the d-functions (cf. (B.43)), we obtain [168, 169]

$$\left\langle \widetilde{T}^{ij}_{mn,m_1 n_1} \right\rangle = \delta_{mm_1} \delta_{nn_1} t^{ij}_n \tag{1.118}$$

with

$$t^{ij}_n = \frac{1}{2n+1} \sum_{m'=-n}^{n} T^{ij}_{m'n,m'n} \,. \tag{1.119}$$

The above relation provides a simple analytical expression for the orientation-averaged transition matrix in terms of the transition matrix in the particle coordinate system. The orientation-averaged $\langle \boldsymbol{T}^{ij} \rangle$ matrices are diagonal and their elements do not depend on the azimuthal indices m and m_1.

Orientation-Averaged Extinction and Scattering Cross-Sections

In view of the optical theorem, the orientation-averaged extinction cross-section is (cf. (1.88) with $|\boldsymbol{E}_{\mathrm{e}0}| = 1$)

$$\langle C_{\mathrm{ext}} \rangle = \frac{4\pi}{k_{\mathrm{s}}} \mathrm{Im} \left\{ \left\langle \boldsymbol{e}^*_{\mathrm{pol}} \cdot \boldsymbol{E}_{\mathrm{s}\infty} (\boldsymbol{e}_z) \right\rangle \right\} \,.$$

Considering the expansion of the far-field pattern in the global coordinate system (cf. (1.96)), taking the average and using the expression of the orientation-averaged transition matrix (cf. (1.118) and (1.119)), gives

$$
\left\langle \boldsymbol{e}_{\mathrm{pol}}^* \cdot \boldsymbol{E}_{\mathrm{s}\infty} \left(\boldsymbol{e}_z\right) \right\rangle = \frac{1}{k_{\mathrm{s}}} \sum_{n,m} (-\mathrm{j})^{n+1} \left[\left(t_n^{11} \widetilde{a}_{mn} + t_n^{12} \widetilde{b}_{mn} \right) \boldsymbol{e}_{\mathrm{pol}}^* \cdot \boldsymbol{m}_{mn} \left(\boldsymbol{e}_z\right) \right.
$$

$$
\left. + \mathrm{j} \left(t_n^{21} \widetilde{a}_{mn} + t_n^{22} \widetilde{b}_{mn} \right) \boldsymbol{e}_{\mathrm{pol}}^* \cdot \boldsymbol{n}_{mn} \left(\boldsymbol{e}_z\right) \right] ,
$$

where the summation over the index m involves the values -1 and 1. In the next chapter we will show that for axisymmetric particles, $T_{-mn,-mn}^{ij} = -T_{mn,mn}^{ij}$ and $T_{0n,0n}^{ij} = 0$ for $i \neq j$, while for particles with a plane of symmetry, $T_{mn,mn}^{ij} = 0$ for $i \neq j$. Thus, for macroscopically isotropic and mirror-symmetric media, (1.119) gives $t_n^{12} = t_n^{21} = 0$. Further, using the expressions of the incident field coefficients (cf. (1.26))

$$
\begin{aligned}
\widetilde{a}_{mn} &= 4j^n \boldsymbol{e}_{\mathrm{pol}} \cdot \boldsymbol{m}_{mn}^* \left(\boldsymbol{e}_z\right) , \\
\widetilde{b}_{mn} &= -4j^{n+1} \boldsymbol{e}_{\mathrm{pol}} \cdot \boldsymbol{n}_{mn}^* \left(\boldsymbol{e}_z\right) ,
\end{aligned}
\tag{1.120}
$$

and the special values of the vector spherical harmonics in the forward direction

$$
\begin{aligned}
\boldsymbol{m}_{mn} \left(\boldsymbol{e}_z\right) &= \frac{\sqrt{2n+1}}{4} \left(\mathrm{j}m\boldsymbol{e}_x - \boldsymbol{e}_y\right) , \\
\boldsymbol{n}_{mn} \left(\boldsymbol{e}_z\right) &= \frac{\sqrt{2n+1}}{4} \left(\boldsymbol{e}_x + \mathrm{j}m\boldsymbol{e}_y\right) ,
\end{aligned}
\tag{1.121}
$$

we obtain [163]

$$
\begin{aligned}
\left\langle C_{\mathrm{ext}} \right\rangle &= -\frac{2\pi}{k_{\mathrm{s}}^2} \mathrm{Re} \left\{ \sum_{n=1}^{\infty} (2n+1) \left(t_n^{11} + t_n^{22} \right) \right\} , \\
&= -\frac{2\pi}{k_{\mathrm{s}}^2} \mathrm{Re} \left\{ \sum_{n=1}^{\infty} \sum_{m=-n}^{n} T_{mn,mn}^{11} + T_{mn,mn}^{22} \right\} .
\end{aligned}
\tag{1.122}
$$

The above relation shows that the orientation-averaged extinction cross-section for macroscopically isotropic and mirror-symmetric media is determined by the diagonal elements of the transition matrix in the particle coordinate system. The same result can be established if we consider an ensemble of randomly oriented particles (with $t_n^{12} \neq 0$ and $t_n^{21} \neq 0$) illuminated by a linearly polarized plane wave (with real polarization vector $\boldsymbol{e}_{\mathrm{pol}}$).

