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An "exact" geometric-optics approach for computing the optical properties of large absorbing particles

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ABSTRACT

Based on the principles of geometric optics, the ray-tracing technique has been extensively used to compute the single-scattering properties of particles whose sizes are much larger than the wavelength of the incident wave. However, the inhomogeneity characteristics of internal waves within an absorbing particle, which stem from a complex index of refraction, have not been fully taken into consideration in the geometric ray-tracing approaches reported in the literature for computing the scattering properties of absorbing particles. In this paper, we first demonstrate that electromagnetic fields associated with an absorbing particle can be decomposed into the TE and TM modes. Subsequently, on the basis of Maxwell's equations and electromagnetic boundary conditions for the TE-mode electric field and the TM-mode magnetic field, we derive generalized Fresnel reflection and refraction coefficients, which differ from conventional formulae and do not involve complex angles. Additionally, a recurrence formulism is developed for the computation of the scattering phase matrix of an absorbing particle within the framework of the conventional geometric ray-tracing method. We further present pertinent numerical examples for the phase function and the degree of linear polarization in conjunction with light scattering by individual absorbing spheres, and discuss the deviation of the geometric optics solutions from the exact Lorenz–Mie results with respect to size parameter and complex refractive index.

1. Introduction

The single-scattering properties of nonspherical particles are fundamental to various applications in remote sensing research and climate radiative forcing analysis involving aerosols and clouds containing ice crystals [1,2]. In the last three decades, the conventional geometric ray-tracing technique [3–9] and its improved forms [10,11] have been extensively used to compute the optical properties of nonspherical dielectric particles much larger than the wavelength of the incident wave. However, in the geometric ray-tracing methods reported in the literature for computing the single-scattering properties of absorbing dielectric particles, a unique physical property of localized waves within an absorbing particle, referred to as wave inhomogeneity, has not been fully considered.

The inhomogeneity of an electromagnetic wave is related to the wave characteristics such that the planes of constant phase are not parallel to those of constant amplitude [12–16]. This wave feature leads to complex angles in the

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conventional Snell law that defines the incident, reflection and refraction directions. However, a complex angle involving an imaginary number does not have a straightforward geometric meaning within the context of ray-tracing calculations in the real-number domain for the propagation directions of geometric optics rays. Moreover, an inhomogeneous electromagnetic wave does not satisfy a simple transverse-wave condition that requires the corresponding electric and magnetic field vectors to be perpendicular to the propagation direction of constant phase or amplitude. For a non-absorbing particle, electromagnetic waves within the particle are transverse waves for which the three directions along the electric field vector, magnetic field vector and wave propagation are orthogonal. However, in the case of an absorbing particle, an internal electromagnetic wave can be decomposed into a transverse electric (TE) component and a transverse magnetic (TM) component. The electric vector is perpendicular to the direction of wave propagation in the TE mode, whereas the magnetic vector is perpendicular to the direction of wave propagation in the TM mode.

In this study, we derive the generalized Fresnel formulas for the TE-mode and TM-mode field components for various orders of reflection–refraction events associated with an absorbing particle. In the generalized Fresnel formulas for the calculations of the electric and magnetic field amplitudes associated with the reflected and transmitted rays, we follow the effective refractive index concept [17] to circumvent the difficulty that stems from the complex angles in the conventional Snell law for absorbing particles. We also formulate a geometric ray-tracing approach in terms of the generalized Fresnel formulas coupled with various transformation matrices to fully account for the wave inhomogeneity effects on the reflection and refraction of a localized wave characterized as a geometric ray. Furthermore, we present some pertinent numerical examples and compare the geometric optics solutions to the Lorenz–Mie results for the phase function and the degree of linear polarization in conjunction with light scattering by individual absorbing spheres for size parameters in the geometric optics regime.

2. Generalized Fresnel formulas for inhomogeneous waves

In this section, we derive the Fresnel formulas for the electric and magnetic fields in the TE and TM modes, respectively, on the basis of the general electromagnetic boundary conditions for two adjacent media with a plane interface and the two Maxwell curl equations [18] given by

$$\nabla \times \vec{E}(\vec{r},t) = -\frac{\mu}{c}\frac{\partial \vec{H}(\vec{r},t)}{\partial t}, \tag{1}$$

$$\nabla \times \vec{H}(\vec{r},t) = \frac{\varepsilon}{c}\frac{\partial \vec{E}(\vec{r},t)}{\partial t}, \tag{2}$$

where μ and ε are permeability and permittivity, respectively. For our purpose, we should consider a non-ferromagnetic particle such that $\mu = 1$. In this case, the permittivity is then given by

$$\varepsilon = m^2, \tag{3}$$

where m is the index of refraction which is 1 outside the particle and a complex quantity within the particle. We further assume that the time-dependence of the waves is harmonic and can be expressed in the form of $e^{-ik_o ct}$, where $k_o = 2\pi/\lambda$ and λ is the wavelength in a vacuum. For formulation simplicity, in the following discussions we will only consider the spatial components of the electromagnetic fields. Thus, for the spatial domain outside the particle, we have

$$\nabla \times \vec{E}(\vec{r}) = ik_o \vec{H}(\vec{r}), \tag{4}$$

$$\nabla \times \vec{H}(\vec{r}) = -ik_o \vec{E}(\vec{r}). \tag{5}$$

But for the spatial domain inside the particle, the two curl equations are given by

$$\nabla \times \vec{E}(\vec{r}) = ik_o \vec{H}(\vec{r}), \tag{6}$$

$$\nabla \times \vec{H}(\vec{r}) = -ik_o m^2 \vec{E}(\vec{r}). \tag{7}$$

Fig. 1 defines the geometric configuration for the first-order reflection–refraction event when the transmission of an incident ray is from air into the particle. The unit vectors $\hat{e}_{i,1}$, $\hat{e}_{r,1}$ and $\hat{e}_{t,1}$ represent the directions of the incident, reflected and refracted rays, respectively; $\hat{\beta}_1$ is a unit vector with the direction pointing onto the paper; $\hat{e}_{f,1}$ is a unit vector on the incident plane, a plane containing the incident, reflected and refracted rays and parallel to the particle surface; $\hat{n}_1$ is a local unit vector normal to the particle surface; the unit vectors $\hat{\alpha}_{i,1}$, $\hat{\alpha}_{r,1}$ and $\hat{\alpha}_{t,1}$ are defined by the following relations:

$$\hat{\alpha}_{i,1} = \hat{e}_{i,1} \times \hat{\beta}_1, \tag{8}$$

$$\hat{\alpha}_{r,1} = \hat{e}_{r,1} \times \hat{\beta}_1, \tag{9}$$

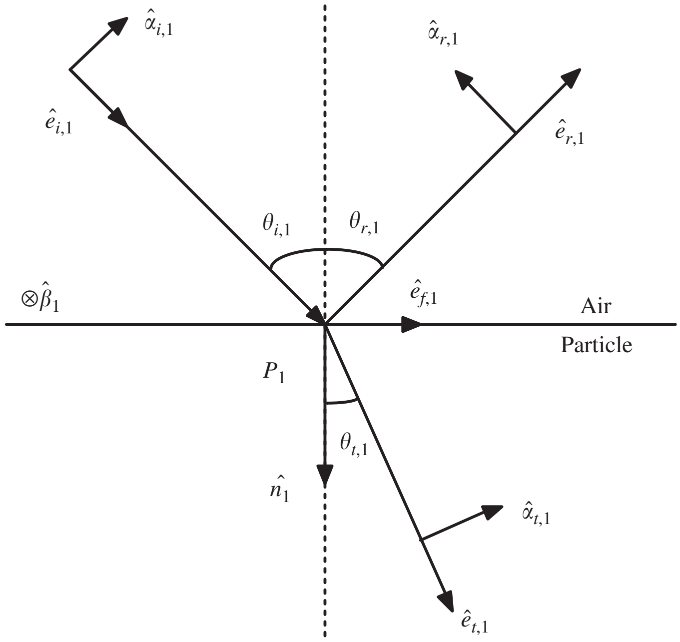

Fig. 1. The geometric configuration for the first-order incident, reflected and refracted rays at point P_1 when the refraction of an incident ray is from the air into the particle.

$$\hat{\alpha}_{t,1} = \hat{e}_{t,1} \times \hat{\beta}_1. \tag{10}$$

Following Ref. [17], the electric and magnetic vectors associated with the incident, reflected and refracted rays with respect to the incident point P_1 can be expressed as follows:

$$\begin{bmatrix} \vec{E}_{i,1}(\vec{r}) \\ \vec{H}_{i,1}(\vec{r}) \end{bmatrix} = \begin{bmatrix} \vec{E}_{oi,1} \\ \vec{H}_{oi,1} \end{bmatrix} \exp[ik_o\hat{e}_{i,1}(\vec{r}-\vec{r}_1)], \tag{11}$$

$$\begin{bmatrix} \vec{E}_{r,1}(\vec{r}) \\ \vec{H}_{r,1}(\vec{r}) \end{bmatrix} = \begin{bmatrix} \vec{E}_{or,1} \\ \vec{H}_{or,1} \end{bmatrix} \exp[ik_o\hat{e}_{r,1}(\vec{r}-\vec{r}_1)], \tag{12}$$

$$\begin{bmatrix} \vec{E}_{t,1}(\vec{r}) \\ \vec{H}_{t,1}(\vec{r}) \end{bmatrix} = \begin{bmatrix} \vec{E}_{ot,1} \\ \vec{H}_{ot,1} \end{bmatrix} \exp[ik_o(\hat{e}_{t,1}N_{r,1} + iN_{n,1}\hat{n}_1)(\vec{r}-\vec{r}_1)], \tag{13}$$

where $\vec{r}_1$ is the position vector of point P_1, and $N_{r,1}$ and $N_{n,1}$ are the effective refractive indices defined in Yang and Liou [17]. Note that, for simplicity, $N^*_{n,j}$ in Ref. [17], where $j = 1,2,3\ldots$, is denoted as $N_{n,j}$ in the present formulation. In Eq. (11), $\vec{E}_{oi,1}$ and $\vec{H}_{oi,1}$ are defined by

$$\begin{bmatrix} \vec{E}_{oi,1} \\ \vec{H}_{oi,1} \end{bmatrix} = \begin{bmatrix} \vec{E}_0 \\ \vec{H}_0 \end{bmatrix} \exp(ik_o\hat{e}_{i,1} \cdot \vec{r}_1), \tag{14}$$

where $\vec{E}_0$ and $\vec{H}_0$ are the amplitude vectors of the incident electric and magnetic fields, respectively.

