



Electromagnetic scattering by discrete random media. III: The vector radiative transfer equation

Adrian Doicu^{a,*}, Michael I. Mishchenko^b

^aDeutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Methodik der Fernerkundung (IMF), Oberpfaffenhofen 82234, Germany

^bNASA Goddard Institute for Space Studies, 2880 Broadway, New York, NY 10025, United States

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ABSTRACT

A vector radiative transfer equation with an additional source term typical of dense media is obtained. The analysis includes (i) the derivation of an integral equation for the correlation matrix of the exciting field coefficients accounting for the correlation between the particles, (ii) the derivation of an integral representation for the specific coherency dyadic in terms of this matrix, and (iii) the simplification of the integral equation for the correlation matrix and of the integral representation for the specific coherency dyadic by employing a series of approximations which are characteristic of sparse media.

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1. Introduction

In this paper we continue the analysis initiated in Refs. [1] and [2] by focusing on the computation of the configuration average of energetic quantities which are quadratic in the field amplitudes. The configuration average of an energetic quantity must be computed explicitly, because the process of averaging cannot be expected to commute with the nonlinear operation of squaring the absolute value of a field quantity.

In the case of a sparse medium, the scattered radiation can be represented as a sum of two terms. One term corresponds to the incoherent part of the scattered radiation and is described by the well-known vector radiative transfer equation obtained by summing the ladder diagrams in the diagrammatic representation of the Bethe–Salpeter equation. The second term corresponds to the coherent part of the scattered radiation, arising from the interference of pairs of conjugate waves propagating along the same self-avoiding paths but in opposite directions, and is obtained by summing the cyclical diagrams. In the case of a dense medium, the radiation scattered by the medium can no longer be expressed as a sum of only two terms. A significant additional contribution to the radiation scattered by the medium can come from, e.g., the interference between single and double scattered, double scattered and triple scattered waves and so on. Tishkovets and Jokers [3], and Tishkovets and Mishchenko [4] extended the approach developed for sparse media to dense media, by also representing the scattered radiation as the sum of an incoherent and a coherent part,

but by taking into account the correlations between the particles. A comprehensive review of these results can be found in Ref. [5]. The analysis is performed in a circular-polarization basis under the assumption that the observation point is outside the discrete random medium and is focused on the computation of the reflection and transmission matrices of the layer.

In this study we analyze the incoherent part of the scattered radiation at an observation point which is inside the discrete random medium. In a linear-polarization basis, we aim to derive a vector radiative transfer equation by taking into account the correlation between the particles. Because a rigorous derivation of this equation is a very challenging task, we adopt a simplified approach. To explain the main assumption of our method we recapitulate some results established in Ref. [2].

Consider a discrete random medium in the form of a group of N identical spherical particles of radius a centered at $\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N$, and distributed throughout a domain D confined to a laterally infinite plane-parallel layer with the imaginary (non-scattering) boundaries $z = 0$ and $z = H$. The wavenumbers of the non-absorbing, non-magnetic background medium and the particles are k_1 and $k_2 = mk_1$, respectively, where m is the relative refractive index of the particles. Denote by $f = n_0 V_0$ the particle volume concentration, where $n_0 = N/V$ is the particle number concentration, V is the volume of the discrete random medium, and $V_0 = (4/3)\pi a^3$ is the volume of each particle. Let the particulate medium be illuminated by a plane electromagnetic wave with the propagation direction $\hat{\mathbf{s}} = \hat{\mathbf{s}}(\theta_0, \varphi_0)$ and the amplitude $\mathcal{E}_0(\hat{\mathbf{s}})$, that is,

$$\mathbf{E}_0(\mathbf{r}) = \mathcal{E}_0(\hat{\mathbf{s}}) e^{ik_1 \hat{\mathbf{s}} \cdot \mathbf{r}}, \quad (1)$$

* Corresponding author.

E-mail address: adrian.doicu@dlr.de (A. Doicu).

$$\mathcal{E}_0(\hat{\mathbf{s}}) = \mathcal{E}_{0\theta}\hat{\boldsymbol{\theta}}(\hat{\mathbf{s}}) + \mathcal{E}_{0\varphi}\hat{\boldsymbol{\varphi}}(\hat{\mathbf{s}}), \quad (2)$$

where $\mathbf{j} = \sqrt{-1}$, $(\hat{\mathbf{s}}, \hat{\boldsymbol{\theta}}(\hat{\mathbf{s}}), \hat{\boldsymbol{\varphi}}(\hat{\mathbf{s}}))$ is the spherical unit-vector basis, and $\mathcal{E}_{0\theta}$ and $\mathcal{E}_{0\varphi}$ are the polarized components of the amplitude vector. Denote by $\mathbf{E}_{\text{sct}i}(\mathbf{r})$ the field scattered by particle i at the observation point \mathbf{r} , by $\mathbf{E}_{\text{inti}}(\mathbf{r})$ the field inside particle i , and by $\mathbf{E}_{\text{exci}}(\mathbf{r})$ the field exciting particle i . If the observation point is outside of any particle, the total field is the sum of the incident and all scattered fields, i.e.,

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \sum_{i=1}^N \mathbf{E}_{\text{sct}i}(\mathbf{r}), \quad (3)$$

while inside particle i , the total field is the internal field $\mathbf{E}_{\text{inti}}(\mathbf{r})$ when excited by $\mathbf{E}_{\text{exci}}(\mathbf{r})$. In a compact notation, the total field can be written as

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \sum_{i=1}^N \mathbf{E}_{\text{sct}i}(\mathbf{r}) + \sum_{i=1}^N [1 - \alpha(\mathbf{r} - \mathbf{R}_i)] [\mathbf{E}_{\text{inti}}(\mathbf{r}) - \mathbf{E}_{\text{exci}}(\mathbf{r})], \quad (4)$$

where $\alpha(\mathbf{r} - \mathbf{R}_i)$ is the indicator function

$$\alpha(\mathbf{r} - \mathbf{R}_i) = \begin{cases} 0, & \mathbf{r} \in D_a(\mathbf{R}_i) \\ 1, & \mathbf{r} \notin D_a(\mathbf{R}_i) \end{cases}, \quad (5)$$

and $D_a(\mathbf{R}_i)$ is a sphere of radius a centered at \mathbf{R}_i (the domain occupied by particle i). Taking the configuration average of Eq. (4), we found that for an external observation point \mathbf{r} situated in the domains $z \leq -a$ or $z \geq H + a$, the coherent field is

$$\mathbf{E}_c(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + n_0 \int_D \langle \mathbf{E}_{\text{sct}i}(\mathbf{r}) \rangle_i d^3\mathbf{R}_i, \quad (6)$$

while for an internal observation point \mathbf{r} situated in the domain $a \leq z \leq H - a$, the coherent field is

$$\mathbf{E}_c(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + n_0 \int_{D-D_a(\mathbf{r})} \langle \mathbf{E}_{\text{sct}i}(\mathbf{r}) \rangle_i d^3\mathbf{R}_i + n_0 \int_{D_a(\mathbf{r})} [\langle \mathbf{E}_{\text{inti}}(\mathbf{r}) \rangle_i - \langle \mathbf{E}_{\text{exci}}(\mathbf{r}) \rangle_i] d^3\mathbf{R}_i, \quad (7)$$

where $D_a(\mathbf{r})$ is a complete sphere of radius a centered at \mathbf{r} . The first integral in Eq. (7) corresponds to the configurations in which the observation point \mathbf{r} is external to all particles, while the second integral gives the inside contribution. In Ref. [2], Eq. (6) has been used to compute the coherent fields reflected and transmitted by the layer, and Eq. (7) has been used to compute the coherent field inside the layer. A simplified method for computing the coherent field inside the layer relies on the sparse-medium approximation for the integration domain, i.e.,

$$\int_{D-D_a(\mathbf{r})} d^3\mathbf{R}_i \approx \int_D d^3\mathbf{R}_i. \quad (8)$$

This means that in Eq. (7), the integrals over $D_a(\mathbf{r})$ are neglected, or equivalently, that the particles are treated as point scatterers. For the coherent field computed by this method, we found that (i) the boundary conditions for the electric fields are satisfied, (ii) for normal incidence and an oblique φ -polarized incidence, the coherent field is a superposition of plane electromagnetic waves, while (iii) for an oblique θ -polarized incidence, the coherent field is not divergence free. However, for small values of the volume concentration, the deviations from a divergence free field are not significant. In fact, the approximation (8) implies that the total field is given by Eq. (3), and that the coherent field inside the layer is given by Eq. (6); both equations are valid when the observation point is outside of any particle.

Taking account of these results we make the following simplifications:

1. we adopt the representation (3) for the total field, i.e., the total field sums the contributions of the incident and all scattered fields, and
2. in some parts of the proof and when taking the configuration average, we apply the sparse-medium approximation for the integration domain (8).

The resulting vector radiative transfer equation will inherit the main features of the equation for sparse media but will include an additional source term which is typical of dense media.

2. Coherency dyadic

The coherency dyadic is defined by the relation

$$\bar{\mathbf{C}}(\mathbf{r}) = \langle \mathbf{E}(\mathbf{r}) \otimes \mathbf{E}^*(\mathbf{r}) \rangle, \quad (9)$$

where \otimes is the dyadic product sign and the asterisk denotes complex conjugation. Representing the field scattered by particle i as the sum of a configuration-averaged part $\langle \mathbf{E}_{\text{sct}i}(\mathbf{r}) \rangle$ and a fluctuating part $\mathcal{E}_{\text{sct}i}(\mathbf{r})$, i.e.,

$$\mathbf{E}_{\text{sct}i}(\mathbf{r}) = \langle \mathbf{E}_{\text{sct}i}(\mathbf{r}) \rangle + \mathcal{E}_{\text{sct}i}(\mathbf{r}), \quad (10)$$

we express the total field $\mathbf{E}(\mathbf{r})$ as (cf. Eq. (3))

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_c(\mathbf{r}) + \mathcal{E}_{\text{sct}}(\mathbf{r}), \quad (11)$$

where

$$\mathbf{E}_c(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \sum_i \langle \mathbf{E}_{\text{sct}i}(\mathbf{r}) \rangle \quad (12)$$

is the coherent field, and (cf. Eq. (10))

$$\mathcal{E}_{\text{sct}}(\mathbf{r}) = \sum_i \mathcal{E}_{\text{sct}i}(\mathbf{r}) = \sum_i \mathbf{E}_{\text{sct}i}(\mathbf{r}) - \sum_i \langle \mathbf{E}_{\text{sct}i}(\mathbf{r}) \rangle, \quad (13)$$

or equivalently,

$$\mathcal{E}_{\text{sct}}(\mathbf{r}) = \mathbf{E}_{\text{sct}}(\mathbf{r}) - \langle \mathbf{E}_{\text{sct}}(\mathbf{r}) \rangle, \quad (14)$$

where $\mathbf{E}_{\text{sct}}(\mathbf{r}) = \sum_i \mathbf{E}_{\text{sct}i}(\mathbf{r})$, is the diffuse scattered field. In Eqs. (12) and (13), the summations run implicitly from 1 to N . Taking into account that $\langle \mathcal{E}_{\text{sct}}(\mathbf{r}) \rangle = 0$, we obtain the following representation for the coherency dyadic:

$$\bar{\mathbf{C}}(\mathbf{r}) = \mathbf{E}_c(\mathbf{r}) \otimes \mathbf{E}_c^*(\mathbf{r}) + \langle \mathcal{E}_{\text{sct}}(\mathbf{r}) \otimes \mathcal{E}_{\text{sct}}^*(\mathbf{r}) \rangle = \bar{\mathbf{C}}_c(\mathbf{r}) + \bar{\mathcal{C}}_d(\mathbf{r}), \quad (15)$$

where

$$\bar{\mathbf{C}}_c(\mathbf{r}) = \mathbf{E}_c(\mathbf{r}) \otimes \mathbf{E}_c^*(\mathbf{r}) \quad (16)$$

is the coherent part of the coherency dyadic, and

$$\bar{\mathcal{C}}_d(\mathbf{r}) = \langle \mathcal{E}_{\text{sct}}(\mathbf{r}) \otimes \mathcal{E}_{\text{sct}}^*(\mathbf{r}) \rangle \quad (17)$$