For an arbitrary excitation, the scattering cross-section can be expressed in the global coordinate system as

$$
C_{\mathrm{scat}} = \frac{\pi}{k_{\mathrm{s}}^2} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left| \widetilde{f}_{mn} \right|^2 + \left| \widetilde{g}_{mn} \right|^2 = \frac{\pi}{k_s^2} \widetilde{\boldsymbol{s}}^\dagger \widetilde{\boldsymbol{s}} ,
$$

whence, using the $\boldsymbol{T}$-matrix equation $\widetilde{\boldsymbol{s}} = \widetilde{\boldsymbol{T}}\widetilde{\boldsymbol{e}}$, we obtain

$$\langle C_{\mathrm{scat}} \rangle = \frac{\pi}{k_{\mathrm{s}}^2} \widetilde{\boldsymbol{e}}^\dagger \left\langle \widetilde{\boldsymbol{T}}^\dagger \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) \widetilde{\boldsymbol{T}} \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) \right\rangle \widetilde{\boldsymbol{e}} \, .$$

Since

$$\widetilde{\boldsymbol{T}} \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) = \mathcal{R}^{\mathrm{T}} \left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}} \right) \boldsymbol{T} \mathcal{R}^{\mathrm{T}} \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) \, ,$$

$$\widetilde{\boldsymbol{T}}^\dagger \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) = \mathcal{R}^* \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) \boldsymbol{T}^\dagger \mathcal{R}^* \left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}} \right) \, ,$$

and in view of (B.54) and (B.55),

$$\mathcal{R}^* \left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}} \right) = \left(\mathcal{R}^{\mathrm{T}} \left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}} \right) \right)^{-1} \, ,$$

$$\mathcal{R}^* \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) = \mathcal{R}^{\mathrm{T}} \left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}} \right) \, ,$$

we see that

$$\widetilde{\boldsymbol{T}}^\dagger \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) \widetilde{\boldsymbol{T}} \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) = \mathcal{R}^{\mathrm{T}} \left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}} \right) \boldsymbol{T}^\dagger \boldsymbol{T} \mathcal{R}^{\mathrm{T}} \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}} \right) \, .$$

The above equation is similar to (1.115), and taking the average, we obtain

$$\left\langle \left(\boldsymbol{T}^\dagger \boldsymbol{T} \right)^{ij}_{mn,m_1 n_1} \right\rangle = \delta_{mm_1} \delta_{nn_1} \widetilde{t}_n^{ij} \, ,$$

where

$$\widetilde{t}_n^{ij} = \frac{1}{2n+1} \sum_{m'=-n}^{n} \left(\boldsymbol{T}^\dagger \boldsymbol{T} \right)^{ij}_{m'n,m'n}$$

or explicitly,

$$\widetilde{t}_n^{11} = \frac{1}{2n+1} \sum_{m'=-n}^{n} \sum_{n_1=1}^{\infty} \sum_{m_1=-n_1}^{n_1} \left| T_{m_1 n_1, m'n}^{11} \right|^2 + \left| T_{m_1 n_1, m'n}^{21} \right|^2 \, ,$$

$$\widetilde{t}_n^{12} = \frac{1}{2n+1} \sum_{m'=-n}^{n} \sum_{n_1=1}^{\infty} \sum_{m_1=-n_1}^{n_1} T_{m_1 n_1, m'n}^{11*} T_{m_1 n_1, m'n}^{12}$$

$$+ T_{m_1 n_1, m'n}^{21*} T_{m_1 n_1, m'n}^{22} \, ,$$

$$\widetilde{t}_n^{21} = \widetilde{t}_n^{12*} \, ,$$

$$\widetilde{t}_n^{22} = \frac{1}{2n+1} \sum_{m'=-n}^{n} \sum_{n_1=1}^{\infty} \sum_{m_1=-n_1}^{n_1} \left| T_{m_1 n_1, m'n}^{12} \right|^2 + \left| T_{m_1 n_1, m'n}^{22} \right|^2 \, .$$

The orientation-averaged scattering cross-section then becomes

$$\langle C_{\mathrm{scat}}\rangle = \frac{\pi}{k_{\mathrm{s}}^2}\sum_{n,m}\widetilde{t}_n^{11}\left|\widetilde{a}_{mn}\right|^2 + \widetilde{t}_n^{12}\widetilde{a}_{mn}^*\widetilde{b}_{mn}$$

$$+\widetilde{t}_n^{21}\widetilde{a}_{mn}\widetilde{b}_{mn}^* + \widetilde{t}_n^{22}\left|\widetilde{b}_{mn}\right|^2 , \qquad (1.123)$$

where as before, the summation over the index m involves the values -1 and 1. For macroscopically isotropic and mirror-symmetric media, $\widetilde{t}_n^{12} = \widetilde{t}_n^{21} = 0$, and using (1.120) and (1.121), we obtain [120, 162]

$$\langle C_{\mathrm{scat}}\rangle = \frac{2\pi}{k_{\mathrm{s}}^2}\sum_{n=1}^{\infty}(2n+1)\left(\widetilde{t}_n^{11} + \widetilde{t}_n^{22}\right)$$

$$= \frac{2\pi}{k_{\mathrm{s}}^2}\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\sum_{n_1=1}^{\infty}\sum_{m_1=-n_1}^{n_1}\left|T_{m_1 n_1, mn}^{11}\right|^2 + \left|T_{m_1 n_1, mn}^{12}\right|^2$$

$$+\left|T_{m_1 n_1, mn}^{21}\right|^2 + \left|T_{m_1 n_1, mn}^{22}\right|^2 . \qquad (1.124)$$

Thus, the orientation-averaged scattering cross-section for macroscopically isotropic and mirror-symmetric media is proportional to the sum of the squares of the absolute values of the transition matrix in the particle coordinate system. The same result holds true for an ensemble of randomly oriented particles illuminated by a linearly polarized plane wave.

Despite the derivation of simple analytical formulas, the above analysis shows that the orientation-averaged extinction and scattering cross-sections for macroscopically isotropic and mirror-symmetric media do not depend on the polarization state of the incident wave. The orientation-averaged extinction and scattering cross-sections are invariant with respect to rotations and translations of the coordinate system and using these properties, Mishchenko et al. [169] have derived several invariants of the transition matrix.