The reflected and refracted field vectors in Eqs. (12) and (13) can be determined from the electromagnetic boundary conditions [14,15] at the particle surface. For the TE mode, we have from Eqs. (11)–(13) the following expressions:

$$\vec{E}_{i,1}(\vec{r}) = E_{oi,1\perp}\hat{\beta}_1 \exp[ik_o\hat{e}_{i,1}(\vec{r}-\vec{r}_1)], \tag{15}$$

$$\vec{H}_{i,1}\left(\vec{r}\right) = \frac{1}{ik_o}\nabla \times \vec{E}_{i,1}(\vec{r}) = E_{oi,1\perp}\hat{\alpha}_{i,1} \exp\left[ik_o\hat{e}_{i,1}(\vec{r}-\vec{r}_1)\right], \tag{16}$$

$$\vec{E}_{r,1}(\vec{r}) = E_{or,1\perp}\hat{\beta}_1 \exp[ik_o\hat{e}_{r,1}(\vec{r}-\vec{r}_1)], \tag{17}$$

$$\vec{H}_{r,1}(\vec{r}) = \frac{1}{ik_o}\nabla \times \vec{E}_{r,1}(\vec{r}) = E_{or,1\perp}\hat{\alpha}_{r,1}\ \exp[ik_o\hat{e}_{r,1}(\vec{r} - \vec{r})], \tag{18}$$

$$\vec{E}_{t,1}(\vec{r}) = E_{ot,1\perp}\hat{\beta}_1\ \exp[ik_o(\hat{e}_{t,1}N_{r,1} + iN_{n,1}\hat{n}_1)(\vec{r} - \vec{r}_1)], \tag{19}$$

$$\vec{H}_{t,1}(\vec{r}) = \frac{1}{ik_o}\nabla \times \vec{E}_{t,1}(\vec{r}) = E_{ot,1\perp}(\hat{\alpha}_{t,1}N_{r,1} + iN_{n,1}\hat{e}_{f,1})\ \exp[ik_o(\hat{e}_{t,1}N_{r,1} + iN_{n,1}\hat{n}_1)(\vec{r} - \vec{r}_1)]. \tag{20}$$

The electromagnetic boundary conditions at $\vec{r} = \vec{r}_1$ for the TE mode require that

$$\hat{\beta}_1 \cdot \vec{E}_{i,1}(\vec{r}_1) + \hat{\beta}_1 \cdot \vec{E}_{r,1}(\vec{r}_1) = \hat{\beta}_1 \cdot \vec{E}_{t,1}(\vec{r}_1), \tag{21}$$

$$\hat{e}_{f,1} \cdot \vec{H}_{i,1}(\vec{r}_1) + \hat{e}_{f,1} \cdot \vec{H}_{r,1}(\vec{r}_1) = \hat{e}_{f,1} \cdot \vec{H}_{t,1}(\vec{r}_1), \tag{22}$$

which lead to the following relations:

$$E_{oi,1\perp} + E_{or,1\perp} = E_{ot,1\perp}, \tag{23}$$

$$E_{oi,1\perp}\cos\theta_{i,1} - E_{or,1\perp}\cos\theta_{r,1} = E_{ot,1\perp}(N_{r,1}\cos\theta_{t,1} + iN_{n,1}), \tag{24}$$

where $\theta_{i,1}$, $\theta_{r,1}$ and $\theta_{t,1}$ are the angles of incidence, reflection and refraction, respectively, as defined in Fig. 1. These are real quantities that can be related in terms of an effective refractive index $N_{r,1}$ via a generalized form of Snell's law [17]. Consequently, this approach alleviates the difficulty associated with the complex refraction angle that results from the conventional formulism. On the basis of Eqs. (23) and (24), we obtain the coefficients of transmission and reflection for the TE-mode electric fields as follows:

$$T_{E,1} = \frac{E_{ot,1\perp}}{E_{oi,1\perp}} = \frac{\cos\theta_{i,1} + \cos\theta_{r,1}}{\cos\theta_{r,1} + N_{r,1}\cos\theta_{t,1} + iN_{n,1}}, \tag{25}$$

$$R_{E,1} = \frac{E_{or,1\perp}}{E_{oi,1\perp}} = \frac{\cos\theta_{i,1} - (N_{r,1}\cos\theta_{t,1} + iN_{n,1})}{\cos\theta_{r,1} + N_{r,1}\cos\theta_{t,1} + iN_{n,1}}. \tag{26}$$

For the TM mode, we have

$$\vec{H}_{i,1}(\vec{r}) = H_{oi,1\perp}\hat{\beta}_1\ \exp[ik_o\hat{e}_{i,1}(\vec{r} - \vec{r}_1)], \tag{27}$$

$$\vec{E}_{i,1}(\vec{r}) = -\frac{1}{ik_o}\nabla \times \vec{H}_{i,1}(\vec{r}) = -\hat{\alpha}_{i,1}H_{oi,1\perp}\exp[ik_o\hat{e}_{i,1}(\vec{r} - \vec{r}_1)], \tag{28}$$

$$\vec{H}_{r,1}(\vec{r}) = H_{or,1\perp}\hat{\beta}_1\ \exp[ik_o\hat{e}_{r,1}(\vec{r} - \vec{r}_1)], \tag{29}$$

$$\vec{E}_{r,1}(\vec{r}) = -\frac{1}{ik_o}\nabla \times \vec{H}_{r,1}(\vec{r}) = -\hat{\alpha}_{r,1}H_{or,1\perp}\ \exp[ik_o\hat{e}_{r,1}(\vec{r} - \vec{r}_1)], \tag{30}$$

$$\vec{H}_{t,1}(\vec{r}) = H_{ot,1\perp}\hat{\beta}_1\ \exp[ik_o(\hat{e}_{t,1}N_{r,1} + iN_{n,1}\hat{n}_1)(\vec{r} - \vec{r}_1)], \tag{31}$$

$$\vec{E}_{t,1}(\vec{r}) = -\frac{1}{ik_o m^2}\nabla \times \vec{H}_{t,1}(\vec{r}) = -\frac{1}{m^2}(N_{r,1}\hat{\alpha}_{t,1} + iN_{n,1}\hat{e}_{f,1})H_{ot,1\perp}\ \exp[ik_o(\hat{e}_{t,1}N_{r,1} + iN_{n,1}\hat{n}_1)(\vec{r} - \vec{r}_1)]. \tag{32}$$

The boundary conditions at $\vec{r} = \vec{r}_1$ for the TM mode require the following relations:

$$\hat{\beta}_1 \cdot \vec{H}_{i,1}(\vec{r}_1) + \hat{\beta}_1 \cdot \vec{H}_{r,1}(\vec{r}_1) = \hat{\beta}_1 \cdot \vec{H}_{t,1}(\vec{r}_1), \tag{33}$$

$$\hat{e}_{f,1} \cdot \vec{E}_{i,1}(\vec{r}_1) + \hat{e}_{f,1} \cdot \vec{E}_{r,1}(\vec{r}_1) = \hat{e}_{f,1} \cdot \vec{E}_{t,1}(\vec{r}_1). \tag{34}$$

As a result of these two boundary conditions, we have the following two equations:

$$H_{oi,1\perp} + H_{or,1\perp} = H_{ot,1\perp}, \tag{35}$$

$$H_{oi,1\perp}\cos\theta_{i,1} - H_{or,1\perp}\cos\theta_{r,1} = \frac{1}{m^2}(N_{r,1}\cos\theta_{t,1} + iN_{n,1})H_{ot,1\perp}. \tag{36}$$

From Eqs. (35) and (36), we obtain the transmission and reflection coefficients for the TM-mode magnetic field as follows:

$$T_{M,1} = \frac{H_{ot,1\perp}}{H_{oi,1\perp}} = \frac{m^2(\cos\theta_{i,1} + \cos\theta_{r,1})}{m^2\cos\theta_{r,1} + N_{r,1}\cos\theta_{t,1} + iN_{n,1}}, \tag{37}$$

$$R_{M,1} = \frac{H_{or,1\perp}}{H_{oi,1\perp}} = \frac{m^2 \cos\theta_{i,1} - (N_{r,1}\cos\theta_{t,1} + iN_{n,1})}{m^2 \cos\theta_{r,1} + N_{r,1}\cos\theta_{t,1} + iN_{n,1}}. \tag{38}$$

Fig. 2 shows the geometric configuration for the jth ($j \geqslant 2$) reflection–refraction event when the refraction of an incident ray is from the particle to air. All the unit vectors defined in Fig. 2 have the same meanings as those displayed in Fig. 1. Note that the unit vector $\hat{n}_j$ in Fig. 2 has the direction pointing into the particle. For the jth-order reflection–refraction event, the electric and magnetic fields for the incident ray can be expressed in the form

$$\begin{bmatrix} \vec{E}_{i,j}(\vec{r}) \\ \vec{H}_{i,j}(\vec{r}) \end{bmatrix} = \begin{bmatrix} \vec{E}_{oi,j} \\ \vec{H}_{oi,j} \end{bmatrix} \exp[ik_o(\hat{e}_{i,j}N_{r,j-1} + i\hat{n}_{j-1}N_{n,j-1})(\vec{r} - \vec{r}_j)]. \tag{39}$$

For $j = 2$, the amplitude vectors of the second-order incident ray are as follows:

$$\begin{bmatrix} \vec{E}_{oi,2} \\ \vec{H}_{oi,2} \end{bmatrix} = \begin{bmatrix} \vec{E}_{ot,1} \\ \vec{H}_{ot,1} \end{bmatrix} \exp[ik_o(\hat{e}_{t,1}N_{r,1} + i\hat{n}_1 N_{n,1})(\vec{r}_2 - \vec{r}_1)]. \tag{40}$$

For $j \geqslant 3$, the amplitude vectors of the jth-order incident ray are as follows:

$$\begin{bmatrix} \vec{E}_{oi,j} \\ \vec{H}_{oi,j} \end{bmatrix} = \begin{bmatrix} \vec{E}_{or,j-1} \\ \vec{H}_{or,j-1} \end{bmatrix} \exp[ik_o(\hat{e}_{r,j-1}N_{r,j-1} + i\hat{n}_{j-1}N_{n,j-1})(\vec{r}_j - \vec{r}_{j-1})]. \tag{41}$$

The jth-order reflected and refracted electric and magnetic field vectors are given by

$$\begin{bmatrix} \vec{E}_{r,j}(\vec{r}) \\ \vec{H}_{r,j}(\vec{r}) \end{bmatrix} = \begin{bmatrix} \vec{E}_{or,j} \\ \vec{H}_{or,j} \end{bmatrix} \exp[ik_o(\hat{e}_{r,j}N_{r,j} + i\hat{n}_j N_{n,j})(\vec{r} - \vec{r}_j)], \tag{42}$$

$$\begin{bmatrix} \vec{E}_{t,j}(\vec{r}) \\ \vec{H}_{t,j}(\vec{r}) \end{bmatrix} = \begin{bmatrix} \vec{E}_{ot,j} \\ \vec{H}_{ot,j} \end{bmatrix} \exp[ik_o\hat{e}_{t,j}(\vec{r} - \vec{r}_j)], \tag{43}$$

where the effective refractive indices, $N_{r,j}$ and $N_{n,j}$, can be determined by the recurrence formulae derived by Yang and Liou [17].