is the diffuse coherency dyadic. Using Eq. (13) we find that in terms of appropriate probability density functions and conditional configuration averages, the diffuse coherency dyadic (17) can be written as

$$\bar{\mathcal{C}}_d(\mathbf{r}) = \bar{\mathcal{C}}_{dL}(\mathbf{r}) + \bar{\mathcal{C}}_{dC}(\mathbf{r}), \quad (18)$$

where

$$\begin{aligned} \bar{\mathcal{C}}_{dL}(\mathbf{r}) &= \sum_i \langle \mathbf{E}_{\text{sct}i}(\mathbf{r}) \otimes \mathbf{E}_{\text{sct}i}^*(\mathbf{r}) \rangle \\ &= n_0 \int_D \langle \mathbf{E}_{\text{sct}i}(\mathbf{r}) \otimes \mathbf{E}_{\text{sct}i}^*(\mathbf{r}) \rangle_i d^3\mathbf{R}_i \end{aligned} \quad (19)$$

is the diffuse ladder coherency dyadic, and

$$\bar{\mathcal{C}}_{dC}(\mathbf{r}) = \sum_i \sum_{j \neq i} \langle \mathbf{E}_{\text{sct}i}(\mathbf{r}) \otimes \mathbf{E}_{\text{sct}j}^*(\mathbf{r}) \rangle$$

$$\begin{aligned}
& - \sum_i \sum_j \langle \mathbf{E}_{\text{scti}}(\mathbf{r}) \rangle \otimes \langle \mathbf{E}_{\text{sctj}}^*(\mathbf{r}) \rangle \\
& = n_0^2 \int_D \langle \mathbf{E}_{\text{scti}}(\mathbf{r}) \otimes \mathbf{E}_{\text{sctj}}^*(\mathbf{r}) \rangle_{ij} g(\mathbf{R}_i, \mathbf{R}_j) d^3 \mathbf{R}_j d^3 \mathbf{R}_i \\
& - n_0^2 \int_D \langle \mathbf{E}_{\text{scti}}(\mathbf{r}) \rangle_i \langle \mathbf{E}_{\text{sctj}}^*(\mathbf{r}) \rangle_j d^3 \mathbf{R}_j d^3 \mathbf{R}_i,
\end{aligned} \quad (20)$$

with $g(\mathbf{R}_i, \mathbf{R}_j)$ being the pair correlation function, is the diffuse cross coherency dyadic. Observe that in Eqs. (19) and (20), the sparse-medium approximation for the integration domain (8) has been applied. Finally, defining the ladder coherency dyadic by the relation

$$\begin{aligned}
\bar{\mathbf{C}}_L(\mathbf{r}) & = \bar{\mathbf{C}}_c(\mathbf{r}) + \bar{\mathcal{C}}_{\text{dL}}(\mathbf{r}) \\
& = \bar{\mathbf{C}}_c(\mathbf{r}) + n_0 \int_D \langle \mathbf{E}_{\text{scti}}(\mathbf{r}) \otimes \mathbf{E}_{\text{scti}}^*(\mathbf{r}) \rangle_i d^3 \mathbf{R}_i
\end{aligned} \quad (21)$$

yields the representation

$$\bar{\mathbf{C}}(\mathbf{r}) = \bar{\mathbf{C}}_L(\mathbf{r}) + \bar{\mathcal{C}}_{\text{dC}}(\mathbf{r}) = \bar{\mathbf{C}}_c(\mathbf{r}) + \bar{\mathcal{C}}_{\text{dL}}(\mathbf{r}) + \bar{\mathcal{C}}_{\text{dC}}(\mathbf{r}). \quad (22)$$

Thus, the coherency dyadic is written as the sum of two terms: the configuration average of the dyadic product of the field scattered by one particle i in the presence of other particles (the ladder term $\bar{\mathbf{C}}_L$), and the correlation of the fields scattered by two distinct particles i and j (the cross term $\bar{\mathcal{C}}_{\text{dC}}$).

Hereafter we will use a matrix-form representation for the dyadic product $\mathbf{E}_{\text{scti}}(\mathbf{r}) \otimes \mathbf{E}_{\text{sctj}}^*(\mathbf{r})$, where

$$\mathbf{E}_{\text{scti}}(\mathbf{r}) = \mathbf{X}_3^T(k_1 \mathbf{r}_i) \mathbf{T} \mathbf{e}_i, \quad (23)$$

$\mathbf{X}_3(k_1 \mathbf{r})$ is the column vector of the radiating vector spherical wave functions, \mathbf{T} is the transition matrix of a spherical particle, and \mathbf{e}_i is the vector of the exciting field coefficients. More specifically, for the vectors $\mathbf{X} = \sum_{i=1}^3 X_i \hat{\mathbf{e}}_i$ and $\mathbf{Y} = \sum_{i=1}^3 Y_i \hat{\mathbf{e}}_i$, where X_i and Y_i are three-dimensional column vectors, and the column vectors \mathbf{x} and \mathbf{y} , we consider the vectors

$$\mathbf{a} = \mathbf{x}^T \mathbf{X} = \mathbf{X}^T \mathbf{x} = \sum_{i=1}^3 a_i \hat{\mathbf{e}}_i, \quad (24)$$

$$a_i = \mathbf{x}^T X_i = X_i^T \mathbf{x}, \quad (25)$$

and

$$\mathbf{b} = \mathbf{y}^T \mathbf{Y} = \mathbf{Y}^T \mathbf{y} = \sum_{i=1}^3 b_i \hat{\mathbf{e}}_i, \quad (26)$$

$$b_i = \mathbf{y}^T Y_i = Y_i^T \mathbf{y}, \quad (27)$$

so that by means of Eqs. (25) and (27), we express the dyadic product $\mathbf{a} \otimes \mathbf{b}$ in matrix form as

$$\begin{aligned}
\mathbf{a} \otimes \mathbf{b} & = [\hat{\mathbf{e}}_1 \quad \hat{\mathbf{e}}_2 \quad \hat{\mathbf{e}}_3] \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \begin{bmatrix} b_1 & b_2 & b_3 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{e}}_1 \\ \hat{\mathbf{e}}_2 \\ \hat{\mathbf{e}}_3 \end{bmatrix} \\
& = [\hat{\mathbf{e}}_1 \quad \hat{\mathbf{e}}_2 \quad \hat{\mathbf{e}}_3] \begin{bmatrix} X_1^T \\ X_2^T \\ X_3^T \end{bmatrix} \mathbf{y}^T [\mathbf{Y}_1 \quad \mathbf{Y}_2 \quad \mathbf{Y}_3] \begin{bmatrix} \hat{\mathbf{e}}_1 \\ \hat{\mathbf{e}}_2 \\ \hat{\mathbf{e}}_3 \end{bmatrix} \\
& = \mathbf{X}^T \mathbf{y}^T \mathbf{Y}.
\end{aligned}$$

In this regard, the matrix-form representation for the dyadic product $\mathbf{E}_{\text{scti}}(\mathbf{r}) \otimes \mathbf{E}_{\text{sctj}}^*(\mathbf{r})$ is (cf. Eq. (23))

$$\mathbf{E}_{\text{scti}}(\mathbf{r}) \otimes \mathbf{E}_{\text{sctj}}^*(\mathbf{r}) = \mathbf{X}_3^T(k_1 \mathbf{r}_i) \mathbf{T} \mathbf{e}_i \mathbf{e}_j^T \mathbf{X}_3^*(k_1 \mathbf{r}_j), \quad (28)$$

where the dagger stands for “hermitian transpose” and $\mathbf{e}_i \mathbf{e}_j^T$ is the matrix of the exciting field coefficients. The diffuse coherency dyadics can then be written as

$$\bar{\mathcal{C}}_{\text{dL}}(\mathbf{r}) = n_0 \int_D \mathbf{X}_3^T(k_1 \mathbf{r}_i) \mathbf{T} \langle \mathbf{e}_i \mathbf{e}_i^T \rangle_i \mathbf{T}^\dagger \mathbf{X}_3^*(k_1 \mathbf{r}_i) d^3 \mathbf{R}_i, \quad (29)$$

and

$$\begin{aligned}
\bar{\mathcal{C}}_{\text{dC}}(\mathbf{r}) & = n_0^2 \int_D \mathbf{X}_3^T(k_1 \mathbf{r}_i) \mathbf{T} \langle \mathbf{e}_i \mathbf{e}_j^T \rangle_{ij} \mathbf{T}^\dagger \mathbf{X}_3^*(k_1 \mathbf{r}_j) g(\mathbf{R}_i, \mathbf{R}_j) d^3 \mathbf{R}_j d^3 \mathbf{R}_i \\
& - n_0^2 \int_D \mathbf{X}_3^T(k_1 \mathbf{r}_i) \mathbf{T} \langle \mathbf{e}_i \rangle_i \langle \mathbf{e}_j^T \rangle_j \mathbf{T}^\dagger \mathbf{X}_3^*(k_1 \mathbf{r}_j) d^3 \mathbf{R}_j d^3 \mathbf{R}_i,
\end{aligned} \quad (30)$$

with $\mathbf{R}_i = \mathbf{r} - \mathbf{r}_i$.

The main quantity describing the vector radiative transfer is the diffuse ladder specific coherency dyadic $\bar{\Sigma}_{\text{dL}}$, defined by

$$\bar{\mathcal{C}}_{\text{dL}}(\mathbf{r}) = \int \bar{\Sigma}_{\text{dL}}(\mathbf{r}, -\hat{\mathbf{p}}) d^2 \hat{\mathbf{p}}. \quad (31)$$

The components of the diffuse ladder specific coherency dyadic are the elements of the diffuse ladder specific coherency column vector which, in turn, determine the photopolarimetric signal of a detector. Therefore, the above equation provides an important link between the radiative transfer theory ($\bar{\Sigma}_{\text{dL}}$) and the electromagnetic scattering theory ($\bar{\mathcal{C}}_{\text{dL}}$). According to Eq. (21), the ladder specific coherency dyadic $\bar{\Sigma}_L$, defined by

$$\bar{\mathbf{C}}_L(\mathbf{r}) = \int \bar{\Sigma}_L(\mathbf{r}, -\hat{\mathbf{p}}) d^2 \hat{\mathbf{p}}, \quad (32)$$

is related to $\bar{\Sigma}_{\text{dL}}$ by

$$\bar{\Sigma}_L(\mathbf{r}, -\hat{\mathbf{p}}) = \bar{\Sigma}_{\text{dL}}(\mathbf{r}, -\hat{\mathbf{p}}) + \delta(\hat{\mathbf{p}} + \hat{\mathbf{s}}) \bar{\mathbf{C}}_c(\mathbf{r}). \quad (33)$$

3. Integral equation for the ladder correlation matrix of the exciting field coefficients

In this section, we derive an integral equation for the so-called ladder correlation matrix of the exciting field coefficients, and then employ a series of approximations to transform this integral equation into a form that is suitable for a numerical analysis.