Orientation-Averaged Extinction Matrix

To compute the orientation-averaged extinction matrix it is necessary to evaluate the orientation-averaged quantities $\langle S_{pq}(\boldsymbol{e}_z, \boldsymbol{e}_z)\rangle$. Taking into account the expressions of the elements of the amplitude matrix (cf. (1.97)), the equation of the orientation-averaged transition matrix (cf. (1.118) and (1.119)) and the expressions of the vector spherical harmonics in the forward direction (cf. (1.121)), we obtain

$$\langle S_{\theta\beta}(\boldsymbol{e}_z, \boldsymbol{e}_z)\rangle = \langle S_{\varphi\alpha}(\boldsymbol{e}_z, \boldsymbol{e}_z)\rangle = -\frac{\mathrm{j}}{2k_{\mathrm{s}}}\sum_{n=1}^{\infty}(2n+1)\left(t_n^{11} + t_n^{22}\right) ,$$

$$\langle S_{\theta\alpha}(\boldsymbol{e}_z, \boldsymbol{e}_z)\rangle = -\langle S_{\varphi\beta}(\boldsymbol{e}_z, \boldsymbol{e}_z)\rangle = -\frac{1}{2k_{\mathrm{s}}}\sum_{n=1}^{\infty}(2n+1)\left(t_n^{12} + t_n^{21}\right) .$$

Inserting these expansions into the equations specifying the elements of the extinction matrix (cf. (1.79)), we see that the nonzero matrix elements are

$$\langle K_{ii}\rangle = -\frac{2\pi}{k_{\mathrm{s}}^2}\mathrm{Re}\left\{\sum_{n=1}^{\infty}(2n+1)\left(t_n^{11}+t_n^{22}\right)\right\}, \quad i=1,2,3,4 \qquad (1.125)$$

and

$$\begin{aligned} \langle K_{14}\rangle = \langle K_{41}\rangle &= \frac{2\pi}{k_{\mathrm{s}}^2}\mathrm{Re}\left\{\sum_{n=1}^{\infty}(2n+1)\left(t_n^{12}+t_n^{21}\right)\right\}, \\ \langle K_{23}\rangle = -\langle K_{32}\rangle &= \frac{2\pi}{k_{\mathrm{s}}^2}\mathrm{Im}\left\{\sum_{n=1}^{\infty}(2n+1)\left(t_n^{12}+t_n^{21}\right)\right\}. \end{aligned} \qquad (1.126)$$

In terms of the elements of the extinction matrix, the orientation-averaged extinction cross-section is (cf. (1.89))

$$\langle C_{\mathrm{ext}}\rangle = \frac{1}{I_{\mathrm{e}}}\left[\langle K_{11}\rangle I_{\mathrm{e}} + \langle K_{14}\rangle V_{\mathrm{e}}\right],$$

while for macroscopically isotropic and mirror-symmetric media, the identities $t_n^{12}=t_n^{21}=0$, imply

$$\langle K_{14}\rangle = \langle K_{41}\rangle = \langle K_{23}\rangle = \langle K_{32}\rangle = 0.$$

In this specific case, the orientation-averaged extinction matrix becomes diagonal with diagonal elements being equal to the orientation-averaged extinction cross-section per particle, $\langle\boldsymbol{K}\rangle = \langle C_{\mathrm{ext}}\rangle\boldsymbol{I}$.

Orientation-Averaged Scattering Matrix

By definition, the orientation-averaged scattering matrix is the orientation-averaged phase matrix with $\beta=0$ and $\alpha=\varphi=0$. In the present analysis we consider the calculation of the general orientation-averaged phase matrix $\langle\boldsymbol{Z}(\boldsymbol{e}_r,\boldsymbol{e}_k;\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}})\rangle$ without taking into account the specific choice of the incident and scattering directions. We give guidelines for computing the quantities of interest, but we do not derive a final formula for the average phase matrix.

According to the definition of the phase matrix we see that the orientation-averaged quantities $\langle S_{pq}(\boldsymbol{e}_r,\boldsymbol{e}_k)S_{p_1q_1}^*(\boldsymbol{e}_r,\boldsymbol{e}_k)\rangle$, with $p,p_1=\theta,\varphi$ and $q,q_1=\beta,\alpha$, need to be computed. In view of (1.99), we have

$$\begin{aligned} &\left\langle S_{pq}\left(\boldsymbol{e}_r,\boldsymbol{e}_k\right)S_{p_1q_1}^*\left(\boldsymbol{e}_r,\boldsymbol{e}_k\right)\right\rangle \\ &= \frac{16}{k_{\mathrm{s}}^2}\left\langle\left(\boldsymbol{v}_{q_1}^{\dagger}\left(\boldsymbol{e}_k\right)\widetilde{\boldsymbol{T}}^{\mathrm{T}}\left(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}}\right)\boldsymbol{v}_{p_1}\left(\boldsymbol{e}_r\right)\right)^*\boldsymbol{v}_p^{\mathrm{T}}\left(\boldsymbol{e}_r\right)\widetilde{\boldsymbol{T}}\left(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}}\right)\boldsymbol{v}_q^*\left(\boldsymbol{e}_k\right)\right\rangle \\ &= \frac{16}{k_{\mathrm{s}}^2}\boldsymbol{v}_{q_1}^{\mathrm{T}}\left(\boldsymbol{e}_k\right)\left\langle\widetilde{\boldsymbol{T}}^{\dagger}\left(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}}\right)\boldsymbol{v}_{p_1}^*\left(\boldsymbol{e}_r\right)\boldsymbol{v}_p^{\mathrm{T}}\left(\boldsymbol{e}_r\right)\widetilde{\boldsymbol{T}}\left(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}}\right)\right\rangle\boldsymbol{v}_q^*\left(\boldsymbol{e}_k\right), \end{aligned}$$

where, as before, $\widetilde{\boldsymbol{T}}$ stands for the transition matrix in the global coordinate system. Defining the matrices

$$\boldsymbol{V}_{pp_1}(\boldsymbol{e}_r) = \boldsymbol{v}_{p_1}^*(\boldsymbol{e}_r)\,\boldsymbol{v}_p^{\mathrm{T}}(\boldsymbol{e}_r)$$

and

$$\boldsymbol{A}_{pp_1}(\boldsymbol{e}_r) = \left\langle \widetilde{\boldsymbol{T}}^\dagger(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}})\,\boldsymbol{V}_{pp_1}(\boldsymbol{e_r})\widetilde{\boldsymbol{T}}(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}}) \right\rangle ,$$

we see that

$$\left\langle S_{pq}(\boldsymbol{e}_r,\boldsymbol{e}_k)\,S_{p_1 q_1}^*(\boldsymbol{e}_r,\boldsymbol{e}_k) \right\rangle = \frac{16}{k_s^2}\boldsymbol{v}_{q_1}^{\mathrm{T}}(\boldsymbol{e}_k)\,\boldsymbol{A}_{pp_1}(\boldsymbol{e}_r)\,\boldsymbol{v}_q^*(\boldsymbol{e}_k)\ . \qquad (1.127)$$