For the jth-order TE mode, we have

$$\vec{E}_{i,j}(\vec{r}) = E_{oi,j\perp}\hat{\beta}_j \exp[ik_o(\hat{e}_{i,j}N_{r,j-1} + i\hat{n}_{j-1}N_{n,j-1})(\vec{r} - \vec{r}_j)], \tag{44}$$

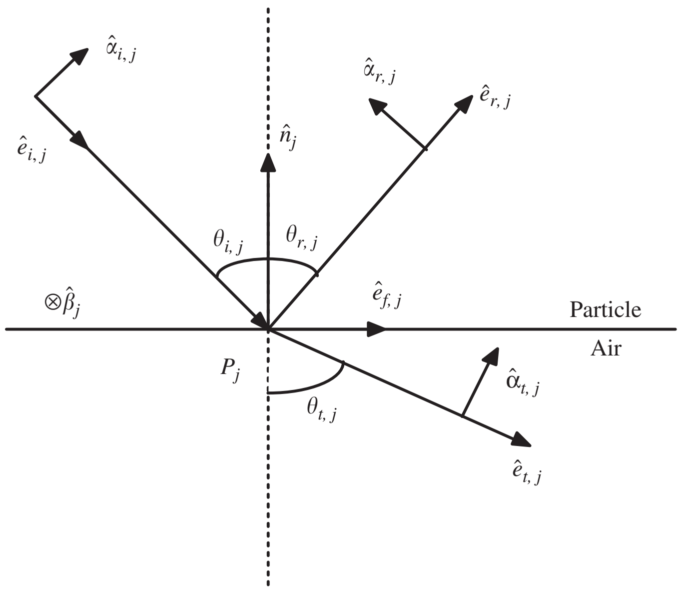

Fig. 2. The geometric configuration for the jth-order incident, reflected and refracted rays at point P_j when the refraction of an incident ray is from the particle into the air.

$$\vec{H}_{i,j}(\vec{r}) = \frac{1}{ik_o}\nabla \times \vec{E}_{i,j}(\vec{r}) = [N_{r,j-1}\hat{\alpha}_{i,j} + iN_{n,j-1}(\hat{n}_{j-1} \times \hat{\beta}_j)]E_{oi,j\perp} \exp[ik_o(\hat{e}_{i,j}N_{r,j-1} + i\hat{n}_{j-1}N_{n,j-1})(\vec{r} - \vec{r}_j)], \tag{45}$$

$$\vec{E}_{r,j}(\vec{r}) = E_{or,j\perp}\hat{\beta}_j \exp[ik_o(\hat{e}_{r,j}N_{r,j} + i\hat{n}_jN_{n,j})(\vec{r} - \vec{r}_j)], \tag{46}$$

$$\vec{H}_{r,j}(\vec{r}) = \frac{1}{ik_o}\nabla \times \vec{E}_{r,j}(\vec{r}) = [N_{r,j}\hat{\alpha}_{r,j} - iN_{n,j}\hat{e}_{f,j}]E_{or,j\perp} \exp[ik_o(\hat{e}_{r,j}N_{r,j} + i\hat{n}_jN_{n,j})(\vec{r} - \vec{r}_j)], \tag{47}$$

$$\vec{E}_{t,j}(\vec{r}) = E_{ot,j\perp}\hat{\beta}_j \exp[ik_o\hat{e}_{t,j}(\vec{r} - \vec{r}_j)], \tag{48}$$

$$\vec{H}_{t,j}(\vec{r}) = \frac{1}{ik_o}\nabla \times \vec{E}_{t,j}(\vec{r}) = \hat{\alpha}_{t,j}E_{ot,j\perp} \exp[ik_o\hat{e}_{t,j}(\vec{r} - \vec{r}_j)]. \tag{49}$$

The electromagnetic boundary conditions at point P_j require the following relationships:

$$\hat{\beta}_j \cdot \vec{E}_{i,j}(\vec{r}_j) + \hat{\beta}_j \cdot \vec{E}_{r,j}(\vec{r}_j) = \hat{\beta}_j \cdot \vec{E}_{t,j}(\vec{r}_j), \tag{50}$$

$$\hat{e}_{f,j} \cdot \vec{H}_{i,j}(\vec{r}_j) + \hat{e}_{f,j} \cdot \vec{H}_{r,j}(\vec{r}_j) = \hat{e}_{f,j} \cdot \vec{H}_{t,j}(\vec{r}_j). \tag{51}$$

Eqs. (50) and (51) can be simplified as follows:

$$E_{oi,j\perp} + E_{or,j\perp} = E_{ot,j\perp}, \tag{52}$$

$$(N_{r,j-1} \cos \theta_{i,j} - iN_{n,j-1}\hat{n}_{j-1} \cdot \hat{n}_j)E_{oi,j\perp} - (N_{r,j} \cos \theta_{r,j} + iN_{n,j})E_{or,j\perp} = E_{ot,j\perp} \cos \theta_{t,j}. \tag{53}$$

After some algebraic manipulations, we can obtain from Eqs. (52) and (53) the transmission and reflection coefficients for the jth-order TM-mode electric fields as follows:

$$T_{E,j} = \frac{E_{ot,j\perp}}{E_{oi,j\perp}} = \frac{N_{r,j} \cos \theta_{r,j} + iN_{n,j} + N_{r,j-1} \cos \theta_{i,j} - iN_{n,j-1}\hat{n}_{j-1} \cdot \hat{n}_j}{N_{r,j} \cos \theta_{r,j} + iN_{n,j} + \cos \theta_{t,j}}, \tag{54}$$

$$R_{E,j} = \frac{E_{or,j\perp}}{E_{oi,j\perp}} = \frac{N_{r,j-1} \cos \theta_{i,j} - iN_{n,j-1}\hat{n}_{j-1} \cdot \hat{n}_j - \cos \theta_{t,j}}{N_{r,j} \cos \theta_{r,j} + iN_{n,j} + \cos \theta_{t,j}}. \tag{55}$$

For the TM mode associated with the jth-order reflection–refraction events, we have

$$\vec{H}_{i,j}(\vec{r}) = H_{oi,j\perp}\hat{\beta}_j \exp[ik_o(\hat{e}_{i,j}N_{r,j-1} + i\hat{n}_{j-1}N_{n,j-1})(\vec{r} - \vec{r}_j)], \tag{56}$$

$$\begin{aligned}\vec{E}_{i,j}(\vec{r}) &= -\frac{1}{ik_om^2}\nabla \times \vec{H}_{i,j}(\vec{r}) \\ &= -\frac{1}{m^2}[N_{r,j-1}\hat{\alpha}_{i,j} + iN_{n,j-1}(\hat{n}_{j-1} \times \hat{\beta}_j)]H_{oi,j\perp} \exp[ik_o(\hat{e}_{i,j}N_{r,j-1} + i\hat{n}_{j-1}N_{n,j-1})(\vec{r} - \vec{r}_j)],\end{aligned} \tag{57}$$

$$\vec{H}_{r,j}(\vec{r}) = H_{or,j\perp}\hat{\beta}_j \exp[ik_o(\hat{e}_{r,j}N_{r,j} + i\hat{n}_jN_{n,j})(\vec{r} - \vec{r}_j)], \tag{58}$$

$$\vec{E}_{r,j}(\vec{r}) = -\frac{1}{ik_om^2}\nabla \times \vec{H}_{r,j}(\vec{r}) = -\frac{1}{m^2}[N_{r,j}\hat{\alpha}_{r,j} - iN_n\hat{e}_{f,j}]H_{or,j\perp} \exp[ik_o(\hat{e}_{r,j}N_{r,j} + i\hat{n}_jN_{n,j})(\vec{r} - \vec{r}_j)], \tag{59}$$

$$\vec{H}_{t,j}(\vec{r}) = H_{ot,j\perp}\hat{\beta}_j \exp[ik_o\hat{e}_{t,j}(\vec{r} - \vec{r}_j)], \tag{60}$$

$$\vec{E}_{t,j}(\vec{r}) = -\frac{1}{ik_o}\nabla \times \vec{H}_{t,j}(\vec{r}) = -\hat{\alpha}_{t,j}H_{ot,j\perp} \exp[ik_o\hat{e}_{t,j}(\vec{r} - \vec{r}_j)]. \tag{61}$$

The boundary conditions at point P_j are as follows:

$$\hat{\beta}_j \cdot \vec{H}_{i,j}(\vec{r}_j) + \hat{\beta}_j \cdot \vec{H}_{r,j}(\vec{r}_j) = \hat{\beta}_j \cdot \vec{H}_{t,j}(\vec{r}_j), \tag{62}$$

$$\hat{e}_{f,j} \cdot \vec{E}_{i,j}(\vec{r}_j) + \hat{e}_{f,j} \cdot \vec{E}_{r,j}(\vec{r}_j) = \hat{e}_{f,j} \cdot \vec{E}_{t,j}(\vec{r}_j). \tag{63}$$

Eqs. (62) and (63) can be written in more explicit forms as follows:

$$H_{oi,j\perp} + H_{or,j\perp} = H_{ot,j\perp}, \tag{64}$$

$$(N_{r,j-1} \cos \theta_{i,j} - iN_{n,j-1}\hat{n}_{j-1} \cdot \hat{n}_j)H_{oi,j\perp} - (N_{r,j} \cos \theta_{r,j} + iN_{n,j})H_{or,j\perp} = H_{ot,j\perp}m^2 \cos \theta_{t,j}. \tag{65}$$