3.1. Derivation

Multiplying the equation for the exciting field coefficients (cf. Eq. (37) of Ref. [1])

$$\mathbf{e}_i = \mathbf{e}_{0i} + \sum_{j \neq i} Q(k_1 \mathbf{R}_{ij}) \mathbf{e}_j \quad (34)$$

by its complex conjugate, where $\mathbf{e}_{0i} = \exp(jk_1 \hat{\mathbf{s}} \cdot \mathbf{R}_i) \mathbf{e}_0$, \mathbf{e}_0 is the column vector of the incident field coefficients, $Q(k_1 \mathbf{R}_{ij}) = \mathcal{T}_{31}^T(k_1 \mathbf{R}_{ij}) \mathbf{T}$, and $\mathcal{T}_{31}(k_1 \mathbf{R}_{ij})$ is the translation matrix relating the radiating and the regular vector spherical wave functions $\mathbf{X}_3(k_1 \mathbf{r}_j)$ and $\mathbf{X}_1(k_1 \mathbf{r}_i)$, respectively, that is, $\mathbf{X}_3(k_1 \mathbf{r}_j) = \mathcal{T}_{31}(k_1 \mathbf{R}_{ij}) \mathbf{X}_1(k_1 \mathbf{r}_i)$ for $\mathbf{r}_j = \mathbf{r}_i + \mathbf{R}_{ij}$ and $r_i < R_{ij}$, and using the following rule for computing the conditional configuration average of a function $f(\mathbf{r}, \Lambda_N)$ with the position of particle i held fixed (cf. Eq. (62) of Ref. [1]):

$$\begin{aligned}
\langle f(\mathbf{r}, \Lambda_N) \rangle_i & = \int_D \langle f(\mathbf{r}, \Lambda_N) \rangle_{ij} p(\mathbf{R}_j | \mathbf{R}_i) d^3 \mathbf{R}_j \\
& = \int_D \langle f(\mathbf{r}, \Lambda_N) \rangle_{ijk} p(\mathbf{R}_j, \mathbf{R}_k | \mathbf{R}_i) d^3 \mathbf{R}_k d^3 \mathbf{R}_j,
\end{aligned} \quad (35)$$

we obtain

$$\begin{aligned}
\langle \mathbf{e}_i \mathbf{e}_i^T \rangle_i & = \mathbf{e}_{0i} \langle \mathbf{e}_i^T \rangle_i + \langle \mathbf{e}_i \rangle_i \mathbf{e}_{0i}^\dagger - \mathbf{e}_{0i} \mathbf{e}_{0i}^\dagger \\
& + \sum_{j \neq i} \int_D Q(k_1 \mathbf{R}_{ij}) \langle \mathbf{e}_j \mathbf{e}_j^T \rangle_{ij} Q^\dagger(k_1 \mathbf{R}_{ij}) p(\mathbf{R}_j | \mathbf{R}_i) d^3 \mathbf{R}_j \\
& + \sum_{j \neq i} \sum_{k \neq i, j} \int_D Q(k_1 \mathbf{R}_{ij}) \langle \mathbf{e}_j \mathbf{e}_k^T \rangle_{ijk} Q^\dagger(k_1 \mathbf{R}_{ik}) \\
& \times p(\mathbf{R}_j, \mathbf{R}_k | \mathbf{R}_i) d^3 \mathbf{R}_k d^3 \mathbf{R}_j,
\end{aligned} \quad (36)$$

where $p(\mathbf{R}_j, \mathbf{R}_k | \mathbf{R}_i) = p(\mathbf{R}_j | \mathbf{R}_i) p(\mathbf{R}_k | \mathbf{R}_j, \mathbf{R}_i)$ is the conditional probability of finding the particles at \mathbf{R}_j and \mathbf{R}_k with respect to a particle at \mathbf{R}_i . The above integral equation is simplified as follows.

- Eq. (36) involves correlation functions of higher orders. In practice, these functions are unknown unless some approximations are made or the statistics is Gaussian. In the first case, higher-order statistics can be completely ignored, while in the second case, higher-order correlation functions can be written in terms of products of lower-order ones. The first option is adopted in our analysis. As statistics higher than the pair statistics has not been employed in the truncation of the hierarchy of equations for the coherent field, we neglect the terms involving $p(\mathbf{R}_j, \mathbf{R}_k | \mathbf{R}_i)$. The resulting equation is similar to the equation associated with a continuous random medium with Gaussian fluctuations of the physical properties, when all correlation functions can be written in terms of the pair correlation function.

- For a large geometrical thickness H , we approximate the conditional configuration average of the exciting field coefficients $\langle e_i \rangle_i$ by that of a dense semi-infinite medium. In this case, $\langle e_i \rangle_i$ can be computed either by using

- the dense-medium relation

$$\langle e_i \rangle_i = e^{i\mathbf{K}\mathbf{R}_i} e, \quad (37)$$

where \mathbf{K} is given by (cf. Eq. (126) of Ref. [1])

$$\mathbf{K} = k_1 \hat{\mathbf{s}} + (K_z - k_1 \cos \theta_0) \hat{\mathbf{z}}, \quad (38)$$

$$K_z = \sqrt{K^2 - k_1^2 \sin^2 \theta_0}, \quad (39)$$

and both K and e are computed from the generalized Lorentz–Lorenz law and the generalized Ewald–Oseen extinction theorem for a dense semi-infinite discrete random medium, or

- the sparse-medium approximation

$$\langle e_i \rangle_i = e^{i\mathbf{K}_0 \cdot \mathbf{R}_i} e_0, \quad (40)$$

where the effective incident wave vector \mathbf{K}_0 is given by (cf. Eq. (211) of Ref. [2])

$$\mathbf{K}_0 = k_1 \hat{\mathbf{s}} + (K - k_1) \frac{\hat{\mathbf{z}}}{\cos \theta_0}, \quad (41)$$

and the effective wave number K is computed from the generalized Lorentz–Lorenz law for a dense semi-infinite discrete random medium.

Note that for a dense medium, K satisfies the following equation of the generalized Ewald–Oseen extinction theorem (cf. Eq. (166) of Ref. [2]):

$$K = k_1 - j \frac{\pi n_0}{k_1^2} \sum_n (2n+1) (T_n^1 x_{+n}^1 + T_n^2 x_{+n}^2), \quad (42)$$

while for a sparse medium, K satisfies Eq. (42) with $x_{+n}^{1,2} = 1$. It is obvious that the representation (40) simplifies the calculation because the vector e needs not to be computed; it is sufficient to solve the dispersion equation for the effective wavenumber K . For this reason and because the volume concentration is assumed to be rather small, we adopt the simplified representation (40) for $\langle e_i \rangle_i$.

- In accordance with the generalized Ewald–Oseen extinction theorem, at a certain depth within the medium, the incident wave transforms into a coherent wave which propagates into the effective medium. This applies also in the case of a wave propagating from one scatterer to another. In order to describe the propagation of the scattered waves in an effective medium, we

- make the replacement

$$Q(k_1 \mathbf{R}_{ij}) \rightarrow Q(K \mathbf{R}_{ij}) = e^{j(K-k_1)R_{ij}} Q(k_1 \mathbf{R}_{ij}), \quad (43)$$

and

- substitute $k_1 \hat{\mathbf{s}}$ in the expression of the incident field coefficients $e_{0i} = \exp(jk_1 \hat{\mathbf{s}} \cdot \mathbf{R}_i) e_0$ with \mathbf{K}_0 , or equivalently and in view of Eq. (40), make the change

$$e_{0i} = e^{jk_1 \hat{\mathbf{s}} \cdot \mathbf{R}_i} e_0 \rightarrow e^{j\mathbf{K}_0 \cdot \mathbf{R}_i} e_0 = \langle e_i \rangle_i. \quad (44)$$

The replacement (43) is equivalent to the following replacement for the radiating spherical wave functions (see Eqs. (67), and (69)–(71) below):

$$u_{mn}^3(k_1 \mathbf{r}) \rightarrow u_{mn}^3(K \mathbf{r}) = e^{j(K-k_1)r} u_{mn}^3(k_1 \mathbf{r}), \quad (45)$$

meaning that

$$h_n(k_1 r) = \frac{e^{jk_1 r}}{k_1 r} \tilde{h}_n(k_1 r) \rightarrow h_n(Kr) = \frac{e^{jKr}}{k_1 r} \tilde{h}_n(k_1 r), \quad (46)$$

where $u_{mn}^3(k_1 \mathbf{r})$ are the radiating spherical wave functions, $\tilde{h}_n(x)$ are the spherical Hankel functions of argument x , and $\tilde{h}_n(x)$ are the modified Hankel functions characterizing the near field between the particles and satisfying the same recurrence relation as h_n with the initial values $\tilde{h}_0(x) = -j$ and $\tilde{h}_1(x) = -(1+j/x)$ [3].

- In the spirit of the quasi-crystalline approximation, we use

$$\langle e_j e_i^\dagger \rangle_{ij} = \langle e_j e_j^\dagger \rangle_j, \quad (47)$$

which is the analog of the quasi-crystalline approximation for the exciting field coefficients $\langle e_j \rangle_{ij} = \langle e_j \rangle_j$.

In this setting, we use the conditional probability $p(\mathbf{R}_j | \mathbf{R}_i) = (1/V)g(R_{ij})$, where $g(R_{ij})$ is the pair correlation function, to obtain the following integral equation for the ladder correlation matrix of the exciting field coefficients:

$$\langle e_i e_i^\dagger \rangle_i = \langle e_i \rangle_i \langle e_i^\dagger \rangle_i + n_0 \int_D Q(K \mathbf{R}_{ij}) \langle e_j e_j^\dagger \rangle_j Q^\dagger(K \mathbf{R}_{ij}) g(R_{ij}) d^3 \mathbf{R}_j. \quad (48)$$

Recall that $g(R_{ij})$ is non-zero in the domain $D - D_{2a}(\mathbf{R}_i)$, where $D_{2a}(\mathbf{R}_i)$ is a sphere of radius $2a$ centered at \mathbf{R}_i . The iterated solution of Eq. (48) is

$$\begin{aligned} \langle e_i e_i^\dagger \rangle_i &= \langle e_i \rangle_i \langle e_i^\dagger \rangle_i + n_0 \int_D Q(K \mathbf{R}_{ij}) \langle e_j \rangle_j \langle e_j^\dagger \rangle_j \\ &\quad \times Q^\dagger(K \mathbf{R}_{ij}) g(R_{ij}) d^3 \mathbf{R}_j \\ &\quad + n_0^2 \int_D Q(K \mathbf{R}_{ij}) Q(K \mathbf{R}_{jk}) \langle e_k \rangle_k \langle e_k^\dagger \rangle_k Q^\dagger(K \mathbf{R}_{jk}) Q^\dagger(K \mathbf{R}_{ij}) \\ &\quad \times g(R_{jk}) g(R_{ij}) d^3 \mathbf{R}_k d^3 \mathbf{R}_j + \dots, \end{aligned} \quad (49)$$

and in a diagrammatic representation, Eq. (49) is equivalent to the correlated ladder approximation for $\langle e_i e_i^\dagger \rangle_i$:

$$\langle e_i e_i^\dagger \rangle_i = \begin{array}{c} i \\ \circ \end{array} \begin{array}{c} \longleftarrow \\ \longrightarrow \end{array} \begin{array}{c} \circ \\ i \end{array} + \begin{array}{c} i \\ \circ \end{array} \begin{array}{c} \longleftarrow \\ \longrightarrow \end{array} \begin{array}{c} \circ \\ \sum j \end{array} \begin{array}{c} \longleftarrow \\ \longrightarrow \end{array} \begin{array}{c} \circ \\ i \end{array} + \begin{array}{c} i \\ \circ \end{array} \begin{array}{c} \longleftarrow \\ \longrightarrow \end{array} \begin{array}{c} \circ \\ \sum j \end{array} \begin{array}{c} \longleftarrow \\ \longrightarrow \end{array} \begin{array}{c} \circ \\ \sum k \end{array} \begin{array}{c} \longleftarrow \\ \longrightarrow \end{array} \begin{array}{c} \circ \\ i \end{array} + \dots$$

where

$$\langle e_i \rangle_i = \begin{array}{c} i \\ \circ \end{array} \begin{array}{c} \longleftarrow \\ \longrightarrow \end{array}, \quad Q(K \mathbf{R}_{ij}) = \begin{array}{c} i \\ \circ \end{array} \begin{array}{c} \longleftarrow \\ \longrightarrow \end{array} \begin{array}{c} j \\ \circ \end{array}, \quad \text{and} \quad g(R_{ij}) = \begin{array}{c} i \\ \circ \end{array} \begin{array}{c} \longleftarrow \\ \longrightarrow \end{array} \begin{array}{c} j \\ \circ \end{array}.$$

The previous results can also be obtained by employing the technique described in Refs. [3,5]. This approach involves the following steps.