Using the block-matrix decomposition

$$\boldsymbol{X} = \begin{bmatrix} \boldsymbol{X}^{11} & \boldsymbol{X}^{12} \\ \boldsymbol{X}^{21} & \boldsymbol{X}^{22} \end{bmatrix} ,$$

where $\boldsymbol{X}$ stands for $\boldsymbol{V}_{pp_1}$ and $\boldsymbol{A}_{pp_1}$, we express the submatrices of $\boldsymbol{A}_{pp_1}$ as

$$\boldsymbol{A}_{pp_1}^{11} = \left\langle \widetilde{\boldsymbol{T}}^{11\dagger}\boldsymbol{V}_{pp_1}^{11}\widetilde{\boldsymbol{T}}^{11} + \widetilde{\boldsymbol{T}}^{11\dagger}\boldsymbol{V}_{pp_1}^{12}\widetilde{\boldsymbol{T}}^{21} + \widetilde{\boldsymbol{T}}^{21\dagger}\boldsymbol{V}_{pp_1}^{21}\widetilde{\boldsymbol{T}}^{11} + \widetilde{\boldsymbol{T}}^{21\dagger}\boldsymbol{V}_{pp_1}^{22}\widetilde{\boldsymbol{T}}^{21} \right\rangle ,$$

$$\boldsymbol{A}_{pp_1}^{12} = \left\langle \widetilde{\boldsymbol{T}}^{11\dagger}\boldsymbol{V}_{pp_1}^{11}\widetilde{\boldsymbol{T}}^{12} + \widetilde{\boldsymbol{T}}^{11\dagger}\boldsymbol{V}_{pp_1}^{12}\widetilde{\boldsymbol{T}}^{22} + \widetilde{\boldsymbol{T}}^{21\dagger}\boldsymbol{V}_{pp_1}^{21}\widetilde{\boldsymbol{T}}^{12} + \widetilde{\boldsymbol{T}}^{21\dagger}\boldsymbol{V}_{pp_1}^{22}\widetilde{\boldsymbol{T}}^{22} \right\rangle ,$$

$$\boldsymbol{A}_{pp_1}^{21} = \left\langle \widetilde{\boldsymbol{T}}^{12\dagger}\boldsymbol{V}_{pp_1}^{11}\widetilde{\boldsymbol{T}}^{11} + \widetilde{\boldsymbol{T}}^{12\dagger}\boldsymbol{V}_{pp_1}^{12}\widetilde{\boldsymbol{T}}^{21} + \widetilde{\boldsymbol{T}}^{22\dagger}\boldsymbol{V}_{pp_1}^{21}\widetilde{\boldsymbol{T}}^{11} + \widetilde{\boldsymbol{T}}^{22\dagger}\boldsymbol{V}_{pp_1}^{22}\widetilde{\boldsymbol{T}}^{21} \right\rangle ,$$

$$\boldsymbol{A}_{pp_1}^{22} = \left\langle \widetilde{\boldsymbol{T}}^{12\dagger}\boldsymbol{V}_{pp_1}^{11}\widetilde{\boldsymbol{T}}^{12} + \widetilde{\boldsymbol{T}}^{12\dagger}\boldsymbol{V}_{pp_1}^{12}\widetilde{\boldsymbol{T}}^{22} + \widetilde{\boldsymbol{T}}^{22\dagger}\boldsymbol{V}_{pp_1}^{21}\widetilde{\boldsymbol{T}}^{12} + \widetilde{\boldsymbol{T}}^{22\dagger}\boldsymbol{V}_{pp_1}^{22}\widetilde{\boldsymbol{T}}^{22} \right\rangle .$$

$$(1.128)$$

It is apparent that each matrix product in the above equations is of the form

$$\boldsymbol{W}_{pp_1}(\boldsymbol{e}_r) = \left\langle \widetilde{\boldsymbol{T}}^{kl\dagger}(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}})\,\boldsymbol{V}_{pp_1}^{uv}(\boldsymbol{e}_r)\,\widetilde{\boldsymbol{T}}^{ij}(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}}) \right\rangle , \qquad (1.129)$$

where the permissive values of the index pairs (i,j), (k,l) and (u,v) follow from (1.128). The elements of the $\boldsymbol{W}_{pp_1}$ matrix are given by

$$(W_{pp_1})_{\widetilde{m}_1\widetilde{n}_1,m_1 n_1}(\boldsymbol{e}_r) = \sum_{\widetilde{n},\widetilde{m}}\sum_{n,m} \left\langle \widetilde{T}_{mn,m_1 n_1}^{ij}(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}})\,\widetilde{T}_{mn,\widetilde{m}_1\widetilde{n}_1}^{kl*}(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}}) \right\rangle$$

$$\times \left(V_{pp_1}^{uv}\right)_{\widetilde{m}\widetilde{n},mn}(\boldsymbol{e}_r) , \qquad (1.130)$$

and the rest of our analysis concerns with the computation of the term

$$\mathcal{T} = \left\langle \widetilde{T}_{mn,m_1 n_1}^{ij}(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}})\,\widetilde{T}_{mn,\widetilde{m}_1\widetilde{n}_1}^{kl*}(\alpha_{\mathrm{p}},\beta_{\mathrm{p}},\gamma_{\mathrm{p}}) \right\rangle . \qquad (1.131)$$

It should be mentioned that for notation simplification we omit to indicate the dependency of $\mathcal{T}$ on the matrix indices.