From Eqs. (64) and (65), the transmission and reflection coefficients for the TM-mode magnetic fields are given by

$$T_{H,j} = \frac{H_{ot,j\perp}}{H_{oi,j\perp}} = \frac{N_r \cos\theta_{r,j} + iN_{n,j} + N_{r,j-1}\cos\theta_{i,j} - iN_{n,j-1}\hat{n}_{j-1}\cdot\hat{n}_j}{N_{r,j}\cos\theta_{r,j} + iN_{n,j} + m^2\cos\theta_{t,j}}, \tag{66}$$

$$R_{H,j} = \frac{H_{or,j\perp}}{H_{oi,j\perp}} = \frac{N_{r,j-1}\cos\theta_{i,j} - iN_{n,j-1}\hat{n}_{j-1}\cdot\hat{n}_j - m^2\cos\theta_{t,j}}{N_{r,j}\cos\theta_{r,j} + iN_{n,j} + m^2\cos\theta_{t,j}}. \tag{67}$$

Eqs. (25), (26), (54), and (55) represent the generalized Fresnel coefficients for the electric fields in the TE mode for a general dielectric particle with absorption, whereas Eqs. (37), (38), (66), and (67) are their counterparts for the magnetic fields in the TM mode. Evidently, unlike the conventional Fresnel formulae, the present formulation of the reflection and refraction coefficients does not involve complex angles in the case of a complex refractive index. In the case when the imaginary refractive index $m_i = 0$, it is straightforward to convert the reflection and refraction coefficients for the TM mode magnetic field components to their counterparts for the corresponding electric field components parallel to the incident plane. After the conversion, the generalized Fresnel formulae for the electric field components reduce to the conventional Fresnel formulae presented in many texts [18,19]. Note that an alternative approach has been suggested by Chang et al. [16] to calculate the Fresnel coefficients and ray propagation associated with an absorbing medium.

3. An "exact" ray-tracing approach for an absorbing particle

Fig. 3 schematically illustrates the incident and scattering configurations associated with the jth-order scattered ray. Note that the first-order scattered rays represent external reflections, while higher-order scattered rays denote ray transmissions. In Fig. 3, the unit vector $\hat{e}_{s,j}$ denotes the direction of the jth-order scattered ray and the term $\hat{\beta}_{s,j}$ is a unit vector normal to the scattering plane, which can be determined by

$$\hat{\beta}_{s,j} = \frac{\hat{e}_{s,j}\times\hat{z}}{|\hat{e}_{s,j}\times\hat{z}|}, \tag{68}$$

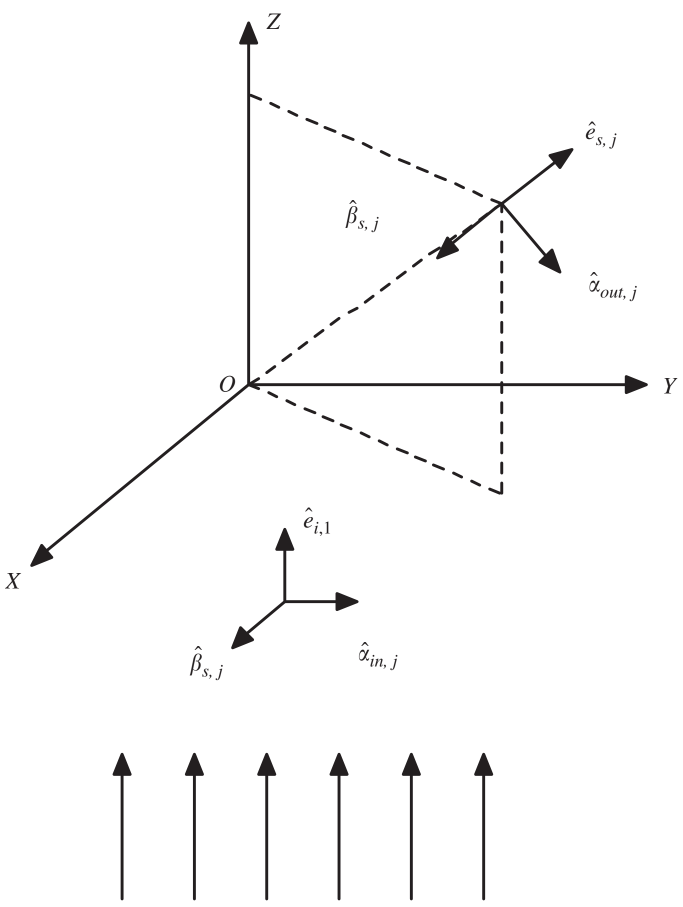

Fig. 3. The incident and scattering geometries involved in the ray-tracing computation.

where $\hat{z}$ denotes a unit vector pointing along the z-axis. In Eq. (68), this term cannot be determined in the exact forward or backward direction, i.e. $\hat{e}_{s,j} = \pm\hat{z}$. In this case, we define

$$\hat{\beta}_{s,j} = \hat{x}, \tag{69}$$

where $\hat{x}$ is a unit vector pointing along the x-axis. In Fig. 3, $\hat{\alpha}_{out,j}$ and $\hat{\alpha}_{in,j}$ are defined as follows:

$$\hat{\alpha}_{out,j} = \hat{e}_{s,j} \times \hat{\beta}_{s,j}, \tag{70}$$

$$\hat{\alpha}_{in,j} = \hat{e}_{i,1} \times \hat{\beta}_{s,j}. \tag{71}$$

The scattered electric field associated with the jth-order scattered rays can be expressed in the form

$$\begin{bmatrix} E_{s,j//} \\ E_{s,j\perp} \end{bmatrix} = \begin{bmatrix} A_{2,j} & A_{3,j} \\ A_{4,j} & A_{1,j} \end{bmatrix} \begin{bmatrix} E_{0,j//} \\ E_{0,j\perp} \end{bmatrix} \exp(ik_0 r), \tag{72}$$

where $E_{0,j//}$ and $E_{0,j\perp}$ are the parallel and perpendicular components of the incident electric amplitude vector, respectively, defined in reference to the scattering plane. $A_{1,j}$, $A_{2,j}$, $A_{3,j}$, and $A_{4,j}$ are the four elements of the scattering matrix associated with the jth-order scattered rays. The present notation convention for the scattering matrix associated with an individual scattered ray is similar to that for the scattering matrix defined by van de Hulst [19]. The key step in ray-tracing calculations is to determine the scattering matrix defined in Eq. (72) in terms of recurrence formulae.

Referring to the geometry defined in Fig. 1 and using Eqs. (4)–(7), we can express the first-order incident electric field as follows:

$$\vec{E}_{i,1} = E_{i,1\perp}\hat{\beta}_1 - (\hat{e}_{i,1} \times \hat{\beta}_1)H_{i,1\perp} = E_{i,1\perp}\hat{\beta}_1 - \hat{\alpha}_{i,1}H_{i,1\perp}, \tag{73}$$

$$\vec{H}_{i,1} = H_{i,1\perp}\hat{\beta}_1 + (\hat{e}_{i,1} \times \hat{\beta}_1)E_{i,1\perp} = H_{i,1\perp}\hat{\beta}_1 + \hat{\alpha}_{i,1}E_{i,1\perp}. \tag{74}$$

The corresponding reflected and refracted electric fields, decomposed with respect to the incident plane, can be expressed in the forms

$$\begin{bmatrix} H_{r,1\perp} \\ E_{r,1\perp} \end{bmatrix} = \begin{bmatrix} R_{H,1} & 0 \\ 0 & R_{E,1} \end{bmatrix} \begin{bmatrix} H_{i,1\perp} \\ E_{i,1\perp} \end{bmatrix} \exp[ik_o\hat{e}_{r,j}(\vec{r} - \vec{r}_1)], \tag{75}$$

$$\begin{bmatrix} H_{t,1\perp} \\ E_{t,1\perp} \end{bmatrix} = \begin{bmatrix} T_{H,1} & 0 \\ 0 & T_{E,1} \end{bmatrix} \begin{bmatrix} H_{i,1\perp} \\ E_{i,1\perp} \end{bmatrix} \exp[ik_o(\hat{e}_{r,j}N_{r,1} + iN_{n,1}\hat{n}_1)(\vec{r} - \vec{r}_1)]. \tag{76}$$

Furthermore, the externally reflected electric field vector can be written as follows:

$$\vec{E}_{r,1} = E_{r,1\perp}\hat{\beta}_1 - (\hat{e}_{r,1} \times \hat{\beta}_1)H_{r,1\perp} = E_{r,1\perp}\hat{\beta}_1 - \hat{\alpha}_{r,1}H_{r,1\perp} = E_{r,1\perp}\hat{\beta}_1 + E_{r,1//}\hat{\alpha}_{r,1}, \tag{77}$$

where $E_{r,1\parallel} = -H_{r,1\perp}$ and the refracted electric and magnetic vectors can be expressed by the following equations:

$$\begin{aligned} \vec{E}_{t,1} &= E_{t,1\perp}\hat{\beta}_1 + \left[-\frac{(N_{r,1}\hat{e}_{t,1} + iN_{n,1}\hat{n}_1) \times \hat{\beta}_1}{m^2}\right]H_{t,1\perp} \\ &= E_{t,1\perp}\hat{\beta}_1 + \left(-\frac{N_{r,1}\hat{\alpha}_{t,1} + iN_{n,1}\hat{e}_{f,1}}{m^2}\right)H_{t,1\perp}, \end{aligned} \tag{78}$$

$$\vec{H}_{t,1} = H_{t,1\perp}\hat{\beta}_1 + (N_{r,1}\hat{e}_{t,1} + iN_{n,1}\hat{n}_1) \times \hat{\beta}_1 E_{t,1\perp} = H_{t,1\perp}\hat{\beta}_1 + (N_{r,1}\hat{\alpha}_{t,1} + iN_{n,1}\hat{e}_{f,1})E_{t,1\perp}. \tag{79}$$