- Consider the series representation for e_i (cf. Eq. (45) of Ref. [1])

$$e_i = e_{0i} + \sum_{j \neq i} Q(k_1 \mathbf{R}_{ij}) e_{0j} + \sum_{j \neq i} \sum_{k \neq i, j} Q(k_1 \mathbf{R}_{ij}) Q(k_1 \mathbf{R}_{jk}) e_{0k} + \dots,$$

in which $Q(k_1 \mathbf{R}_{ij})$ and e_{0i} are replaced by $Q(K\mathbf{R}_{ij})$ and $\langle e_i \rangle_i$, respectively, that is,

$$e_i = \langle e_i \rangle_i + \sum_{j \neq i} Q(K\mathbf{R}_{ij}) \langle e_j \rangle_j + \sum_{j \neq i} \sum_{k \neq i, j} Q(K\mathbf{R}_{ij}) Q(K\mathbf{R}_{jk}) \langle e_k \rangle_k + \dots \quad (50)$$

2. Multiply Eq. (50) by its complex conjugate; the matrix product will contain terms corresponding to different diagrams in the diagrammatic representation of the Bethe–Salpeter equation, e.g., ladder diagrams arising from the interference of pairs of conjugate waves propagating along the same self-avoiding path in the same direction, cyclical diagrams corresponding to the interference of pairs of conjugate waves propagating along the same self-avoiding path but in opposite directions, diagrams corresponding to the interference between single and double scattered waves, double scattered and triple scattered waves, and so on. Retain in the matrix product $e_i e_i^\dagger$ only the terms corresponding to the ladder diagrams; the result is

$$e_i e_i^\dagger = \langle e_i \rangle_i \langle e_i^\dagger \rangle_i + \sum_{j \neq i} Q(K\mathbf{R}_{ij}) \langle e_j \rangle_j \langle e_j^\dagger \rangle_j Q^\dagger(K\mathbf{R}_{ji}) + \sum_{j \neq i} \sum_{k \neq i, j} Q(K\mathbf{R}_{ij}) Q(K\mathbf{R}_{jk}) \langle e_k \rangle_k \langle e_k^\dagger \rangle_k \times Q^\dagger(K\mathbf{R}_{jk}) Q^\dagger(K\mathbf{R}_{ij}) + \dots, \quad (51)$$

showing that $e_i e_i^\dagger$ is the iterated solution of the equation

$$e_i e_i^\dagger = \langle e_i \rangle_i \langle e_i^\dagger \rangle_i + \sum_{j \neq i} Q(K\mathbf{R}_{ij}) e_j e_j^\dagger Q^\dagger(K\mathbf{R}_{ji}). \quad (52)$$

3. Take the conditional configuration average of Eq. (52) with the position of particle i held fixed, and use the quasi-crystalline approximation (47) to obtain the integral equation (48).

A short comment is in order. If we take the conditional configuration average of Eq. (51) and approximate higher-order correlation functions by products of pair correlation functions we obtain the iterated solution (49), and so, the integral equation (48). Specifically, this means for example, that for the third term on the right-hand side of Eq. (51), we use

$$p(\mathbf{R}_j, \mathbf{R}_k | \mathbf{R}_i) = p(\mathbf{R}_j | \mathbf{R}_i) p(\mathbf{R}_k | \mathbf{R}_j, \mathbf{R}_i) \approx p(\mathbf{R}_j | \mathbf{R}_i) p(\mathbf{R}_k | \mathbf{R}_j), \quad (53)$$

while for the fourth term corresponding to the chain $i \leftarrow j \leftarrow k \leftarrow l$, we use

$$\begin{aligned} p(\mathbf{R}_j, \mathbf{R}_k, \mathbf{R}_l | \mathbf{R}_i) &= p(\mathbf{R}_j | \mathbf{R}_i) p(\mathbf{R}_k, \mathbf{R}_l | \mathbf{R}_j, \mathbf{R}_i) \\ &= p(\mathbf{R}_j | \mathbf{R}_i) p(\mathbf{R}_k | \mathbf{R}_j, \mathbf{R}_i) p(\mathbf{R}_l | \mathbf{R}_k, \mathbf{R}_j, \mathbf{R}_i) \\ &\approx p(\mathbf{R}_j | \mathbf{R}_i) p(\mathbf{R}_k | \mathbf{R}_j) p(\mathbf{R}_l | \mathbf{R}_k). \end{aligned} \quad (54)$$

The approximations (53) and (54) are equivalent to the assumption that the chain of particles is a Markov chain with the transition probability determined by the pair correlation function, e.g., for the chain of particles $i \leftarrow j \leftarrow k \leftarrow l$, we have $p(\mathbf{R}_k | \mathbf{R}_j, \mathbf{R}_i) = p(\mathbf{R}_k | \mathbf{R}_j)$ and $p(\mathbf{R}_l | \mathbf{R}_k, \mathbf{R}_j, \mathbf{R}_i) = p(\mathbf{R}_l | \mathbf{R}_k)$. Therefore, only for a Markov chain, the configuration average of the series (51) can be summed up to yield the integral equation (48). In this context, it is obvious that the Markov-chain approximation is equivalent to the quasi-crystalline approximation (47) which is used when taking the conditional configuration average of Eq. (52) and deriving the integral equation (48).

According to Eq. (29), the diffuse ladder coherency dyadic $\mathcal{C}_{dL}(\mathbf{r})$ is determined by the ladder correlation matrix $\langle e_i e_i^\dagger \rangle_i$, while in view of Eq. (30), the diffuse cross coherency dyadic $\mathcal{C}_{dC}(\mathbf{r})$ is determined by the so-called cross correlation matrix $\langle e_i e_j^\dagger \rangle_{ij}$. Recall that the diffuse cross coherency dyadic is associated with the sum

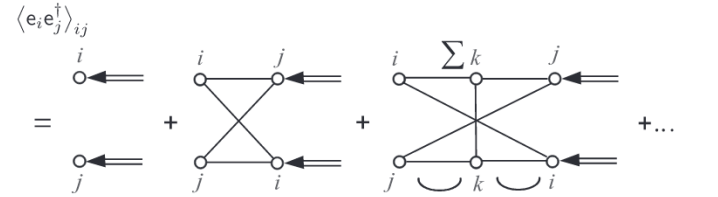
of the cyclical diagrams describing the interference of two waves propagating along the same self-avoiding path connecting scatterers i and j , but in opposite directions. For reasons of comparison, we conclude this section with some remarks on the computation of the cross correlation matrix $\langle e_i e_j^\dagger \rangle_{ij}$. Making use of the series representation for e_i given by Eq. (50), retaining in the matrix product $e_i e_j^\dagger$ only the terms corresponding to cyclical diagrams, i.e.,

$$\begin{aligned} e_i e_j^\dagger &= \langle e_i \rangle_i \langle e_j^\dagger \rangle_j + Q(K\mathbf{R}_{ij}) \langle e_j \rangle_j \langle e_i^\dagger \rangle_i Q^\dagger(K\mathbf{R}_{ji}) \\ &+ \sum_{k \neq i, j} Q(K\mathbf{R}_{ik}) Q(K\mathbf{R}_{kj}) \langle e_j \rangle_j \langle e_i^\dagger \rangle_i Q^\dagger(K\mathbf{R}_{ki}) Q^\dagger(K\mathbf{R}_{jk}) \\ &+ \sum_{k \neq i, j} \sum_{l \neq i, j, k} Q(K\mathbf{R}_{ik}) Q(K\mathbf{R}_{kl}) Q(K\mathbf{R}_{lj}) \langle e_j \rangle_j \langle e_i^\dagger \rangle_i \\ &\times Q^\dagger(K\mathbf{R}_{li}) Q^\dagger(K\mathbf{R}_{lk}) Q^\dagger(K\mathbf{R}_{jl}) + \dots, \end{aligned} \quad (55)$$

and taking the conditional configuration average while holding the positions of the i th and j th particles fixed, we obtain

$$\begin{aligned} \langle e_i e_j^\dagger \rangle_{ij} &= \langle e_i \rangle_i \langle e_j^\dagger \rangle_j + Q(K\mathbf{R}_{ij}) \langle e_j \rangle_j \langle e_i^\dagger \rangle_i Q^\dagger(K\mathbf{R}_{ji}) \\ &+ \sum_{k \neq i, j} \int_D Q(K\mathbf{R}_{ik}) Q(K\mathbf{R}_{kj}) \langle e_j \rangle_j \langle e_i^\dagger \rangle_i \\ &\times Q^\dagger(K\mathbf{R}_{ki}) Q^\dagger(K\mathbf{R}_{jk}) p(\mathbf{R}_k | \mathbf{R}_i, \mathbf{R}_j) d^3 \mathbf{R}_k \\ &+ \sum_{k \neq i, j} \sum_{l \neq i, j, k} \int_D Q(K\mathbf{R}_{ik}) Q(K\mathbf{R}_{kl}) Q(K\mathbf{R}_{lj}) \langle e_j \rangle_j \langle e_i^\dagger \rangle_i \\ &\times Q^\dagger(K\mathbf{R}_{li}) Q^\dagger(K\mathbf{R}_{lk}) Q^\dagger(K\mathbf{R}_{jl}) \\ &\times p(\mathbf{R}_k, \mathbf{R}_l | \mathbf{R}_i, \mathbf{R}_j) d^3 \mathbf{R}_l d^3 \mathbf{R}_k + \dots \end{aligned} \quad (56)$$

The above series which sums up all single scattering processes between particles i and j is illustrated diagrammatically as



where

$$\langle e_i \rangle_i = i \leftarrow, \quad Q(K\mathbf{R}_{ij}) = i \xrightarrow{j}, \quad \text{and} \quad p(\mathbf{R}_k | \mathbf{R}_i, \mathbf{R}_j) = i \curvearrowright k \curvearrowleft j.$$

Even when approximating higher-order statistics by lower-order statistics, it is not possible to sum up the cyclical diagrams in Eq. (56) and to interpret $\langle e_i e_j^\dagger \rangle_{ij}$ as an iterated solution of an integral equation. However, this can be done for an external observation point situated in the far-field region of the entire particulate medium when the summation is performed by invoking the reciprocity principle. In fact, the reciprocity principle is applied to the series for e_j^\dagger , i.e., we consider a series in which the wave propagation direction is reversed. As a result, the cyclical diagrams are transformed into ladder diagrams involving only pair correlation functions [4].

3.2. Simplification

In the integral equation (48), the conditional configuration average of the exciting field coefficients $\langle e_i \rangle_i$ is given by Eq. (40); hence, we have

$$\langle e_i \rangle_i \langle e_i^\dagger \rangle_i = e^{-K_0 z_i} E_{L0}, \quad (57)$$

where

$$E_{L0} = e_0 e_0^\dagger, \quad (58)$$

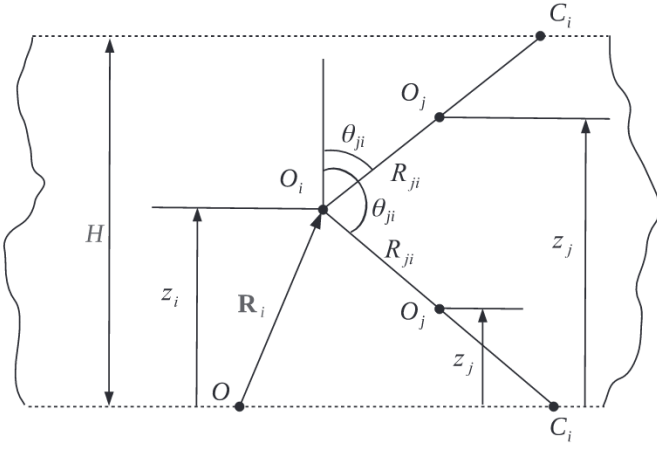


Fig. 1. The integration domain for computing $X_L(z_i)$.

(x_i, y_i, z_i) are the Cartesian coordinates of \mathbf{R}_i ,

$$\kappa_0 = \frac{\kappa}{\cos \theta_0}, \quad \kappa = j(K - K^*) = 2K'', \quad (59)$$

and $K'' = \text{Im}(K)$. Because the source term in the integral equation (48) depends only on z_i and, by assumption, the scattering medium is statistically homogeneous in horizontal directions, we look for a solution in the form

$$\langle \mathbf{e}_i \mathbf{e}_i^\dagger \rangle_i = X_L(z_i), \quad (60)$$

where hereafter the (Hermitian) matrix $X_L(z_i)$ stands for the ladder correlation matrix of the exciting field coefficients. Making the change of variables $\mathbf{R}_{ji} = \mathbf{R}_j - \mathbf{R}_i$, and using Eq. (43), we express the integral equation (48) as

$$X_L(z_i) = e^{-\kappa_0 z_i} E_{L0} + n_0 \int_{D-D_{2a}(z_i)} e^{-\kappa R_{ji}} Q(-k_1 \mathbf{R}_{ji}) X_L(z_j) \times Q^\dagger(-k_1 \mathbf{R}_{ji}) g(R_{ji}) d^3 \mathbf{R}_{ji}, \quad (61)$$

where $D_{2a}(z_i)$ is a sphere of radius $2a$ centered at z_i , $(R_{ji}, \theta_{ji}, \varphi_{ji})$ are the spherical coordinates of \mathbf{R}_{ji} , and $z_j = z_i + R_{ji} \cos \theta_{ji}$. The integral in Eq. (61) is computed by choosing the origin of a local coordinate system at the center of particle i as shown in Fig. 1.