Using the rotation transformation rule for the transition matrix (cf. (1.116)), we obtain

$$\mathcal{T} = \frac{1}{8\pi^2} \sum_{m'=-n}^{n} \sum_{m_1'=-n_1}^{n_1} \sum_{\widetilde{m}'=-\widetilde{n}}^{\widetilde{n}} \sum_{\widetilde{m}_1'=-\widetilde{n}_1}^{\widetilde{n}_1} \left[\int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} D_{m'm}^n \left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}}\right) \right.$$

$$\times D_{m_1 m_1'}^{n_1} \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}}\right) D_{\widetilde{m}'\widetilde{m}}^{\widetilde{n}*} \left(-\gamma_{\mathrm{p}}, -\beta_{\mathrm{p}}, -\alpha_{\mathrm{p}}\right)$$

$$\left. \times D_{\widetilde{m}_1 \widetilde{m}_1'}^{\widetilde{n}_1 *} \left(\alpha_{\mathrm{p}}, \beta_{\mathrm{p}}, \gamma_{\mathrm{p}}\right) \sin\beta_{\mathrm{p}} \, \mathrm{d}\beta_{\mathrm{p}} \, \mathrm{d}\alpha_{\mathrm{p}} \, \mathrm{d}\gamma_{\mathrm{p}} \right] T_{m'n,m_1'n_1}^{ij} T_{\widetilde{m}'\widetilde{n},\widetilde{m}_1'\widetilde{n}_1}^{kl*} .$$

Taking into account the definition of the Wigner D-functions (cf. (B.34)) and integrating over α_{p} and γ_{p}, yields

$$\mathcal{T} = \frac{1}{2} \sum_{m'=-n}^{n} \sum_{m_1'=-n_1}^{n_1} \sum_{\widetilde{m}'=-\widetilde{n}}^{\widetilde{n}} \sum_{\widetilde{m}_1'=-\widetilde{n}_1}^{\widetilde{n}_1} \delta_{m_1-m,\widetilde{m}_1-\widetilde{m}} \delta_{m_1'-m',\widetilde{m}_1'-\widetilde{m}'} \Delta$$

$$\times \left[\int_0^{\pi} d_{m'm}^n \left(-\beta_{\mathrm{p}}\right) d_{\widetilde{m}'\widetilde{m}}^{\widetilde{n}} \left(-\beta_{\mathrm{p}}\right) d_{m_1 m_1'}^{n_1} \left(\beta_{\mathrm{p}}\right) d_{\widetilde{m}_1 \widetilde{m}_1'}^{\widetilde{n}_1} \left(\beta_{\mathrm{p}}\right) \sin\beta_{\mathrm{p}} \, \mathrm{d}\beta_{\mathrm{p}} \right]$$

$$\times T_{m'n,m_1'n_1}^{ij} T_{\widetilde{m}'\widetilde{n},\widetilde{m}_1'\widetilde{n}_1}^{kl*} ,$$

where $d_{mm'}^n$ are the Wigner d-functions defined in Appendix B,

$$\Delta = \Delta_{m'm} \Delta_{\widetilde{m}'\widetilde{m}} \Delta_{m_1 m_1'} \Delta_{\widetilde{m}_1 \widetilde{m}_1'} ,$$

and $\Delta_{mm'}$ is given by (B.36). To compute the integral

$$\mathcal{I} = \frac{1}{2} \delta_{m_1-m,\widetilde{m}_1-\widetilde{m}} \delta_{m_1'-m',\widetilde{m}_1'-\widetilde{m}'}$$

$$\times \int_0^{\pi} d_{m'm}^n \left(-\beta_{\mathrm{p}}\right) d_{\widetilde{m}'\widetilde{m}}^{\widetilde{n}} \left(-\beta_{\mathrm{p}}\right) d_{m_1 m_1'}^{n_1} \left(\beta_{\mathrm{p}}\right) d_{\widetilde{m}_1 \widetilde{m}_1'}^{\widetilde{n}_1} \left(\beta_{\mathrm{p}}\right) \sin\beta_{\mathrm{p}} \, \mathrm{d}\beta_{\mathrm{p}} ,$$

we use the symmetry relations (cf. (B.39) and (B.41))

$$d_{m'm}^n(-\beta_{\mathrm{p}}) = d_{mm'}^n(\beta_{\mathrm{p}}) = (-1)^{m+m'} d_{-m-m'}^n(\beta_{\mathrm{p}}) ,$$

$$d_{\widetilde{m}'\widetilde{m}}^{\widetilde{n}}(-\beta_{\mathrm{p}}) = d_{\widetilde{m}\widetilde{m}'}^{\widetilde{n}}(\beta_{\mathrm{p}}) = (-1)^{\widetilde{m}+\widetilde{m}'} d_{-\widetilde{m}-\widetilde{m}'}^{\widetilde{n}}(\beta_{\mathrm{p}}) ,$$

the expansions of the d-functions products $d_{m_1 m_1'}^{n_1} d_{-m-m'}^n$ and $d_{\widetilde{m}_1 \widetilde{m}_1'}^{\widetilde{n}_1} d_{-\widetilde{m}-\widetilde{m}'}^{\widetilde{n}}$ given by (B.47), and the orthogonality property of the d-functions (cf. (B.43)).

We obtain

$$
\mathcal{I} = (-1)^{m+m'+\widetilde{m}+\widetilde{m}'}(-1)^{n+n_1+\widetilde{n}+\widetilde{n}_1}\delta_{m_1-m,\widetilde{m}_1-\widetilde{m}}\delta_{m_1'-m',\widetilde{m}_1'-\widetilde{m}'}
$$

$$
\times \sum_{u=u_{\min}}^{u_{\max}} \frac{1}{2u+1} C_{m_1 n_1,-mn}^{m_1-mu} C_{-m_1' n_1,m'n}^{m'-m_1'u} C_{\widetilde{m}_1\widetilde{n}_1,-\widetilde{m}\widetilde{n}}^{\widetilde{m}_1-\widetilde{m}u} C_{-\widetilde{m}_1'\widetilde{n}_1,\widetilde{m}'\widetilde{n}}^{\widetilde{m}'-\widetilde{m}_1'u},
$$

where $C_{mn,m_1 n_1}^{m+m_1 u}$ are the Clebsch–Gordan coefficients defined in Appendix B, and

$$
u_{\min} = \max\left(|n-n_1|,|\widetilde{n}-\widetilde{n}_1|,|m_1-m|,|\widetilde{m}_1-\widetilde{m}|,|m'-m_1'|,|\widetilde{m}'-\widetilde{m}_1'|\right),
$$
$$
u_{\max} = \min\left(n+n_1,\widetilde{n}+\widetilde{n}_1\right).
$$