The first-order scattered electric field vector, decomposed in reference to the scattering plane shown in Fig. 3, can be expressed as follows:

$$\begin{aligned} \begin{bmatrix} E_{s,1//} \\ E_{s,1\perp} \end{bmatrix} &= \begin{bmatrix} \hat{\alpha}_{out,1} \cdot \hat{\alpha}_{r,1} & \hat{\alpha}_{out,1} \cdot \hat{\beta}_1 \\ \hat{\beta}_{s,1} \cdot \hat{\alpha}_{r,1} & \hat{\beta}_{s,1} \cdot \hat{\beta}_1 \end{bmatrix} \begin{bmatrix} E_{r,1//} \\ E_{r,1\perp} \end{bmatrix} = \begin{bmatrix} \hat{\alpha}_{out,1} \cdot \hat{\alpha}_{r,1} & \hat{\alpha}_{out,1} \cdot \hat{\beta}_1 \\ \hat{\beta}_{s,1} \cdot \hat{\alpha}_{r,1} & \hat{\beta}_{s,1} \cdot \hat{\beta}_1 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} H_{r,1\perp} \\ E_{r,1\perp} \end{bmatrix} \\ &= \begin{bmatrix} \hat{\alpha}_{out,1} \cdot \hat{\alpha}_{r,1} & \hat{\alpha}_{out,1} \cdot \hat{\beta}_1 \\ \hat{\beta}_{s,1} \cdot \hat{\alpha}_{r,1} & \hat{\beta}_{s,1} \cdot \hat{\beta}_1 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} R_{H,1} & 0 \\ 0 & R_{E,1} \end{bmatrix} \begin{bmatrix} H_{i,1\perp}(\vec{r}_1) \\ E_{i,1\perp}(\vec{r}_1) \end{bmatrix} \exp[ik_o\hat{e}_{r,1}(\vec{r} - \vec{r}_1)], \end{aligned} \tag{80}$$

where the last term can be expressed by

$$\begin{bmatrix} H_{i,1\perp}(\vec{r}_1) \\ E_{i,1\perp}(\vec{r}_1) \end{bmatrix} = \begin{bmatrix} -E_{i,1//}(\vec{r}_1) \\ E_{i,1\perp}(\vec{r}_1) \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{\alpha}_{i,1} \cdot \hat{\alpha}_{in,1} & \hat{\alpha}_{i,1} \cdot \hat{\beta}_{s,1} \\ \hat{\beta}_1 \cdot \hat{\alpha}_{in,1} & \hat{\beta}_1 \cdot \hat{\beta}_{s,1} \end{bmatrix} \begin{bmatrix} E_{0,1//} \\ E_{0,1\perp} \end{bmatrix} \exp(ik_o\hat{e}_{i,1} \cdot \vec{r}_1). \tag{81}$$

Thus, the scattering matrix for externally reflected rays can be written as

$$\begin{bmatrix} A_{2,1} & A_{3,1} \\ A_{4,1} & A_{1,1} \end{bmatrix} = \begin{bmatrix} M_{2,1} & M_{3,1} \\ M_{4,1} & M_{1,1} \end{bmatrix} \exp[ik_o(\hat{e}_{i,1} \cdot \vec{r}_1 - \hat{e}_{r,1} \cdot \vec{r}_1)], \tag{82}$$

$$\begin{bmatrix} M_{2,1} & M_{3,1} \\ M_{4,1} & M_{1,1} \end{bmatrix} = \begin{bmatrix} \hat{\alpha}_{out,1} \cdot \hat{\alpha}_{r,1} & \hat{\alpha}_{out,1} \cdot \hat{\beta}_1 \\ \hat{\beta}_{s,1} \cdot \hat{\alpha}_{r,1} & \hat{\beta}_{s,1} \cdot \hat{\beta}_1 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} R_{H,1} & 0 \\ 0 & R_{E,1} \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{\alpha}_{i,1} \cdot \hat{\alpha}_{in,1} & \hat{\alpha}_{i,1} \cdot \hat{\beta}_{s,1} \\ \hat{\beta}_1 \cdot \hat{\alpha}_{in,1} & \hat{\beta}_{s,1} \cdot \hat{\beta}_1 \end{bmatrix}. \tag{83}$$

For second-order reflection–refraction events, the perpendicular components of the electric and magnetic fields, defined with respect to the incident plan, can be written as follows:

$$\begin{aligned} E_{i,2\perp}(\vec{r}_2) &= \vec{E}_{t,1}(\vec{r}_2)\hat{\beta}_2 = \left[\hat{\beta}_1 E_{t,1\perp}(\vec{r}_2) - \frac{(N_{r,1}\hat{e}_{t,1} + iN_{n,1}\hat{n}_1) \times \hat{\beta}_1}{m^2} H_{t,1\perp}(\vec{r}_2)\right]\hat{\beta}_2 \\ &= (\hat{\beta}_1 \cdot \hat{\beta}_2)E_{t,1\perp}(\vec{r}_2) - \frac{N_{r,1}(\hat{\beta}_2 \cdot \hat{\alpha}_{t,1}) + iN_{n,1}(\hat{e}_{f,1} \cdot \hat{\beta}_2)}{m^2} H_{t,1\perp}(\vec{r}_2), \end{aligned} \tag{84}$$

$$\begin{aligned} H_{i,2\perp}(\vec{r}_2) &= \vec{H}_{t,2}(\vec{r}_2)\hat{\beta}_2 = [\hat{\beta}_1 H_{t,1\perp}(\vec{r}_2) + (N_{r,1}\hat{e}_{t,1} + iN_{n,1}\hat{n}_1) \times \hat{\beta}_1 E_{t,1\perp}(\vec{r}_2)]\hat{\beta}_2 \\ &= (\hat{\beta}_1 \cdot \hat{\beta}_2)H_{t,1\perp}(\vec{r}_2) + [N_{r,1}(\hat{\alpha}_{t,1} \cdot \hat{\beta}_2) + iN_{n,1}(\hat{\beta}_2 \cdot \hat{e}_{f,1})]E_{t,1\perp}(\vec{r}_2). \end{aligned} \tag{85}$$

Alternatively, we may express Eqs. (84) and (85) in a compact matrix form as follows:

$$\begin{bmatrix} H_{i,2\perp}(\vec{r}_2) \\ E_{i,2\perp}(\vec{r}_2) \end{bmatrix} = \begin{bmatrix} \hat{\beta}_1 \cdot \hat{\beta}_2 & N_{r,1}(\hat{\alpha}_{t,1} \cdot \hat{\beta}_2) + iN_{n,1}(\hat{\beta}_1 \cdot \hat{e}_{f,1}) \\ -\dfrac{N_{r,1}(\hat{\alpha}_{t,1} \cdot \hat{\beta}_2) + iN_{n,1}(\hat{\beta}_2 \cdot \hat{e}_{f,1})}{m^2} & \hat{\beta}_1 \cdot \hat{\beta}_2 \end{bmatrix} \begin{bmatrix} H_{t,1\perp}(\vec{r}_2) \\ E_{t,1\perp}(\vec{r}_2) \end{bmatrix}. \tag{86}$$

The corresponding second-order reflected and refracted field vectors can be written in the forms

$$\begin{bmatrix} H_{r,2\perp}(\vec{r}) \\ E_{r,2\perp}(\vec{r}) \end{bmatrix} = \begin{bmatrix} R_{H,2} & 0 \\ 0 & R_{E,2} \end{bmatrix} \begin{bmatrix} H_{i,2\perp}(\vec{r}_2) \\ E_{i,2\perp}(\vec{r}_2) \end{bmatrix} \exp[ik_o(N_{r,2}\hat{e}_{r,1} + iN_{n,2}\hat{n}_2)(\vec{r} - \vec{r}_2)], \tag{87}$$

$$\begin{bmatrix} H_{t,2\perp}(\vec{r}) \\ E_{t,2\perp}(\vec{r}) \end{bmatrix} = \begin{bmatrix} T_{H,2} & 0 \\ 0 & T_{E,2} \end{bmatrix} \begin{bmatrix} H_{i,2\perp}(\vec{r}_2) \\ E_{i,2\perp}(\vec{r}_2) \end{bmatrix} \exp[ik_o\hat{e}_{t,2}(\vec{r} - \vec{r}_2)]. \tag{88}$$

Based on Eq. (88) and some algebraic manipulations similar to the case of $j = 1$, the scattering matrix for the second-order scattered rays can be written as follows:

$$\begin{bmatrix} A_{2,2} & A_{3,2} \\ A_{4,2} & A_{1,2} \end{bmatrix} = \begin{bmatrix} M_{2,2} & M_{3,2} \\ M_{4,2} & M_{1,2} \end{bmatrix} \exp\{ik_o[\hat{e}_{i,1} \cdot \vec{r}_1 + (N_{r,1}\hat{e}_{t,1} + iN_{n,1}\hat{n}_1)(\vec{r}_2 - \vec{r}_1) - \hat{e}_{t,2} \cdot \vec{r}_2]\}, \tag{89}$$

$$\begin{aligned} \begin{bmatrix} M_{2,2} & M_{3,2} \\ M_{4,2} & M_{1,2} \end{bmatrix} &= \left(\frac{\cos\theta_{t,2}\cos\theta_{t,1}}{\cos\theta_{i,2}\cos\theta_{i,1}}\right)^{1/2} \begin{bmatrix} \hat{\alpha}_{out,2} \cdot \hat{\alpha}_{t,2} & \hat{\alpha}_{out,2} \cdot \hat{\beta}_2 \\ \hat{\beta}_{s,2} \cdot \hat{\alpha}_{t,2} & \hat{\beta}_{s,2} \cdot \hat{\beta}_2 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} T_{H,2} & 0 \\ 0 & T_{E,2} \end{bmatrix} \\ &\times \begin{bmatrix} \hat{\beta}_2 \cdot \hat{\beta}_1 & N_{r,1}(\hat{\alpha}_{t,1} \cdot \hat{\beta}_2) + iN_{n,1}(\hat{\beta}_2 \cdot \hat{e}_{f,1}) \\ -\dfrac{N_{r,1}(\hat{\alpha}_{t,1} \cdot \hat{\beta}_2) + iN_{n,1}(\hat{\beta}_2 \cdot \hat{e}_{f,1})}{m^2} & \hat{\beta}_2 \cdot \hat{\beta}_1 \end{bmatrix} \\ &\times \begin{bmatrix} T_{H,1} & 0 \\ 0 & T_{E,1} \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{\alpha}_{i,1} \cdot \hat{\alpha}_{in,2} & \hat{\alpha}_{i,1} \cdot \hat{\beta}_{s,2} \\ \hat{\beta}_2 \cdot \hat{\alpha}_{in,2} & \hat{\beta}_{s,2} \cdot \hat{\beta}_2 \end{bmatrix}. \end{aligned} \tag{90}$$