Tishkovets and Jockers [3] employed various approximations to simplify the integral equation (61) into a form that is suitable for a numerical analysis. Their approach is considered here. Let us express this equation as

$$X_L(z_i) = e^{-\kappa_0 z_i} E_{L0} + (\mathcal{L}_L X_L)(z_i) + (\mathcal{M}_L X_L)(z_i), \quad (62)$$

where \mathcal{L}_L and \mathcal{M}_L are integral operators defined by

$$(\mathcal{L}_L X_L)(z_i) = n_0 \int_{D-D_{2a}(z_i)} e^{-\kappa R_{ji}} Q(-k_1 \mathbf{R}_{ji}) X_L(z_j) Q^\dagger(-k_1 \mathbf{R}_{ji}) \times [g(R_{ji}) - 1] d^3 \mathbf{R}_{ji} \quad (63)$$

and

$$(\mathcal{M}_L X_L)(z_i) = n_0 \int_{D-D_{2a}(z_i)} e^{-\kappa R_{ji}} Q(-k_1 \mathbf{R}_{ji}) X_L(z_j) \times Q^\dagger(-k_1 \mathbf{R}_{ji}) d^3 \mathbf{R}_{ji}, \quad (64)$$

respectively. Next, we switch to a component-form representation for the matrices $(\mathcal{L}_L X_L)(z_i)$ and $(\mathcal{M}_L X_L)(z_i)$. For example, in the case of the matrix

$$(\mathcal{L}_L X_L)(z_i) = [(\mathcal{L}_L X_L)_{mn,m'n'}(z_i)],$$

this representation is

$$(\mathcal{L}_L X_L)_{mn,m'n'}(z_i) = n_0 \sum_{m_1 n_1 m_2 n_2} \int_{D-D_{2a}(z_i)} e^{-\kappa R_{ji}} Q_{mn,m_1 n_1}(-k_1 \mathbf{R}_{ji}) \times X_{L m_1 n_1, m_2 n_2}(z_j) Q_{m_2 n_2, m' n'}^\dagger(-k_1 \mathbf{R}_{ji}) \times [g(R_{ji}) - 1] R_{ji}^2 d^2 \hat{\mathbf{R}}_{ji} dR_{ji}, \quad (65)$$

where

$$Q(-k_1 \mathbf{R}_{ji}) = [Q_{mn,m'n'}(-k_1 \mathbf{R}_{ji})], \\ X_L(z_i) = [X_{Lmn,m'n'}(z_i)].$$

Setting

$$X_L(z_i) = [X_{Lmn,m'n'}(z_i)] = \begin{bmatrix} X_{Lmn,m'n'}^{11}(z_i) & X_{Lmn,m'n'}^{12}(z_i) \\ X_{Lmn,m'n'}^{21}(z_i) & X_{Lmn,m'n'}^{22}(z_i) \end{bmatrix}, \quad (66)$$

using the relation (recall that $Q(-k_1 \mathbf{R}_{ji}) = \mathcal{T}_{31}^T(-k_1 \mathbf{R}_{ji}) \mathcal{T}$)

$$Q_{mn,m_1 n_1}(-k_1 \mathbf{R}_{ji}) = \mathcal{T}_{m_1 n_1, mn}^{31}(-k_1 \mathbf{R}_{ji}) T_{n_1}, \quad (67)$$

where

$$\mathcal{T} = [T_n \delta_{mm'} \delta_{nn'}], \quad [T_n] = \begin{bmatrix} T_n^1 \\ T_n^2 \end{bmatrix}, \quad (68)$$

and taking into account the symmetry relations for the translation matrix,

$$[\mathcal{T}_{m_1 n_1, mn}^{31}(-k_1 \mathbf{R}_{ji})] = [\mathcal{T}_{-mn, -m_1 n_1}^{31}(k_1 \mathbf{R}_{ji})] \\ = \begin{bmatrix} A_{-mn, -m_1 n_1}^3(k_1 \mathbf{R}_{ji}) & B_{-mn, -m_1 n_1}^3(k_1 \mathbf{R}_{ji}) \\ B_{-mn, -m_1 n_1}^3(k_1 \mathbf{R}_{ji}) & A_{-mn, -m_1 n_1}^3(k_1 \mathbf{R}_{ji}) \end{bmatrix}, \quad (69)$$

where (cf. Eq. (18) of Ref. [1])

$$A_{-mn, -m_1 n_1}^3(k_1 \mathbf{R}_{ji}) = c_{nn_1} \sum_{n''} j^{n''} a_1(-m, n | -m_1, n_1 | n'') \times u_{m_1 - m, n''}^3(k_1 \mathbf{R}_{ji}), \quad (70)$$

$$B_{-mn, -m_1 n_1}^3(k_1 \mathbf{R}_{ji}) = c_{nn_1} \sum_{n''} j^{n''} b_1(-m, n | -m_1, n_1 | n'') \times u_{m_1 - m, n''}^3(k_1 \mathbf{R}_{ji}), \quad (71)$$

the coefficients $a_1(\cdot)$ and $b_1(\cdot)$ are given by Eq. (19) of Ref. [1], and

$$c_{nn_1} = \frac{2j^{n_1 - n}}{\sqrt{nn_1(n+1)(n_1+1)}}, \quad (72)$$

we obtain the component-form representation for the integral equation (62):

$$X_{Lmn,m'n'}^{pq}(z_i) = e^{-\kappa_0 z_i} E_{L0mn,m'n'}^{pq} + (\mathcal{L}_L X_L)_{mn,m'n'}^{pq}(z_i) + (\mathcal{M}_L X_L)_{mn,m'n'}^{pq}(z_i), \quad p, q = 1, 2, \quad (73)$$

where $E_{L0mn,m'n'}^{pq}$ are the block-matrix components of E_{L0} ,

$$(\mathcal{L}_L X_L)_{mn,m'n'}^{pq}(z_i) = n_0 \sum_{m_1 n_1 m_2 n_2 n'' n'''} K_{m_1 n_1 m_2 n_2 n'' n'''}^{pqrt} \times \int_{D-D_{2a}(z_i)} e^{-\kappa R_{ji}} u_{m_1 - m, n''}^3(k_1 \mathbf{R}_{ji}) X_{L m_1 n_1, m_2 n_2}^{rt}(z_j) \times u_{m_2 - m', n'''}^3(k_1 \mathbf{R}_{ji}) [g(R_{ji}) - 1] R_{ji}^2 d^2 \hat{\mathbf{R}}_{ji} dR_{ji}, \quad (74)$$

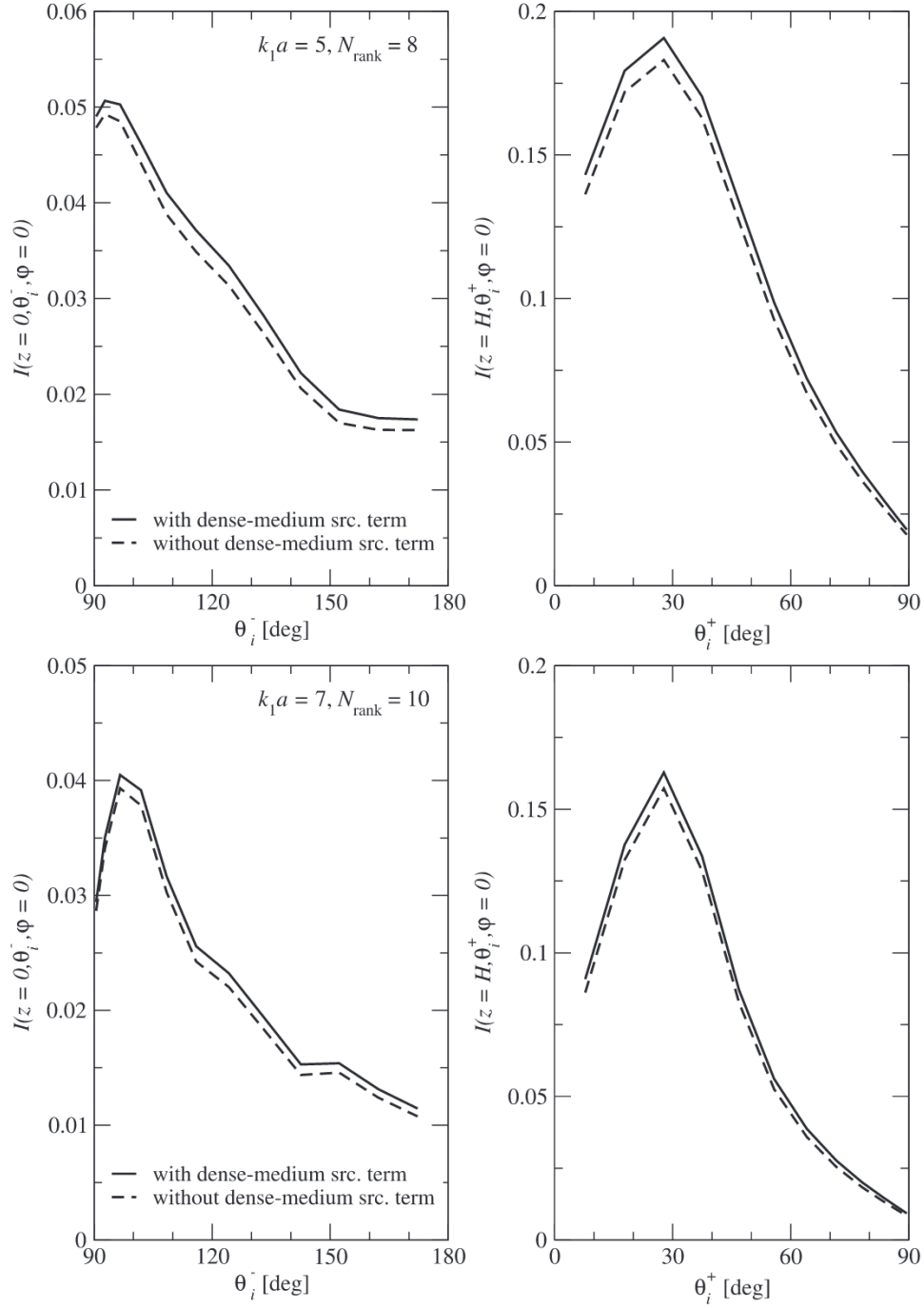


Fig. 2. The specific intensities at the bottom and the top of the layer $I(z=0, \theta_i^-, \varphi=0)$ and $I(z=H, \theta_i^+, \varphi=0)$, respectively. The results correspond to the solution of the radiative transfer equation with (solid curve) and without (dotted curve) the dense-medium source term. The plots in the upper panels corresponds to $k_1 a = 5$, while the plots in the lower panels correspond to $k_1 a = 7$. The incidence angle is $\theta_0 = 30^\circ$, the polarization angle is $\alpha_{\text{pol}} = 45^\circ$, the volume concentration is $f = 0.04$, the layer thickness is $H = 30a$, the wavenumber of the background medium is $k_1 = 10 \mu\text{m}^{-1}$, and the number of Gauss–Legendre quadrature nodes is $N_\mu = 12$.

and

$$\begin{aligned}
 (\mathcal{M}_L X_L)_{mn, m' n'}^{pq}(\mathbf{z}_i) &= n_0 \sum K_{m_1 n_1 m_2 n_2 n'' n'''}^{pqrt} \\
 &\times \int_{D-D_{2a}(\mathbf{z}_i)} e^{-\kappa R_{ji}} u_{m_1-m, n''}^3(k_1 \mathbf{R}_{ji}) X_{L m_1 n_1, m_2 n_2}^{rt}(\mathbf{z}_j) \\
 &\times u_{m_2-m', n'''}^{3*}(k_1 \mathbf{R}_{ji}) R_{ji}^2 d^2 \hat{\mathbf{R}}_{ji} dR_{ji}. \quad (75)
 \end{aligned}$$

In Eqs. (74) and (75), the coefficients $K_{m_1 n_1 m_2 n_2 n'' n'''}^{pqrt}$ are computed as

$$\begin{aligned}
 K_{m_1 n_1 m_2 n_2 n'' n'''}^{pqrt} &= c_{m n_1} c_{n' n_2}^* j^{n''-n'''} t_{pr}(-m, n | -m_1, n_1 | n'') \\
 &\times t_{tq}(-m', n' | -m_2, n_2 | n''') T_{n_1}^r T_{n_2}^{t*}, \quad (76)
 \end{aligned}$$

with

$$t_{11}(\cdot) = t_{22}(\cdot) := a_1(\cdot), \quad (77)$$

$$t_{12}(\cdot) = t_{21}(\cdot) := b_1(\cdot), \quad (78)$$

and the sum should be understood as

$$\sum = \sum_{r,t=1}^2 \sum_{n_1=1}^{N_{\text{rank}}} \sum_{m_1=-n_1}^{n_1} \sum_{n_2=1}^{N_{\text{rank}}} \sum_{m_2=-n_2}^{n_2} \sum_{n''=|n-n_1|}^{n+n_1} \sum_{n'''=|n'-n_2|}^{n'+n_2}, \quad (79)$$

where N_{rank} is the maximum expansion order.