Further, using the symmetry properties of the Clebsch–Gordan coefficients (cf. (B.48) and (B.51)) we arrive at

$$
\mathcal{I} = (-1)^{n+n_1+\widetilde{n}+\widetilde{n}_1}\delta_{m_1-m,\widetilde{m}_1-\widetilde{m}}\delta_{m_1'-m',\widetilde{m}_1'-\widetilde{m}'}
$$

$$
\times \sum_{u=u_{\min}}^{u_{\max}} \frac{2u+1}{(2n_1+1)(2\widetilde{n}_1+1)} C_{m_1-mu,mn}^{m_1 n_1} C_{m'-m_1'u,-m'n}^{-m_1' n_1}
$$

$$
\times C_{\widetilde{m}_1-\widetilde{m}u,\widetilde{m}\widetilde{n}}^{\widetilde{m}_1\widetilde{n}_1} C_{\widetilde{m}'-\widetilde{m}_1'u,-\widetilde{m}'\widetilde{n}}^{-\widetilde{m}_1'\widetilde{n}_1}
$$

and

$$
\mathcal{T} = \sum_{m'=-n}^{n}\sum_{m_1'=-n_1}^{n_1}\sum_{\widetilde{m}'=-\widetilde{n}}^{\widetilde{n}}\sum_{\widetilde{m}_1'=-\widetilde{n}_1}^{\widetilde{n}_1} \Delta\mathcal{I} T_{m'n,m_1'n_1}^{ij} T_{\widetilde{m}'\widetilde{n},\widetilde{m}_1'\widetilde{n}_1}^{kl*}. \quad (1.132)
$$

The orientation-averaged quantities $\langle S_{pq}(\boldsymbol{e}_r,\boldsymbol{e}_k)S_{p_1 q_1}^*(\boldsymbol{e}_r,\boldsymbol{e}_k)\rangle$ can be computed from the set of equations (1.127)–(1.132).

For an incident wave propagating along the Z-axis, the augmented vector of spherical harmonics $\boldsymbol{v}_q(\boldsymbol{e}_z)$ can be computed by using (1.121). Choosing the XZ-plane as the scattering plane, i.e., setting $\varphi = 0$, we see that the matrices $\boldsymbol{V}_{pp_1}(\boldsymbol{e}_r)$ involve only the normalized angular functions $\pi_n^{|m|}(\theta)$ and $\tau_n^{|m|}(\theta)$. The resulting orientation-averaged scattering matrix can be computed at a set of polar angles θ and polynomial interpolation can be used to evaluate the orientation-averaged scattering matrix at any polar angle θ.

For macroscopically isotropic media, the orientation-averaged scattering matrix has sixteen nonzero elements (cf. (1.113)) but only ten of them are independent. For macroscopically isotropic and mirror-symmetric media, the orientation-averaged scattering matrix has a block-diagonal structure (cf. (1.114)), so that only eight elements are nonzero and only six of them are independent. In this case we determine the six quantities $\langle |S_{\theta\beta}(\theta)|^2\rangle$,

$\langle|S_{\theta\alpha}(\theta)|^2\rangle$, $\langle|S_{\varphi\beta}(\theta)|^2\rangle$, $\langle|S_{\varphi\alpha}(\theta)|^2\rangle$, $\langle S_{\theta\beta}(\theta)S^*_{\varphi\alpha}(\theta)\rangle$ and $\langle S_{\theta\alpha}(\theta)S^*_{\varphi\beta}(\theta)\rangle$, and compute the eight nonzero elements by using the relations

$$\langle F_{11}(\theta)\rangle = \frac{1}{2}\left(\left\langle|S_{\theta\beta}(\theta)|^2\right\rangle + \left\langle|S_{\theta\alpha}(\theta)|^2\right\rangle + \left\langle|S_{\varphi\beta}(\theta)|^2\right\rangle + \left\langle|S_{\varphi\alpha}(\theta)|^2\right\rangle\right),$$

$$\langle F_{12}(\theta)\rangle = \frac{1}{2}\left(\left\langle|S_{\theta\beta}(\theta)|^2\right\rangle - \left\langle|S_{\theta\alpha}(\theta)|^2\right\rangle + \left\langle|S_{\varphi\beta}(\theta)|^2\right\rangle - \left\langle|S_{\varphi\alpha}(\theta)|^2\right\rangle\right),$$

$$\langle F_{21}(\theta)\rangle = \langle F_{12}(\theta)\rangle,$$

$$\langle F_{22}(\theta)\rangle = \frac{1}{2}\left(\left\langle|S_{\theta\beta}(\theta)|^2\right\rangle - \left\langle|S_{\theta\alpha}(\theta)|^2\right\rangle - \left\langle|S_{\varphi\beta}(\theta)|^2\right\rangle + \left\langle|S_{\varphi\alpha}(\theta)|^2\right\rangle\right),$$

$$\langle F_{33}(\theta)\rangle = \mathrm{Re}\left\{\left\langle S_{\theta\beta}(\theta)S^*_{\varphi\alpha}(\theta)\right\rangle + \left\langle S_{\theta\alpha}(\theta)S^*_{\varphi\beta}(\theta)\right\rangle\right\},$$

$$\langle F_{34}(\theta)\rangle = \mathrm{Im}\left\{\left\langle S_{\theta\beta}(\theta)S^*_{\varphi\alpha}(\theta)\right\rangle + \left\langle S_{\theta\alpha}(\theta)S^*_{\varphi\beta}(\theta)\right\rangle^*\right\},$$

$$\langle F_{43}(\theta)\rangle = -\langle F_{34}(\theta)\rangle,$$

$$\langle F_{44}(\theta)\rangle = \mathrm{Re}\left\{\left\langle S_{\theta\beta}(\theta)S^*_{\varphi\alpha}(\theta)\right\rangle^* - \left\langle S_{\theta\alpha}(\theta)S^*_{\varphi\beta}(\theta)\right\rangle\right\}.$$