In a strong absorption case, the value of the exponential function in Eq. (89) is quite small for a size parameter in the geometric optics regime such that only external reflections essentially dominate the scattered field. The term $[(\cos\theta_{t,2}\cos\theta_{t,1})/(\cos\theta_{i,2}\cos\theta_{i,1})]^{1/2}$ in Eq. (90) is included to satisfy the law of conservation of energy [12]. Similarly, for the jth ($j \geqslant 3$) order, the scattering matrix can be given as follows:

$$\begin{aligned} \begin{bmatrix} A_{2,j} & A_{3,j} \\ A_{4,j} & A_{1,j} \end{bmatrix} &= \begin{bmatrix} M_{2,j} & M_{3,j} \\ M_{4,j} & M_{1,j} \end{bmatrix} \exp\{ik_o[\hat{e}_{i,1} \cdot \vec{r}_1 + (N_{r,1}\hat{e}_{t,1} + iN_{n,1}\hat{n}_1)(\vec{r}_2 - \vec{r}_1) \\ &+ (N_{r,2}\hat{e}_{r,2} + iN_{n,2}\hat{n}_2)(\vec{r}_3 - \vec{r}_2)\ldots(N_{r,j-1}\hat{e}_{r,j-1} + iN_{n,j-1}\hat{n}_{j-1})(\vec{r}_j - \vec{r}_{j-1}) - \hat{e}_{t,j} \cdot \vec{r}_j]\}, \end{aligned} \tag{91}$$

$$\begin{bmatrix} M_{2,j} & M_{3,j} \\ M_{4,j} & M_{1,j} \end{bmatrix} = \left(\frac{\cos\,\theta_{t,j}\,\cos\,\theta_{r,j-1}\ldots\cos\,\theta_{r,2}\,\cos\,\theta_{t,1}}{\cos\,\theta_{i,j}\,\cos\,\theta_{i,j-1}\ldots\cos\,\theta_{i,2}\,\cos\,\theta_{i,1}} \right)^{1/2} \begin{bmatrix} \hat{\alpha}_{out,j}\cdot\hat{\alpha}_{t,j} & \hat{\alpha}_{out,j}\cdot\hat{\beta}_j \\ \hat{\beta}_{s,j}\cdot\hat{\alpha}_{t,j} & \hat{\beta}_{s,j}\cdot\hat{\beta}_j \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} T_{H,j} & 0 \\ 0 & T_{E,j} \end{bmatrix}$$
$$\times \begin{bmatrix} \hat{\beta}_j\cdot\hat{\beta}_{j-1} & N_{r,j-1}(\hat{\alpha}_{r,j-1}\cdot\hat{\beta}_j) + iN_{n,j-1}(\hat{e}_{f,j-1}\cdot\hat{\beta}_j) \\ -\dfrac{N_{r,j-1}(\hat{\alpha}_{r,j-1}\cdot\hat{\beta}_j) + iN_{n,j-1}(\hat{e}_{f,j-1}\cdot\hat{\beta}_j)}{m^2} & \hat{\beta}_j\cdot\hat{\beta}_{j-1} \end{bmatrix}$$
$$\times \begin{bmatrix} R_{H,j-1} & 0 \\ 0 & R_{E,j-1} \end{bmatrix}$$
$$\times \begin{bmatrix} \hat{\beta}_{j-1}\cdot\hat{\beta}_{j-2} & N_{r,j-2}(\hat{\alpha}_{r,j-2}\cdot\hat{\beta}_{j-1}) + iN_{n,j-2}(\hat{e}_{f,j-2}\cdot\hat{\beta}_{j-1}) \\ -\dfrac{N_{r,j-2}(\hat{\alpha}_{r,j-2}\cdot\hat{\beta}_{j-1}) + iN_{n,j-2}(\hat{e}_{f,j-2}\cdot\hat{\beta}_{j-1})}{m^2} & \hat{\beta}_{j-1}\cdot\hat{\beta}_{j-2} \end{bmatrix}$$
$$\times \begin{bmatrix} R_{H,j-2} & 0 \\ 0 & R_{E,j-2} \end{bmatrix} \cdots \begin{bmatrix} T_{H,1} & 0 \\ 0 & T_{E,1} \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{\alpha}_{i,1}\cdot\hat{\alpha}_{in,j} & \hat{\alpha}_{i,1}\cdot\hat{\beta}_{s,j} \\ \hat{\beta}_j\cdot\hat{\alpha}_{in,j} & \hat{\beta}_j\cdot\hat{\beta}_{s,j} \end{bmatrix}, \tag{92}$$

where the term $[(\cos\,\theta_{t,j}\,\cos\,\theta_{r,j-1}\ldots\cos\,\theta_{r,2}\,\cos\,\theta_{t,1})/(\cos\,\theta_{i,j}\,\cos\,\theta_{i,j-1}\ldots\cos\,\theta_{i,2}\,\cos\,\theta_{i,1})]^{1/2}$ is introduced for the conservation of energy, similar to the case presented in Eq. (90). Note that within an absorbing particle, the angle of incidence can differ from the angle of reflection for a geometric optics ray, as shown by Yang and Liou [17].

Following van de Hulst [19], we express the scattered electric field in terms of the scattering matrix and the incident electric field as follows:

$$\begin{bmatrix} E_{s,//} \\ E_{s,\perp} \end{bmatrix} = \frac{e^{ikr}}{-ikr} \begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix} \begin{bmatrix} E_{0,//} \\ E_{0,\perp} \end{bmatrix}. \tag{93}$$

In the framework of the conventional ray-tracing technique, the scattering matrix can be decomposed into contributions from geometric reflection and refraction (denoted by subscript *ray*) and diffraction (denoted by subscript *dif*) in the form

$$\begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix} = \begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix}_{ray} + \begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix}_{dif}. \tag{94}$$

In the conventional ray-tracing calculation for the single-scattering properties of a dielectric particle, the 4π directional space is discretized in terms of a number of small solid angle elements given by

$$\Delta\Omega_{u,v} = \sin\left(\frac{\theta_{u+1}+\theta_u}{2}\right)(\theta_{u+1}-\theta_u)(\varphi_{v+1}-\varphi_v), \tag{95}$$

where θ_u and φ_v denote discretization nodes of the scattering zenith and azimuthal angles, respectively. In the direction specified by a scattering zenith angle θ_s and an azimuth angle φ_s, the contribution of geometric optics rays to the scattering matrix can be written as follows:

$$\begin{aligned} \begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix}_{ray} &= \sum_p \sum_j \begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix}_{ray,p,j} \\ &= \sum_p \sum_j -ik\left(\frac{\Delta\sigma_{p,j}}{\Delta\Omega_{u,v}}\right)^{1/2} W_{u,v} \begin{bmatrix} A_{2,j} & A_{3,j} \\ A_{4,j} & A_{1,j} \end{bmatrix}_p \quad \text{for} \begin{cases} \theta_s = (\theta_u+\theta_{u+1})/2, \\ \varphi_s = (\varphi_v+\varphi_{v+1})/2, \end{cases} \end{aligned} \tag{96}$$

where the subscript p denotes an incident ray within the particle projected area on a plane normal to the incident direction, the subscript j denotes the jth-order scattered ray whose cross section is $\Delta\sigma_{p,j}$, which is associated with the pth-incident ray, and $W_{u,v}$ is a weight given by

$$W_{u,v} = \begin{cases} 1 & \text{if} \quad \theta_{s,j} \in [\theta_u, \theta_{u+1}] \quad \text{and} \quad \varphi_{s,j} \in [\varphi_u, \varphi_{u+1}], \\ 0 & \text{if} \quad \theta_{s,j} \notin [\theta_u, \theta_{u+1}] \quad \text{or} \quad \varphi_{s,j} \notin [\varphi_u, \varphi_{u+1}]. \end{cases} \tag{97}$$

In Eq. (97), $\theta_{s,j}$ and $\varphi_{s,j}$ represent, respectively, the zenith and azimuthal angles of the direction corresponding to the jth-order outgoing ray specified by the unit vector $\hat{e}_{s,j}$ defined in Fig. 3. The contribution of diffraction to the scattering matrix in Eq. (94) can be calculated via the following formula [20]:

$$\begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix}_{diff} = \frac{k_0^2}{4\pi}\int\!\!\int \exp(-ik_0\hat{r}\cdot\vec{p})d^2\vec{p} \begin{bmatrix} \cos\,\theta_s(1+\cos\,\theta_s) & 0 \\ 0 & \cos\,\theta_s \end{bmatrix}, \tag{98}$$

where the integration domain is the particle projected area on a plane perpendicular to the incident rays.

After the scattering matrix has been determined, computing the scattering phase matrix that relates the scattered Stokes parameters to their incident counterparts is straightforward. Eq. (94) fully accounts for the phase interferences among geometric optics rays and diffraction. In practice, however, the effect of phase inferences on scattering patterns can be neglected, particularly for a polydisperse system consisting of randomly oriented nonspherical particles, because of the required averaging processes relevant to particle orientations and sizes. The phase matrix subject to this simplification can be expressed by

$$P = \frac{\sigma - \sigma_a}{2\sigma - \sigma_a} P_{ray} + \frac{\sigma}{2\sigma - \sigma_a} P_{dif}, \tag{99}$$

where P_{ray} and P_{dif} are the contributions from geometric optics rays and diffraction, respectively. Note that both P_{ray} and P_{dif} in Eq. (99) are normalized such that

$$\frac{1}{2}\int_0^{\pi} P_{ray}(\theta_s)\sin\theta_s\,d\theta_s = 1 \quad \text{and} \quad \frac{1}{2}\int_0^{\pi} P_{dif}(\theta_s)\sin\theta_s\,d\theta_s = 1. \tag{100}$$

In Eq. (99), the quantity P_{ray} can be written as follows:

$$P_{ray} = \sum_p \sum_j P_{ray,p,j}, \tag{101}$$

where $P_{ray,p,j}$ can be directly computed from the first term on the right-hand side in Eq. (96), along with the normalization condition defined in Eq. (100). Likewise, the term $P_{dif}(\theta_s)$ can be directly computed from the diffraction component of the scattering matrix defined in Eq. (98). The quantity σ, in Eq. (99), is the particle projected area, while σ_a is the particle absorption cross-section. In Eq. (99), it is noted, in accordance with the geometric optics approximation within the context of the optical theorem, that the extinction cross-section of a scattering particle is twice its projected area. In the ray-tracing computation, the total absorption of a scattering particle is the sum of the absorption of individual rays given by

$$\begin{aligned}\sigma_a = \sigma - 2^{-1}\sum_p \sigma_{p,1}(|M_{1,1}|^2 + |M_{2,1}|^2 + |M_{3,1}|^2 + |M_{4,1}|^2) \\ - 2^{-1}\sum_p \sum_{j=2} \sigma_{p,j}(|M_{1,j}|^2 + |M_{2,j}|^2 + |M_{3,j}|^2 + |M_{4,j}|^2)\exp\left[-2k_o \sum_{q=1}^{j-1} N_{n,q}\hat{n}_q(\vec{r}_{q+1} - \vec{r}_q)\right].\end{aligned} \tag{102}$$

Eqs. (99)–(102) provide a practical ray-tracing scheme for computing the single-scattering properties of an absorbing particle within the context of the conventional geometric ray-tracing framework.