Computation of the matrix $(\mathcal{L}_L X_L)(z_i)$. Consider the integral

$$\begin{aligned} L_{Lmnmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L) \\ = \int_{D-D_{2a}(z_i)} e^{-\kappa R_{ji}} u_{mn}^3(k_1 \mathbf{R}_{ji}) X_{Lm_1n_1m_2n_2}^{rt}(z_j) \\ \times u_{m'n'}^{3*}(k_1 \mathbf{R}_{ji}) [g(R_{ji}) - 1] R_{ji}^2 d^2 \hat{\mathbf{R}}_{ji} dR_{ji} \end{aligned} \quad (80)$$

and take into account that the function $g(R_{ji}) - 1$ quickly decreases with increasing R_{ji} , so that the volume of integration can be extended to the whole space less a sphere of radius $2a$ around \mathbf{R}_i . Note that the same assumption was made in Ref. [1] to compute the effective wavenumber K . Thus, the integral is determined by the particles in the neighborhood of particle i , and we use the approximation

$$\int_{D-D_{2a}(z_i)} R_{ji}^2 d^2 \hat{\mathbf{R}}_{ji} dR_{ji} \approx \int_{\mathbb{R}^3-D_{2a}(z_i)} R_{ji}^2 d^2 \hat{\mathbf{R}}_{ji} dR_{ji}. \quad (81)$$

Besides, we assume that $(z_j = z_i + R_{ji} \cos \theta_{ji})$:

$$\begin{aligned} X_L^{rt}(z_j) &\approx e^{i(\mathbf{K}_0 - \mathbf{K}_0^*) \cdot \mathbf{R}_{ji}} X_L^{rt}(z_i) \\ &= e^{-\kappa_0(z_j - z_i)} X_L^{rt}(z_i) \\ &= e^{-\kappa_0 R_{ji} \cos \theta_{ji}} X_L^{rt}(z_i). \end{aligned} \quad (82)$$

According to this approximation, we suppose that in the neighborhood of particle i (inside a sphere around particle i whose radius R_0 is determined by the interval $[2a, R_0]$ in which the function $g(R_{ji}) - 1$ is not negligible, e.g., $R_0 \approx 8a$), the matrix X_L decreases exponentially with increasing the optical depth along the incidence direction; for $z_j > z_i$, $X_L(z_j)$ decreases with respect to $X_L(z_i)$ when $\kappa_0(z_j - z_i)$ increases, while for $z_j < z_i$, the reverse is true. The approximation (82) is equivalent to the estimate $X_L(z_i) \approx e^{-\kappa_0 z_i} W$ for some matrix W that does not depend on z_i (observe that the source term in Eq. (62) has the same dependence on z_i). Employing this local approximation, we get

$$L_{Lmnmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L) = L_{Lmnmm'n'}^{rt} X_{Lm_1n_1m_2n_2}^{rt}(z_i),$$

where

$$\begin{aligned} L_{Lmnmm'n'} &= 2\pi \delta_{mm'} \int_0^\pi \left\{ \int_{2a}^\infty e^{-\kappa R_{ji}} e^{-\kappa_0 R_{ji} \cos \theta_{ji}} [g(R_{ji}) - 1] \right. \\ &\quad \times h_n(k_1 R_{ji}) h_{n'}^*(k_1 R_{ji}) R_{ji}^2 dR_{ji} \left. \right\} \\ &\quad \times P_n^{(m)}(\cos \theta_{ji}) P_{n'}^{(m')}(\cos \theta_{ji}) \sin \theta_{ji} d\theta_{ji}, \end{aligned} \quad (83)$$

and $P_n^{(m)}(\cos \theta)$ are the associated Legendre functions of degree n and order m . The integral over the polar angle θ_{ji} in Eq. (83) can be computed analytically. Using the series expansion for the plane wave

$$e^{i(\mathbf{K}_0 - \mathbf{K}_0^*) \cdot \mathbf{R}_{ji}} = e^{i(j\kappa_0) \hat{\mathbf{z}} \cdot \mathbf{R}_{ji}} = \sum_{l=0}^\infty 2j^l \sqrt{\frac{2l+1}{2}} u_{0l}^1(j\kappa_0 R_{ji}), \quad (84)$$

and the spherical harmonic expansion theorem for the associated Legendre functions

$$P_n^{(m)}(\cos \theta) P_{n'}^{(m')}(\cos \theta) = \sum_{l=|n-n'|}^{n+n'} a(m, n | -m, n' | l) P_l(\cos \theta), \quad (85)$$

where $u_{0l}^1(j\kappa_0 R_{ji}) = j_l(j\kappa_0 R_{ji}) P_l(\cos \theta_{ji})$ are the regular spherical wave functions for the azimuthal mode $m=0$, $j_l(x)$ are the spherical Bessel functions of argument x , and $P_n(\cos \theta) = P_n^0(\cos \theta)$ are

the Legendre polynomials, we find

$$L_{Lmnmm'n'} = 4\pi \delta_{mm'} \sum_{l=|n-n'|}^{n+n'} j^l \sqrt{\frac{2l+1}{2}} a(m, n | -m, n' | l) F_{nn'}^l, \quad (86)$$

with

$$\begin{aligned} F_{nn'}^l &= \int_{2a}^\infty e^{-\kappa R_{ji}} [g(R_{ji}) - 1] h_n(k_1 R_{ji}) \\ &\quad \times j_l(j\kappa_0 R_{ji}) h_{n'}^*(k_1 R_{ji}) R_{ji}^2 dR_{ji}. \end{aligned} \quad (87)$$

Thus, the elements of the matrix $(\mathcal{L}_L X_L)(z_i)$ are given by

$$\begin{aligned} (\mathcal{L}_L X_L)_{mn, m'n'}^{pq}(z_i) &= n_0 \sum K_{m_1n_1m_2n_2n''n'''}^{pqrt} L_{Lm_1-mn''m_2-m'n'''} \\ &\quad \times X_{Lm_1n_1m_2n_2}^{rt}(z_i). \end{aligned} \quad (88)$$

Computation of the matrix $(\mathcal{M}_L X_L)(z_i)$. Consider the integral

$$\begin{aligned} M_{Lmnmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L) &= \int_{D-D_{2a}(z_i)} e^{-\kappa R_{ji}} u_{mn}^3(k_1 \mathbf{R}_{ji}) X_{Lm_1n_1m_2n_2}^{rt}(z_j) \\ &\quad \times u_{m'n'}^{3*}(k_1 \mathbf{R}_{ji}) R_{ji}^2 d^2 \hat{\mathbf{R}}_{ji} dR_{ji}. \end{aligned} \quad (89)$$

For a medium with sufficiently weak absorption, this integral is mainly determined by the contribution of the particles located in the far-field region of particle i [5]. Therefore, in Eq. (89) we employ

1. the sparse-medium approximation for the integration domain:

$$\int_{D-D_{2a}(z_i)} R_{ji}^2 d^2 \hat{\mathbf{R}}_{ji} dR_{ji} \approx \int_D R_{ji}^2 d^2 \hat{\mathbf{R}}_{ji} dR_{ji}, \quad (90)$$

and

2. the far-field representation for the radiating spherical wave functions:

$$u_{mn}^3(k_1 \mathbf{R}_{ji}) = (-j)^{n+1} \frac{e^{ik_1 R_{ji}}}{k_1 R_{ji}} Y_{mn}(\hat{\mathbf{R}}_{ji}), \quad R_{ji} \rightarrow \infty, \quad (91)$$

where $Y_{mn}(\hat{\mathbf{R}}_{ji})$ are the spherical harmonics for the direction $\hat{\mathbf{R}}_{ji}$.

We obtain

$$\begin{aligned} M_{Lmnmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L) &= \frac{2\pi}{k_1^2} (-j)^{n'-n} \delta_{mm'} \sum_{b=\pm} \int_{\Theta_b} P_n^{(m)}(\cos \theta_{ij}) P_{n'}^{(m')}(\cos \theta_{ij}) \\ &\quad \times \left[\frac{1}{|\cos \theta_{ij}|} \int_0^H \delta_{b, \text{sgn}(z_i - z_j)} e^{-b\kappa \frac{z_i - z_j}{|\cos \theta_{ij}|}} X_{Lm_1n_1m_2n_2}^{rt}(z_j) dz_j \right] \\ &\quad \times \sin \theta_{ij} d\theta_{ij}, \end{aligned} \quad (92)$$

where Θ_+ and Θ_- are the intervals $[0, \pi/2]$ and $(\pi/2, \pi]$, respectively, $\hat{\mathbf{R}}_{ij} = -\hat{\mathbf{R}}_{ji} = \hat{\mathbf{R}}_{ij}(\theta_{ij}, \varphi_{ij})$, and $\delta_{b, \text{sgn}(z_i - z_j)}$ is the indicator function

$$\delta_{b, \text{sgn}(z_i - z_j)} = \begin{cases} 1, & b = \text{sgn}(z_i - z_j) \\ 0, & b \neq \text{sgn}(z_i - z_j) \end{cases} \quad (93)$$

Thus, the components of the matrix $(\mathcal{M}_L X_L)(z_i)$ are given by

$$\begin{aligned} (\mathcal{M}_L X_L)_{mn, m'n'}^{pq}(z_i) &= n_0 \sum K_{m_1n_1m_2n_2n''n'''}^{pqrt} \\ &\quad \times M_{Lm_1-mn''m_2-m'n'''}^{rtm_1n_1m_2n_2}(z_i; X_L). \end{aligned} \quad (94)$$

Another way of computing $M_{Lmnmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L)$ by means of an integral representation for the radiating spherical wave functions in terms of plane waves is given in Appendix A.

The above method for computing $M_{Lmnmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L)$ is equivalent to the computation of the matrix $(\mathcal{M}_L X_L)(z_i)$ by means of

the relation (cf. Eq. (64) with the sparse-medium approximation for the integration domain (90))

$$(\mathcal{M}_L X_L)(z_i) = n_0 \int_D e^{-\kappa R_{ji}} Q(-k_1 \mathbf{R}_{ji}) X_L(z_j) Q^\dagger(-k_1 \mathbf{R}_{ji}) d^3 \mathbf{R}_{ji}, \quad (95)$$

in which, the far-field approximation

$$Q(-k_1 \mathbf{R}_{ji}) = \frac{e^{ik_1 R_{ji}}}{k_1 R_{ji}} Q_\infty(-\hat{\mathbf{R}}_{ji}), \quad R_{ji} \rightarrow \infty, \quad (96)$$

$$Q_\infty(-\hat{\mathbf{R}}_{ji}) = -4\pi j \mathbf{x}^*(-\hat{\mathbf{R}}_{ji}) \cdot \mathbf{x}^T(-\hat{\mathbf{R}}_{ji}) \mathbf{T} \quad (97)$$

is employed. The result is

$$\begin{aligned} (\mathcal{M}_L X_L)(z_i) &= (4\pi)^2 \frac{n_0}{k_1^2} \sum_{b=\pm} \int_{\Omega_b} \mathbf{x}^*(\hat{\mathbf{R}}_{ij}) \cdot \mathbf{x}^T(\hat{\mathbf{R}}_{ij}) \mathbf{T} \\ &\times \left[\frac{1}{|\cos \theta_{ij}|} \int_0^H \delta_{b, \text{sgn}(z_i - z_j)} e^{-bk \frac{z_i - z_j}{|\cos \theta_{ij}|}} X_L(z_j) dz_j \right] \\ &\times \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{R}}_{ij}) \cdot \mathbf{x}^T(\hat{\mathbf{R}}_{ij}) d^2 \hat{\mathbf{R}}_{ij}, \end{aligned} \quad (98)$$

where $\mathbf{x}(\hat{\mathbf{R}}_{ij})$ is the column vector of the vector spherical harmonics in the direction $\hat{\mathbf{R}}_{ij}$, and Ω_+ and Ω_- are the upper and lower unit hemispheres.