Other scattering characteristics as for instance the orientation-averaged scattering cross-section and the orientation-averaged mean direction of propagation of the scattered field can be expressed in terms of the elements of the orientation-averaged scattering matrix. To derive these expressions we consider the scattering plane characterized by the azimuth angle φ as shown in Fig. 1.15. In the scattering plane, the Stokes vector of the scattered wave is given by $\langle\boldsymbol{I}_s(r\boldsymbol{e}_r)\rangle = (1/r^2)\langle\boldsymbol{F}(\theta)\rangle\boldsymbol{I}'_e$, whence, using the transformation rule of the Stokes vector under coordinate rotation $\boldsymbol{I}'_e = \boldsymbol{L}(\varphi)\boldsymbol{I}_e$, we obtain

$$\langle\boldsymbol{I}_s(r\boldsymbol{e}_r)\rangle = \frac{1}{r^2}\langle\boldsymbol{F}(\theta)\rangle\boldsymbol{L}(\varphi)\boldsymbol{I}_e.$$

Further, taking into account the expression of the Stokes rotation matrix $\boldsymbol{L}$ (cf. (1.23)) we derive

$$\langle I_s(\boldsymbol{e}_r)\rangle = \langle F_{11}(\theta)\rangle I_e + [\langle F_{12}(\theta)\rangle\cos 2\varphi + \langle F_{13}(\theta)\rangle\sin 2\varphi]Q_e$$
$$- [\langle F_{12}(\theta)\rangle\sin 2\varphi - \langle F_{13}(\theta)\rangle\cos 2\varphi]U_e + \langle F_{14}(\theta)\rangle V_e.$$

Integrating over φ, we find that the orientation-averaged scattering cross-section and the orientation-averaged mean direction of propagation of the scattered field are given by

$$\langle C_{\mathrm{scat}}\rangle = \frac{1}{I_e}\int_\Omega \langle I_s(\boldsymbol{e}_r)\rangle\,\mathrm{d}\Omega(\boldsymbol{e}_r)$$

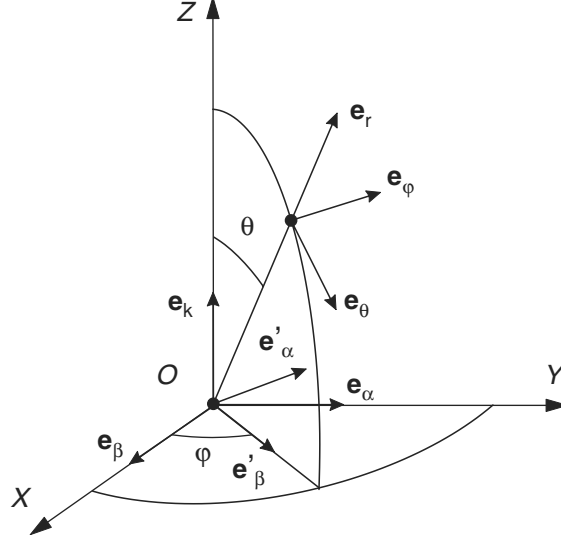$$= \frac{2\pi}{I_e}\int_0^\pi [\langle F_{11}(\theta)\rangle I_e + \langle F_{14}(\theta)\rangle V_e]\sin\theta\,\mathrm{d}\theta$$

Fig. 1.15. Incident and scattering directions e_k and e_r. The incident direction is along the Z-axis and the scattering matrix relates the Stokes vectors of the incident and scattered fields specified relative to the scattering plane characterized by the azimuth angle φ

and

$$
\begin{aligned}
\langle \boldsymbol{g} \rangle &= \frac{1}{\langle C_{\mathrm{scat}} \rangle I_{\mathrm{e}}} \int_{\Omega} \langle I_{\mathrm{s}} \left(\boldsymbol{e}_r \right) \rangle \boldsymbol{e}_r \, \mathrm{d}\Omega \left(\boldsymbol{e}_r \right) \\
&= \frac{2\pi}{\langle C_{\mathrm{scat}} \rangle I_{\mathrm{e}}} \left\{ \int_0^{\pi} \left[\langle F_{11}(\theta) \rangle I_{\mathrm{e}} + \langle F_{14}(\theta) \rangle V_{\mathrm{e}} \right] \sin\theta \cos\theta \, \mathrm{d}\theta \right\} \boldsymbol{e}_z \,,
\end{aligned}
$$

respectively. Because the incident wave propagates along the Z-axis, the nonzero component of $\langle \boldsymbol{g} \rangle$ is the orientation-averaged asymmetry parameter $\langle \cos\Theta \rangle$. In practical computer simulations, we use the decomposition

$$
\langle C_{\mathrm{scat}} \rangle = \frac{1}{I_{\mathrm{e}}} \left(\langle C_{\mathrm{scat}} \rangle_{\mathrm{I}} I_{\mathrm{e}} + \langle C_{\mathrm{scat}} \rangle_{\mathrm{V}} V_{\mathrm{e}} \right) \,,
$$

and compute the quantities $\langle C_{\mathrm{scat}} \rangle_{\mathrm{I}}$ and $\langle C_{\mathrm{scat}} \rangle_{\mathrm{V}}$ by using (1.124) and the relation

$$
\langle C_{\mathrm{scat}} \rangle_{\mathrm{V}} = 2\pi \int_0^{\pi} \langle F_{14}(\theta) \rangle \sin\theta \, \mathrm{d}\theta \,, \tag{1.133}
$$

respectively. These quantities do not depend on the polarization state of the incident wave and can be used to compute the orientation-averaged scattering cross-section for any incident polarization. For the asymmetry parameter we proceed analogously; we use the decomposition

$$\langle\cos\Theta\rangle = \frac{\langle C_{\mathrm{scat}}\rangle_{\mathrm{I}}}{\langle C_{\mathrm{scat}}\rangle}\frac{1}{I_{\mathrm{e}}}\left(\langle\cos\Theta\rangle_{\mathrm{I}}\,I_{\mathrm{e}} + \langle\cos\Theta\rangle_{\mathrm{V}}\,V_{\mathrm{e}}\right),$$

and compute $\langle\cos\Theta\rangle_{\mathrm{I}}$ and $\langle\cos\Theta\rangle_{\mathrm{V}}$ by using the relations