4. Some numerical examples

To illustrate the applicability of the present ray-tracing scheme, we apply this scheme to compute the angular distributions of the scattered energy and degree of linear polarization in conjunction with light scattering by water droplets at infrared and far-infrared wavelengths at which water is considerably absorptive. A comparison of the geometric optics solutions and their Lorenz–Mie counterparts for the single-scattering properties of an ensemble (referred to as polydispersion) of non-absorbing spheres with sizes specified in terms of a gamma function has been reported by Liou and Hansen [21]. Unlike the previous study, however, the present computations have been made for individual spheres (referred to as monodispersion) to match more precisely with Lorenz–Mie results. The formulation of the scattering phase function and the degree of linear polarization within the framework of the conventional geometric optics method for spheres is given in Appendix A.

Fig. 4 shows the angular variations of P_{11} and *DLP* for spheres with size parameters of 25, 50, 100 and 500. The index of refraction used in the computation is $m = 1.218+i0.0508$, corresponding to the refractive index of water at the 10 μm wavelength [22]. In each panel in Fig. 4, a sub-panel shows the zoom-in of the phase function in the range of scattering angles from 0° to 10°. For a size parameter of 25, the ray-tracing solutions for both the phase function and *DLP* deviate substantially from the exact Lorenz–Mie results because of the breakdown of the principles of geometric optics for small particles. However, the accuracies of the ray-tracing solutions are systematically improved with an increase in size parameter. In the case of $x = 500$, the Lorenz–Mie and geometric ray-tracing results are essentially the same, except for several minor differences for *DLP* in forward directions. Note that surface wave and the so-called above- and below-edge effects [23], which are related to some physical processes beyond the applicability domain of the geometric optics method, are not considered in the present ray-tracing computation. Furthermore, the cases considered in this study correspond to strong absorption and many features such as caustics [24,25] associated with resonances [26,27] are substantially diminished.

Fig. 5 is similar to Fig. 4, except for a refractive index of $1.48+i0.393$, which is for water at a far-infrared wavelength of 20 μm [22]. In this case, the imaginary part of the refractive index for the results shown in Fig. 5 is almost one order of magnitude larger than that used for Fig. 4. It is evident from comparison of Figs. 4 and 5 for the case of $x = 25$ that the accuracy of ray-tracing calculations is improved with increasing particle absorption. In Fig. 5, the oscillation patterns in both the phase function and *DLP* are similar for the Lorenz–Mie and geometric optics solutions even for $x = 25$, although the angular locations of the oscillation maxima and minima shifted between the two solutions for scattering angles larger

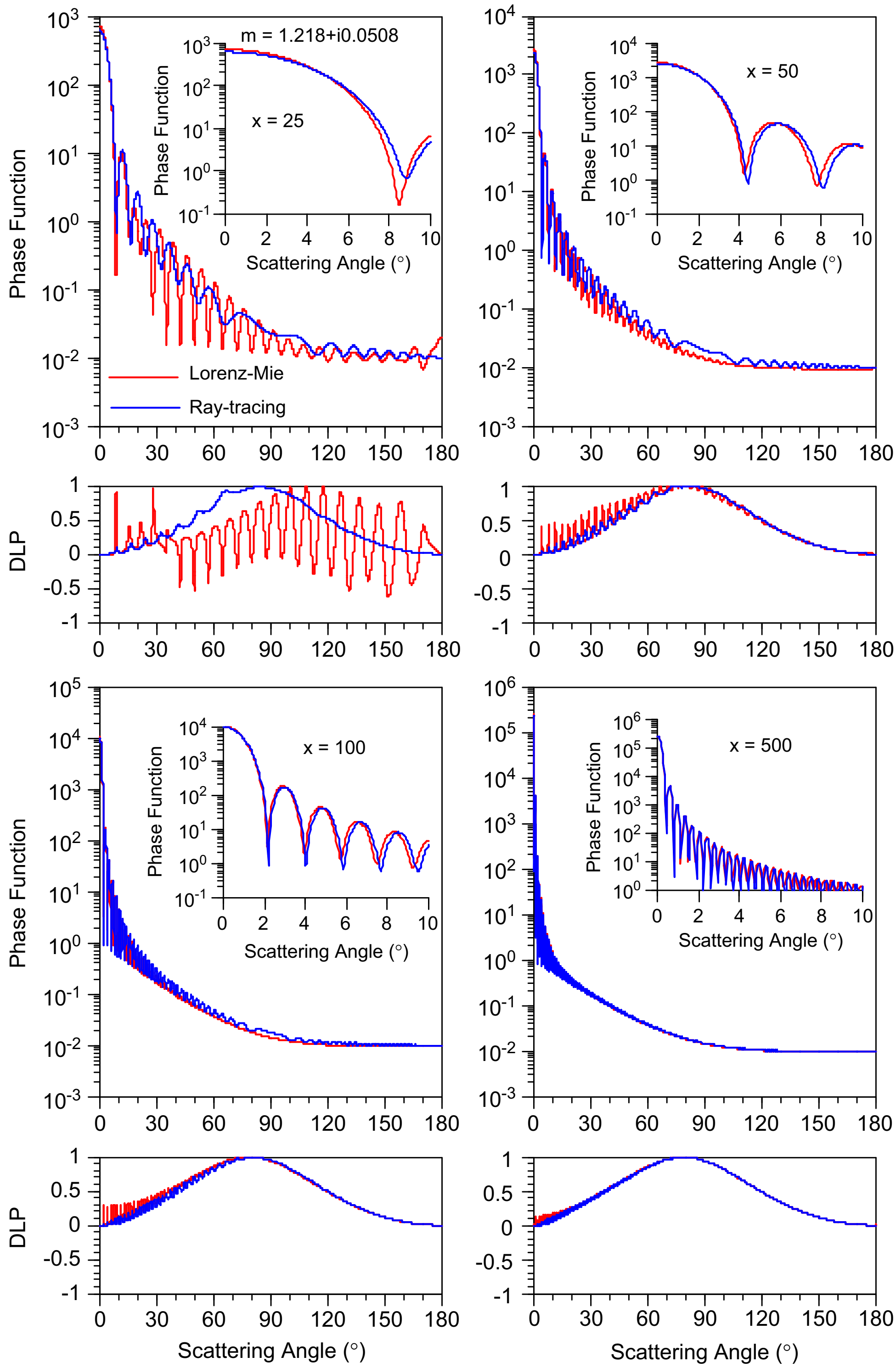

Fig. 4. The angular distributions of phase function and degree of linear polarization for spheres. The refractive index used is 1.218+*i*0.0508 for water at a wavelength of 10 μm.

than about 30°. From Figs. 4 and 5, it can be concluded, with reasonable accuracy, that the geometric-optics method can be applied to a strongly absorbing sphere with a size parameter larger than approximately 50.

5. Summary

When a scattering particle is absorptive, the waves within it are not homogeneous such that the electromagnetic field vectors are not perpendicular to the propagation direction of such waves. However, the electric and magnetic vectors in the

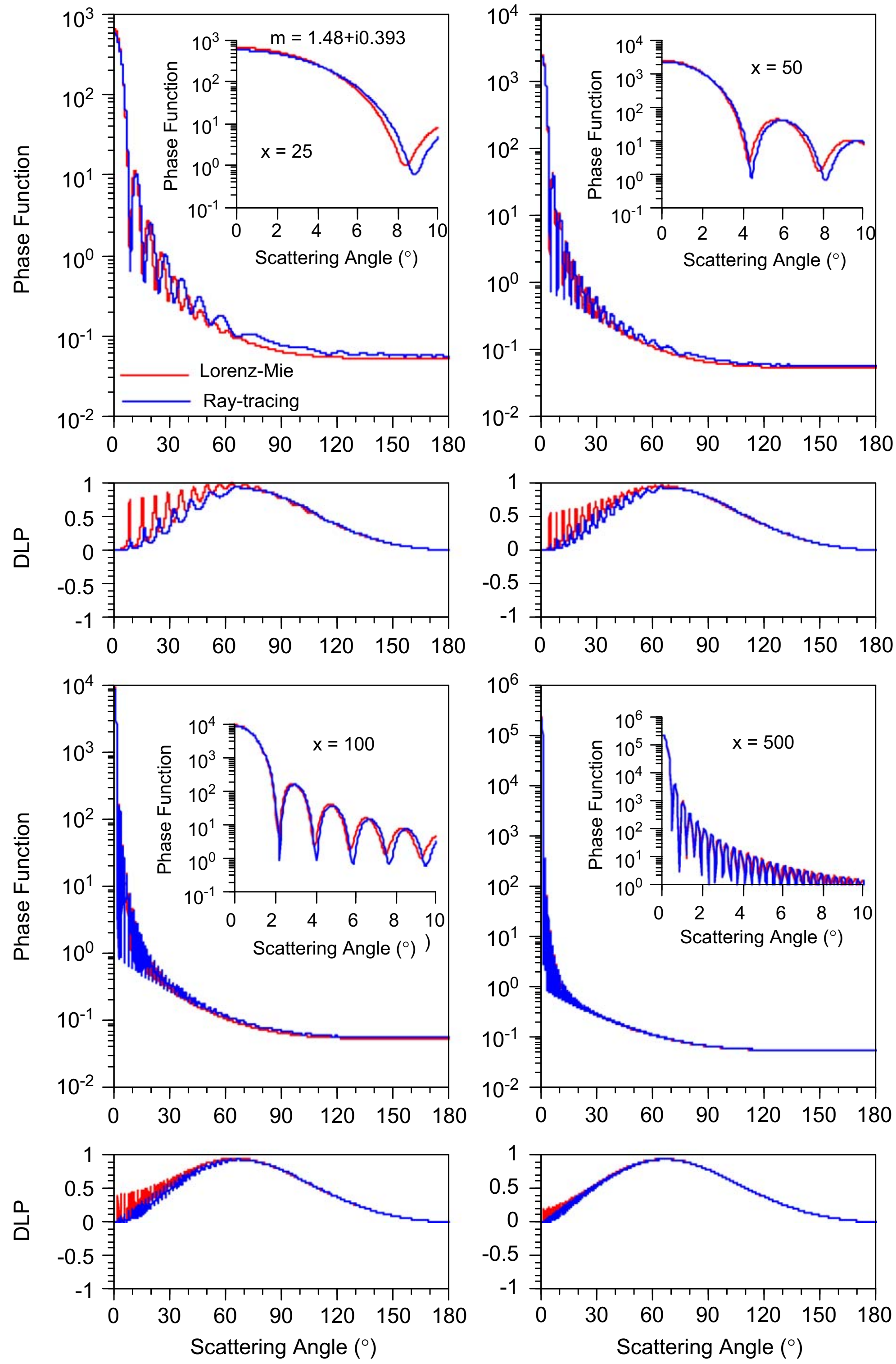

Fig. 5. The angular distributions of phase function and degree of linear polarization for spheres. The refractive index used is 1.48+i0.393 for water at a wavelength of 20 μm.