In the above approach the matrix $(\mathcal{L}_L X_L)(z_i)$ is a characteristic of a dense medium, while the matrix $(\mathcal{M}_L X_L)(z_i)$ is a characteristic of a sparse medium. Obviously, for a sparse medium, we have $g(R_{ji}) = 1$; hence, $(\mathcal{L}_L X_L)(z_i) = 0$ and the integral equation (62) simplifies to that for sparse media.

Some comments are in order.

1. Discretizing the altitude interval $[0, H]$ with a set of N_z points $\{z_i\}_{i=1}^{N_z}$, and computing the integral in the expression for $(\mathcal{M}_L X_L)(z_i)$ by a quadrature method, we are led to a matrix equation which involves the components of all matrices $X_L(z_i)$ at all quadrature points z_i , $i = 1, \dots, N_z$. The solution of this matrix equation by a direct method is computationally expensive because the dimension of the matrix to be inverted is exceedingly high. To deal with this problem, we may solve the integral equation (62) by applying the iteration formula

$$X_L^{(l)}(z_i) = e^{-\kappa_0 z_i} E_{L0} + (\mathcal{L}_L X_L^{(l-1)})(z_i) + (\mathcal{M}_L X_L^{(l-1)})(z_i). \quad (99)$$

In a computer implementation of this approach, we have to store N_z matrices of dimension $2N_{\max} \times 2N_{\max}$, where

$$N_{\max} = N_{\text{rank}} + M_{\text{rank}}(2N_{\text{rank}} - M_{\text{rank}} + 1),$$

while N_{rank} and M_{rank} are the maximum expansion and azimuthal orders, respectively. For particles with moderate values of the size parameter, the memory requirement is manageable, e.g., for a particle with a size parameter $k_1 a = 5$, the choice $N_{\text{rank}} = M_{\text{rank}} = 10$ guarantees convergence, so that for $N_z = 100$, we have to store 100 matrices of dimension 240×240 .

2. If instead of the representation (40) we use the representation (37) for the conditional configuration average of the exciting field coefficients $\langle e_i \rangle_i$, we get

$$\langle e_i \rangle_i \langle e_i^\dagger \rangle_i = e^{-\kappa_z z_i} E_L, \quad (100)$$

where $E_L = ee^\dagger$, and

$$\kappa_z = 2K_z'' = 2\text{Im}(K_z) = 2\text{Im}(\sqrt{K^2 - k^2 \sin^2 \theta_0}). \quad (101)$$

Comparing Eqs. (57) and (100) it is apparent that the above relations remain valid provided that the following replacements are made:

- (a) $e^{-\kappa_0 z_i} E_{L0} \rightarrow e^{-\kappa_z z_i} E_L$ in Eqs. (61), (62), and (99);
- (b) $e^{-\kappa_0 z_i} E_{L0mn, m'n'}^{pq} \rightarrow e^{-\kappa_z z_i} E_{Lmn, m'n'}^{pq}$ in Eq. (73);
- (c) $X_L^{rt}(z_j) \approx e^{-\kappa_z(z_j - z_i)} X_L^{rt}(z_i)$ instead of the approximation (82); and
- (d) $\kappa_0 \rightarrow \kappa_z$ in Eqs. (83), (84), and (87).

4. Diffuse ladder specific coherency dyadic

To derive the expression for the diffuse ladder specific coherency dyadic $\bar{\Sigma}_{\text{dL}}$ we consider the integral representation (29) in which we make the replacement (compare with Eqs. (43) and (45))

$$\mathbf{X}_3(k_1 \mathbf{r}_i) \rightarrow \mathbf{X}_3(K \mathbf{r}_i) = e^{i(K-k_1)r_i} \mathbf{X}_3(k_1 \mathbf{r}_i). \quad (102)$$

Then, by the change of variables $\mathbf{p} = -\mathbf{r}_i = \mathbf{R}_i - \mathbf{r}$, we obtain

$$\bar{\mathcal{C}}_{\text{dL}}(z) = n_0 \int_D \mathbf{X}_3^T(-K \mathbf{p}) \mathbf{T} X_L(z_i) \mathbf{T}^\dagger \mathbf{X}_3(-K \mathbf{p}) d^3 \mathbf{p}, \quad (103)$$

so that by taking into account the definition of the diffuse ladder specific coherency dyadic $\bar{\Sigma}_{\text{dL}}$ as given by Eq. (31), we get, for a specified direction $\hat{\mathbf{p}}$,

$$\bar{\Sigma}_{\text{dL}}(z, -\hat{\mathbf{p}}) = n_0 \int \mathbf{X}_3^T(-K \mathbf{p}) \mathbf{T} X_L(z_i) \mathbf{T}^\dagger \mathbf{X}_3(-K \mathbf{p}) p^2 dp \quad (104)$$

with $\mathbf{p} = p\hat{\mathbf{p}}$ and $z_i = z + p(\hat{\mathbf{p}} \cdot \hat{\mathbf{z}})$.

The diffuse ladder specific coherency dyadic (104), which has been obtained by applying the sparse-medium approximation for the integration domain in Eq. (29), is of the form $\mathbf{X}_3^T(-K p \hat{\mathbf{p}})(\cdot) \mathbf{X}_3(-K p \hat{\mathbf{p}})$ and is therefore not a transverse dyadic. It can be transformed into a transverse dyadic if we assume that the observation point is in the far zone of the group of particles. Under this assumption, we use Eq. (102) and apply the far-field approximation for the vector spherical wave functions $\mathbf{X}_3(-k_1 \mathbf{p})$ to obtain (cf. Eq. (11) of Ref. [1]):

$$\mathbf{X}_3(-K \mathbf{p}) = -j \frac{e^{iKp}}{k_1 p} \mathbf{x}(-\hat{\mathbf{p}}), \quad p \rightarrow \infty. \quad (105)$$

Consequently, from Eq. (104), we find

$$\bar{\Sigma}_{\text{dL}}(z, -\hat{\mathbf{p}}) = \frac{n_0}{k_1^2} \mathbf{x}^T(-\hat{\mathbf{p}}) \mathbf{T} \left[\int e^{-\kappa p} X_L(z_i) dp \right] \mathbf{T}^\dagger \mathbf{x}^*(-\hat{\mathbf{p}}). \quad (106)$$

For the direction $\hat{\mathbf{k}} = -\hat{\mathbf{p}}$ with $\hat{\mathbf{k}} = \hat{\mathbf{k}}(\theta, \varphi)$, we define the upward and downward propagating vectors $\hat{\mathbf{k}}^+$ and $\hat{\mathbf{k}}^-$ by

$$\hat{\mathbf{k}}^+ = \hat{\mathbf{k}}(\theta, \varphi), \quad \theta \in [0, \pi/2], \quad \varphi \in [0, 2\pi], \quad (107)$$

$$\hat{\mathbf{k}}^- = \hat{\mathbf{k}}(\theta, \varphi), \quad \theta \in (\pi/2, \pi], \quad \varphi \in [0, 2\pi] \quad (108)$$

and obtain the equivalent representation

$$\begin{aligned} \bar{\Sigma}_{\text{dL}}(z, \hat{\mathbf{k}}^b) &= \frac{n_0}{k_1^2} \mathbf{x}^T(\hat{\mathbf{k}}^b) \mathbf{T} \left[\frac{1}{|\cos \theta|} \int_0^H \delta_{b, \text{sgn}(z - z_i)} e^{-bk \frac{z - z_i}{|\cos \theta|}} \right. \\ &\times X_L(z_i) dz_i \left. \right] \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{k}}^b). \end{aligned} \quad (109)$$

Another derivation of Eq. (109) relying on an integral representation of the vector spherical wave functions in terms of plane electromagnetic waves is given in Appendix B. The diffuse ladder specific coherency dyadic (109) is of the form $\mathbf{x}^T(-\hat{\mathbf{p}})(\cdot) \mathbf{x}^*(-\hat{\mathbf{p}})$ and is therefore a transverse dyadic.

5. Vector radiative transfer equation

In this section we derive a radiative transfer equation for the diffuse ladder specific coherency dyadic, obtain the expressions for the reflection and transmission matrices of a layer, and discuss iterative schemes for solving the vector radiative transfer equation.

5.1. Derivation

From Eqs. (98) and (109), we get

$$(\mathcal{M}_L X_L)(z_i) = (4\pi)^2 \int \mathbf{x}^*(\hat{\mathbf{k}}) \cdot \bar{\Sigma}_{\text{dL}}(z_i, \hat{\mathbf{k}}) \cdot \mathbf{x}^T(\hat{\mathbf{k}}) d^2 \hat{\mathbf{k}}. \quad (110)$$

Consequently, the integral [equation \(61\)](#) becomes

$$\begin{aligned} \mathbf{X}_L(z_i) = & \mathbf{e}^{-\kappa_0 z_i} \mathbf{E}_{L0} + (4\pi)^2 \int \mathbf{x}^*(\hat{\mathbf{k}}) \cdot \bar{\Sigma}_{dL}(z_i, \hat{\mathbf{k}}) \cdot \mathbf{x}^T(\hat{\mathbf{k}}) d^2 \hat{\mathbf{k}} \\ & + \bar{\mathbf{X}}_L(z_i), \end{aligned} \quad (111)$$

where the elements of the matrix $\bar{\mathbf{X}}_L(z_i) = (\mathcal{L}_L \mathbf{X}_L)(z_i)$, which is a characteristic of a dense medium, are computed from [Eq. \(88\)](#).

Substituting now [Eq. \(111\)](#) in [Eq. \(109\)](#) gives rise to three terms on the right-hand side of the resulting equation; these terms correspond to the three terms on the right-hand side of [Eq. \(111\)](#). For the first term, we identify (cf. [Eq. \(15\)](#) of Ref. [1])

$$-\frac{4\pi j}{k_1} \mathbf{x}^T(\hat{\mathbf{r}}) \mathbf{T} \mathbf{x}^*(\hat{\mathbf{s}}) = \bar{\mathbf{A}}(\hat{\mathbf{r}}, \hat{\mathbf{s}}), \quad (112)$$

where $\bar{\mathbf{A}}(\hat{\mathbf{r}}, \hat{\mathbf{s}})$ is the far-field scattering dyadic, and use the relations (cf. [Eq. \(58\)](#)) $\mathbf{E}_{L0} = \mathbf{e}_0 \mathbf{e}_0^\dagger$ and (cf. [Eq. \(31\)](#) of Ref. [1]) $\mathbf{e}_0 = 4\pi \mathbf{x}^*(\hat{\mathbf{s}}) \cdot \mathcal{E}_0(\hat{\mathbf{s}})$, to obtain

$$\frac{1}{k_1^2} \mathbf{x}^T(\hat{\mathbf{k}}^b) \mathbf{T} \mathbf{e}^{-\kappa_0 z_i} \mathbf{E}_{L0} \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{k}}^b) = \bar{\mathbf{A}}(\hat{\mathbf{k}}^b, \hat{\mathbf{s}}) \cdot \bar{\mathbf{C}}_c(z_i) \cdot \bar{\mathbf{A}}^\dagger(\hat{\mathbf{k}}^b, \hat{\mathbf{s}}), \quad (113)$$

with

$$\begin{aligned} \bar{\mathbf{C}}_c(z_i) = & \mathbf{e}^{-\kappa_0 z_i} \mathcal{E}_0(\hat{\mathbf{s}}) \otimes \mathcal{E}_0^*(\hat{\mathbf{s}}) \\ = & \sum_{\eta, \xi = \theta, \varphi} \mathbf{e}^{-\kappa_0 z_i} \mathcal{E}_{0\eta} \mathcal{E}_{0\xi}^* \hat{\eta}(\hat{\mathbf{s}}) \otimes \hat{\xi}(\hat{\mathbf{s}}). \end{aligned} \quad (114)$$