$$\langle\cos\Theta\rangle_{\mathrm{I}} = \frac{2\pi}{\langle C_{\mathrm{scat}}\rangle_{\mathrm{I}}}\int_0^\pi \langle F_{11}(\theta)\rangle\sin\theta\cos\theta\,\mathrm{d}\theta \tag{1.134}$$

and

$$\langle\cos\Theta\rangle_{\mathrm{V}} = \frac{2\pi}{\langle C_{\mathrm{scat}}\rangle_{\mathrm{I}}}\int_0^\pi \langle F_{14}(\theta)\rangle\sin\theta\cos\theta\,\mathrm{d}\theta\,, \tag{1.135}$$

respectively. For macroscopically isotropic and mirror-symmetric media,

$$\langle F_{14}(\theta)\rangle = 0$$

and consequently, $\langle C_{\mathrm{scat}}\rangle = \langle C_{\mathrm{scat}}\rangle_{\mathrm{I}}$ and $\langle\cos\Theta\rangle = \langle\cos\Theta\rangle_{\mathrm{I}}$.

Another important scattering characteristic is the angular distribution of the scattered field. For an ensemble of randomly oriented particles illuminated by a vector plane wave of unit amplitude and polarization vector $\boldsymbol{e}_{\mathrm{pol}} = e_{\mathrm{pol},\beta}\boldsymbol{e}_\beta + e_{\mathrm{pol},\alpha}\boldsymbol{e}_\alpha$, the differential scattering cross-sections in the scattering plane φ are given by

$$\langle\sigma_{\mathrm{dp}}(\theta)\rangle = \left\langle|E_{\mathrm{s}\infty,\theta}(\theta)|^2\right\rangle = \left\langle|S_{\theta\beta}(\theta)|^2\right\rangle\left|E'_{\mathrm{e}0,\beta}\right|^2$$
$$+ \left\langle|S_{\theta\alpha}(\theta)|^2\right\rangle\left|E'_{\mathrm{e}0,\alpha}\right|^2$$
$$+ 2\mathrm{Re}\left\{\langle S_{\theta\beta}(\theta)S_{\theta\alpha}^*(\theta)\rangle\,E'_{\mathrm{e}0,\beta}E'^*_{\mathrm{e}0,\alpha}\right\} \tag{1.136}$$

and

$$\langle\sigma_{\mathrm{ds}}(\theta)\rangle = \left\langle|E_{\mathrm{s}\infty,\varphi}(\theta)|^2\right\rangle = \left\langle|S_{\varphi\beta}(\theta)|^2\right\rangle\left|E'_{\mathrm{e}0,\beta}\right|^2$$
$$+ \left\langle|S_{\varphi\alpha}(\theta)|^2\right\rangle\left|E'_{\mathrm{e}0,\alpha}\right|^2$$
$$+ 2\mathrm{Re}\left\{\langle S_{\varphi\beta}(\theta)S_{\varphi\alpha}^*(\theta)\rangle\,E'_{\mathrm{e}0,\beta}E'^*_{\mathrm{e}0,\alpha}\right\}, \tag{1.137}$$

where

$$E'_{\mathrm{e}0,\beta} = e_{\mathrm{pol},\beta}\cos\varphi + e_{\mathrm{pol},\alpha}\sin\varphi\,,$$
$$E'_{\mathrm{e}0,\alpha} = -e_{\mathrm{pol},\beta}\sin\varphi + e_{\mathrm{pol},\alpha}\cos\varphi\,.$$

It should be noted that for macroscopically isotropic and mirror-symmetric media,

$$\langle S_{\theta\beta}(\theta)S_{\theta\alpha}^*(\theta)\rangle = 0\,,$$
$$\langle S_{\varphi\beta}(\theta)S_{\varphi\alpha}^*(\theta)\rangle = 0\,,$$

and the expressions of $\langle\sigma_{\mathrm{dp}}(\theta)\rangle$ and $\langle\sigma_{\mathrm{ds}}(\theta)\rangle$ simplify considerably.

In practice, the inequalities

$$\langle F_{11} \rangle \geq |\langle F_{ij} \rangle| \,, \quad i,j = 1,2,3,4 \,,$$

$$(\langle F_{11} \rangle + \langle F_{22} \rangle)^2 - 4 \langle F_{12} \rangle^2 \geq (\langle F_{33} \rangle + \langle F_{44} \rangle)^2 + 4 \langle F_{34} \rangle^2 \,,$$

$$\langle F_{11} \rangle - \langle F_{22} \rangle \geq |\langle F_{33} \rangle - \langle F_{44} \rangle| \,,$$

$$\langle F_{11} \rangle - \langle F_{12} \rangle \geq |\langle F_{22} \rangle - \langle F_{12} \rangle| \,,$$

$$\langle F_{11} \rangle + \langle F_{12} \rangle \geq |\langle F_{22} \rangle + \langle F_{12} \rangle| \,, \tag{1.138}$$

can be used to test the numerically obtained orientation-averaged scattering matrix [104, 169].

It should be emphasized that we do not expand the elements of the orientation-averaged scattering matrix in generalized spherical functions (or Wigner d-functions) and do not exploit the advantage of performing as much work analytically as possible. Therefore, the above averaging procedure is computationally not so fast as the scattering matrix expansion method given by Mishchenko [162]. As noted by Mishchenko et al. [169], the analyticity of the $\boldsymbol{T}$-matrix formulation can be connected with the formalism of expanding scattering matrices in generalized spherical functions to derive an efficient procedure that does not involve any angular variable.

Khlebtsov [120] and Fucile et al. [71] developed a similar formalism that exploit the rotation property of the transition matrix but avoids the expansion of the scattering matrix in generalized spherical functions. Paramonov [182] and Borghese et al. [23] extended the analytical orientation-averaging procedure to arbitrary orientation distribution functions, while the standard averaging approach employing numerical integrations over the orientation angles has been used by Wiscombe and Mugnai [263, 264] and Barber and Hill [8]. A method to compute light scattering by arbitrarily oriented rotationally symmetric particles has been given by Skaropoulos and Russchenberg [212].