TE and TM modes, respectively, are transverse with respect to the wave propagation. Based on Maxwell's equations and the electromagnetic boundary conditions, we have derived the generalized Fresnel formulas for reflection and refraction of the TE-mode electric field and the TM-mode magnetic field. In these formulas, we have employed the concept of effective refractive indices to circumvent the difficulties associated with the complex angles involved in the conventional Snell law in the limit of geometric optics. Furthermore, we have also derived the recurrence equations that are required for computing the scattering matrix of an absorbing particle within the framework of the conventional geometric optics approach. Subject to this framework, the present formulation provides an "exact" ray-tracing scheme that fully accounts for the inhomogeneity of internal waves within an absorbing particle. We applied the present ray-tracing scheme to compute the angular distributions of phase function and the degree of linear polarization associated with the scattering of infrared and far-infrared radiation by individual spheres. We illustrated that the accuracy of the conventional geometric optics method is improved with increasing size parameter and particle absorption.

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Appendix A. Phase function and degree of linear polarization formulated in a ray-tracing method for spheres

Following van de Hulst [19] and Liou and Hansen [21], the scattered field can be decomposed into the contributions from Fraunhofer diffraction and geometric optics rays of various orders. Thus, the phase matrix for a sphere within the context of the geometric optics method can be written as follows:

$$P(\theta) = \sum_{n=0}^{N} [P_{TM}^{(n)}(\theta) + P_{TE}^{(n)}(\theta)], \tag{103}$$

where the subscripts *TM* and *TE* indicate the TM and TE modes, respectively, in the case of an absorbing sphere,. In Eq. (103), $n=0$ indicates the contribution from Fraunhofer diffraction, $n=1$ indicates the contribution from externally reflected rays, and $n\geqslant 2$ indicates the contributions from the rays that undergo $n-2$ internal reflections and two refractions. In practice, the upper limit of the summation in Eq. (103) can be set to be in the order of 10 because the energy carried by higher-order rays is quite small, particularly for an absorbing particle. In the case of a sphere, the scattered Stokes vector can be expressed in the form [28]

$$\begin{bmatrix} I_s(\theta) \\ Q_s(\theta) \\ U_s(\theta) \\ V_s(\theta) \end{bmatrix} = \frac{q_s x^2}{4k_o^2 r^2} \begin{bmatrix} P_{11}(\theta) & P_{12}(\theta) & 0 & 0 \\ P_{12}(\theta) & P_{11}(\theta) & 0 & 0 \\ 0 & 0 & P_{33}(\theta) & -P_{43}(\theta) \\ 0 & 0 & P_{43}(\theta) & P_{33}(\theta) \end{bmatrix} \begin{bmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{bmatrix}, \tag{104}$$

where *I*, *Q*, *U*, and *V* are the four elements of the Stokes vector; the subscripts *s* and *i* in Eq. (104) indicate scattered and incident quantities, respectively; x is the size parameter; q_s is the scattering efficiency; P_{11} is the phase function, which satisfies

$$\frac{1}{2}\int_0^{\pi} P_{11}(\theta) \sin\theta \, d\theta = 1. \tag{105}$$

The quantity q_s in Eq. (104) can be given in terms of the difference between the extinction and absorption efficiencies. In the conventional geometric optics method, the extinction efficiency is assumed to be 2, and the absorption cross-section can be computed from Eq. (102).

We focus on P_{11} and P_{12} so that the contributions of diffraction to the TM and TE components of the phase function from Eqs. (98) and (104) can be expressed in the forms [29]

$$P_{11,TM}^{(0)}(\theta) = \frac{x^2}{8q_s}\left[\frac{2J_1(x\sin\theta)}{x\sin\theta}\right]^2 (\cos\theta + \cos^2\theta)^2, \tag{106}$$

$$P_{11,TE}^{(0)}(\theta) = \frac{x^2}{8q_s}\left[\frac{2J_1(x\sin\theta)}{x\sin\theta}\right]^2 (1 + \cos\theta)^2, \tag{107}$$

where J_1 is the Bessel function of the first kind.

Following van de Hulst [19] and referring to the incidence-scattering configuration in Fig. 6a, we can express the contribution of externally reflected rays to the phase function in the form

$$P_{11,TM}^{(1)}(\theta) = \frac{2|R_{H,1}|^2}{q_s} D, \tag{108}$$

$$P_{11,TE}^{(1)}(\theta) = \frac{2|R_{E,1}|^2}{q_s} D, \tag{109}$$

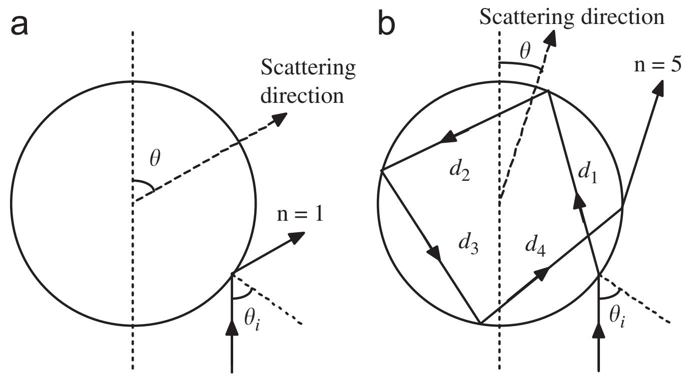

Fig. 6. Incidence scattering configurations for propagations of the first- and fifth-order rays for a sphere.

where the generalized Fresnel reflection coefficients $R_{E,1}$ and $R_{H,1}$ can be computed from Eqs. (26) and (38). The term D is the so-called "divergence" that was first introduced by van de Hulst [19] and it is given by

$$D = \left|\frac{\cos\,\theta_i\,\sin\,\theta_i}{\sin\,\theta(\mathrm{d}\theta/\mathrm{d}\theta_i)}\right|. \tag{110}$$

In van de Hulst's formulation, the complement of θ_i is used. For external reflection, $D = \frac{1}{4}$ because $\theta = \pi - 2\theta_i$.

For a large sphere with strong absorption, the waves refracted into the particle are essentially absorbed and the scattered field is primarily contributed from diffraction and external reflection. In this case, the geometric optics solutions for the phase function and the degree of linear polarization have been presented by Yang et al. [29]. However, the contributions from transmitted rays must be taken into account if particle absorption or size parameter is moderate. Referring to Fig. 6b and following the procedure of van de Hulst [19] and Liou and Hansen [21], we obtain the contribution of the nth-order rays to the phase function as follows:

$$\begin{aligned} P^{(n)}_{11,TE}(\theta) = {} & \frac{2D}{q_s}(1-|R_{E,1}|^2)\frac{\cos\,\theta_{r,2}}{\cos\,\theta_{i,2}}|R_{E,2}|^2\ldots\frac{\cos\,\theta_{r,n-1}}{\cos\,\theta_{i,n-1}}|R_{E,n-1}|^2 \\ & \times\left(1-\frac{\cos\,\theta_{r,n}}{\cos\theta_{i,n}}|R_{E,n}|^2\right)\exp[-4\pi(\tilde{N}_{i,1}d_1+\tilde{N}_{i,2}d_2+\cdots+\tilde{N}_{i,n-1}d_{n-1})/\lambda], \end{aligned} \tag{111}$$

$$\begin{aligned} P^{(n)}_{11,TM}(\theta) = {} & \frac{2D}{q_s}(1-|R_{M,1}|^2)\frac{\cos\,\theta_{r,2}}{\cos\,\theta_{i,2}}|R_{M,2}|^2\cdots\frac{\cos\,\theta_{r,n-1}}{\cos\,\theta_{i,n-1}}|R_{M,n-1}|^2 \\ & \times\left(1-\frac{\cos\,\theta_{r,n}}{\cos\,\theta_{i,n}}|R_{M,n}|^2\right)\exp[-4\pi(\tilde{N}_{i,1}d_1+\tilde{N}_{i,2}d_2+\cdots+\tilde{N}_{i,n-1}d_{n-1})/\lambda], \end{aligned} \tag{112}$$

where the terms $\tilde{N}_{i,1}$ and $\tilde{N}_{i,j}$ (for $j>1$) are given by $N_{n,1}\,\cos\,\theta_{t,1}$ and $N_{n,j}\,\cos\,\theta_{r,j}$, respectively [17]. The terms $\cos\,\theta_{r,j}/\cos\,\theta_{i,j}$ (for $j = 2, 3\ldots n-1$) in Eqs. (111) and (112), which are unity in the case of a non-absorbing sphere, are included for the conservation of energy associated with variations in ray cross-sections in the corresponding reflection–refraction events. The quantity d_j is the distance between the jth-order incident point an the (j+1)th-order incident point, as shown in Fig. 6b.

The P_{12} element of the phase matrix is given by

$$P_{12} = \sum_{n=0}^{N}[P^{(n)}_{11,TM}(\theta) - P^{(n)}_{11,TE}(\theta)]. \tag{113}$$

The degree of linear polarization (DLP) is defined in terms of the negative ratio of the second element (Q) to the first element (I) in the Stokes vector [30], i.e.

$$DLP = -\frac{Q_s}{I_s}. \tag{114}$$

For non-polarized incident light, it can be shown that DLP for a sphere is given by

$$DLP = -\frac{P_{12}}{P_{11}} = -\frac{\sum_{n=0}^{N}[P^{(n)}_{11,TM}(\theta) - P^{(n)}_{11,TE}(\theta)]}{\sum_{n=0}^{N}[P^{(n)}_{11,TM}(\theta) + P^{(n)}_{11,TE}(\theta)]}. \tag{115}$$

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