Note that [Eq. \(114\)](#) is compatible with the representation (cf. [Eq. \(16\)](#)) $\bar{\mathbf{C}}_c(\mathbf{R}_i) = \mathbf{E}_c(\mathbf{R}_i) \otimes \mathbf{E}_c^*(\mathbf{R}_i)$, since for a sparse medium, we have (cf. [Eq. \(213\)](#) of Ref. [2]) $\mathbf{E}_c(\mathbf{R}_i) = \exp(j\mathbf{K}_0 \cdot \mathbf{R}_i) \mathcal{E}_0(\hat{\mathbf{s}})$. For the second term, application of the relation [\(112\)](#) yields

$$\begin{aligned} & \frac{(4\pi)^2}{k_1^2} \mathbf{x}^T(\hat{\mathbf{k}}^b) \mathbf{T} \mathbf{x}^*(\hat{\mathbf{k}}') \cdot \bar{\Sigma}_{dL}(z_i, \hat{\mathbf{k}}') \cdot \mathbf{x}^T(\hat{\mathbf{k}}') \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{k}}^b) \\ = & \bar{\mathbf{A}}(\hat{\mathbf{k}}^b, \hat{\mathbf{k}}') \cdot \bar{\Sigma}_{dL}(z_i, \hat{\mathbf{k}}') \cdot \bar{\mathbf{A}}^\dagger(\hat{\mathbf{k}}^b, \hat{\mathbf{k}}'). \end{aligned} \quad (115)$$

Taking these results into account, we find the following integral form of the vector radiative transfer equation for the diffuse ladder specific coherency dyadic:

$$\begin{aligned} \bar{\Sigma}_{dL}(z, \hat{\mathbf{k}}^b) = & n_0 \frac{1}{|\cos \theta|} \int_0^H \delta_{b, \text{sgn}(z-z_i)} e^{-b\kappa \frac{z-z_i}{|\cos \theta|}} \left[\bar{\mathbf{A}}(\hat{\mathbf{k}}^b, \hat{\mathbf{s}}) \cdot \bar{\mathbf{C}}_c(z_i) \cdot \bar{\mathbf{A}}^\dagger(\hat{\mathbf{k}}^b, \hat{\mathbf{s}}) \right. \\ & + \left. \int \bar{\mathbf{A}}(\hat{\mathbf{k}}^b, \hat{\mathbf{k}}') \cdot \bar{\Sigma}_{dL}(z_i, \hat{\mathbf{k}}') \cdot \bar{\mathbf{A}}^\dagger(\hat{\mathbf{k}}^b, \hat{\mathbf{k}}') d^2 \hat{\mathbf{k}}' \right] dz_i \\ & + \frac{n_0}{k_1^2} \mathbf{x}^T(\hat{\mathbf{k}}^b) \mathbf{T} \left[\frac{1}{|\cos \theta|} \int_0^H \delta_{b, \text{sgn}(z-z_i)} e^{-b\kappa \frac{z-z_i}{|\cos \theta|}} \bar{\mathbf{X}}_L(z_i) dz_i \right] \\ & \times \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{k}}^b). \end{aligned} \quad (116)$$

Differentiating with respect to z and using the results

$$\delta_{b, \text{sgn}(z-z_i)} = \delta_{b+} H(z-z_i) + \delta_{b-} H(z_i-z), \quad (117)$$

$$\frac{dH(z)}{dz} = \delta(z), \quad (118)$$

which imply

$$\begin{aligned} & \frac{d}{dz} \int_0^H f(z_i) \delta_{b, \text{sgn}(z-z_i)} dz_i \\ = & \int_0^H f(z_i) [\delta_{b+} \delta(z-z_i) - \delta_{b-} \delta(z_i-z)] dz_i \\ = & b f(z), \end{aligned} \quad (119)$$

where $H(z)$ is the Heaviside step function, we obtain the differential form of the vector radiative transfer equation:

$$\begin{aligned} \cos \theta \frac{d\bar{\Sigma}_{dL}(z, \hat{\mathbf{k}})}{dz} = & -\kappa \bar{\Sigma}_{dL}(z, \hat{\mathbf{k}}) \\ & + n_0 \bar{\mathbf{A}}(\hat{\mathbf{k}}, \hat{\mathbf{s}}) \cdot \bar{\mathbf{C}}_c(z) \cdot \bar{\mathbf{A}}^\dagger(\hat{\mathbf{k}}, \hat{\mathbf{s}}) + n_0 \bar{\Gamma}(z, \hat{\mathbf{k}}) \\ & + n_0 \int \bar{\mathbf{A}}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') \cdot \bar{\Sigma}_{dL}(z, \hat{\mathbf{k}}') \cdot \bar{\mathbf{A}}^\dagger(\hat{\mathbf{k}}, \hat{\mathbf{k}}') d^2 \hat{\mathbf{k}}'. \end{aligned} \quad (120)$$

In [Eq. \(120\)](#), the dyadic $\bar{\Gamma}(z, \hat{\mathbf{k}})$ possesses the matrix-form representation

$$\bar{\Gamma}(z, \hat{\mathbf{k}}) = \frac{1}{k_1^2} \mathbf{x}^T(\hat{\mathbf{k}}) \mathbf{T} \bar{\mathbf{X}}_L(z) \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{k}}), \quad (121)$$

which means that in the dyadic-form representation

$$\bar{\Gamma}(z, \hat{\mathbf{k}}) = \sum_{\eta, \xi = \theta, \varphi} \Gamma_{\eta\xi}(z, \hat{\mathbf{k}}) \hat{\eta}(\hat{\mathbf{k}}) \otimes \hat{\xi}(\hat{\mathbf{k}}), \quad (122)$$

the components of $\bar{\Gamma}(z, \hat{\mathbf{k}})$ are

$$\Gamma_{\eta\xi}(z, \hat{\mathbf{k}}) = \frac{1}{k_1^2} \mathbf{x}_\eta^T(\hat{\mathbf{k}}) \mathbf{T} \bar{\mathbf{X}}_L(z) \mathbf{T}^\dagger \mathbf{x}_\xi^*(\hat{\mathbf{k}}), \quad (123)$$

where $\mathbf{x}(\hat{\mathbf{k}}) = \sum_{\eta=\theta, \varphi} \mathbf{x}_\eta(\hat{\mathbf{k}}) \hat{\eta}(\hat{\mathbf{k}})$. [Eq. \(120\)](#) is similar to the vector radiative transfer equation for sparse media; the difference is that now, the source dyadic contains the additional term $n_0 \bar{\Gamma}(z, \hat{\mathbf{k}})$ which is characteristic for a dense medium.

To cast the vector radiative transfer [equation \(120\)](#) into a common form, we use the dyadic-form representation for the far-field scattering dyadic

$$\bar{\mathbf{A}}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') = \sum_{\eta, \xi = \theta, \varphi} S_{0\eta\xi}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') \hat{\eta}(\hat{\mathbf{k}}) \otimes \hat{\xi}(\hat{\mathbf{k}}'), \quad (124)$$

where $S_{0\eta\xi}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') = [S_{0\eta\xi}(\hat{\mathbf{k}}, \hat{\mathbf{k}}')]$ is the single-particle amplitude matrix, and obtain

$$\begin{aligned} \cos \theta \frac{d}{dz} \bar{\Sigma}_{dL\eta\xi}(z, \hat{\mathbf{k}}) = & -\kappa \bar{\Sigma}_{dL\eta\xi}(z, \hat{\mathbf{k}}) + n_0 \sum_{\eta', \xi' = \theta, \varphi} S_{0\eta\eta'}(\hat{\mathbf{k}}, \hat{\mathbf{s}}) S_{0\xi\xi'}^*(\hat{\mathbf{k}}, \hat{\mathbf{s}}) C_{c\eta'\xi'}(z) \\ & + n_0 \Gamma_{\eta\xi}(z, \hat{\mathbf{k}}) \\ & + n_0 \sum_{\eta', \xi' = \theta, \varphi} \int S_{0\eta\eta'}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') S_{0\xi\xi'}^*(\hat{\mathbf{k}}, \hat{\mathbf{k}}') \bar{\Sigma}_{dL\eta'\xi'}(z, \hat{\mathbf{k}}') d^2 \hat{\mathbf{k}}', \end{aligned} \quad (125)$$

where

$$\bar{\Sigma}_{dL}(z, \hat{\mathbf{k}}) = \sum_{\eta, \xi = \theta, \varphi} \bar{\Sigma}_{dL\eta\xi}(z, \hat{\mathbf{k}}) \hat{\eta}(\hat{\mathbf{k}}) \otimes \hat{\xi}(\hat{\mathbf{k}}),$$

and (cf. [Eq. \(114\)](#))

$$\bar{\mathbf{C}}_c(z) = \sum_{\eta, \xi = \theta, \varphi} C_{c\eta\xi}(z) \hat{\eta}(\hat{\mathbf{s}}) \otimes \hat{\xi}(\hat{\mathbf{s}}),$$

$$C_{c\eta\xi}(z) = \mathbf{e}^{-\kappa_0 z} \mathcal{E}_{0\eta} \mathcal{E}_{0\xi}^*.$$

The vector radiative transfer [equation \(125\)](#) can also be written as

$$\begin{aligned} \cos \theta \frac{d\mathbf{J}_{dL}(z, \hat{\mathbf{k}})}{dz} = & -\kappa \mathbf{J}_{dL}(z, \hat{\mathbf{k}}) \\ & + n_0 \mathbf{Z}_{JL}(\hat{\mathbf{k}}, \hat{\mathbf{s}}) \mathbf{J}_c(z) + n_0 \mathbf{J}_{dLns}(z, \hat{\mathbf{k}}) \\ & + n_0 \int \mathbf{Z}_{JL}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') \mathbf{J}_{dL}(z, \hat{\mathbf{k}}') d^2 \hat{\mathbf{k}}', \end{aligned} \quad (126)$$

where,

$$\mathbf{J}_{dL(\eta, \xi)}(z, \hat{\mathbf{k}}) = \frac{1}{2} \sqrt{\frac{\varepsilon_1}{\mu_0}} \bar{\Sigma}_{dL\eta\xi}(z, \hat{\mathbf{k}}) \quad (127)$$

are the components of the diffuse ladder specific coherency column vector $J_{dL}(z, \hat{\mathbf{k}}) = [J_{dL(\eta, \xi)}(z, \hat{\mathbf{k}})]$,

$$J_{c(\eta, \xi)}(z) = \frac{1}{2} \sqrt{\frac{\varepsilon_1}{\mu_0}} C_{\eta\xi}(z) \quad (128)$$

are the components of the coherency column vector of the coherent field $J_c(z) = [J_{c(\eta, \xi)}(z)]$,

$$J_{dns(\eta, \xi)}(z, \hat{\mathbf{k}}) = \frac{1}{2} \sqrt{\frac{\varepsilon_1}{\mu_0}} \Gamma_{\eta\xi}(z, \hat{\mathbf{k}}) \quad (129)$$

are the components of the diffuse coherency column vector for a dense medium $J_{dns}(z, \hat{\mathbf{k}}) = [J_{dns(\eta, \xi)}(z, \hat{\mathbf{k}})]$, and

$$Z_{JL(\eta, \xi)(\eta', \xi')}(z, \hat{\mathbf{k}}, \hat{\mathbf{k}}') = S_{0\eta\eta'}(z, \hat{\mathbf{k}}, \hat{\mathbf{k}}') S_{0\xi\xi'}^*(z, \hat{\mathbf{k}}, \hat{\mathbf{k}}'), \quad (130)$$

are the components of the ladder coherency phase matrix

$$Z_{JL}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') = [Z_{JL(\eta, \xi)(\eta', \xi')}(z, \hat{\mathbf{k}}, \hat{\mathbf{k}}')].$$

In Eqs. (127)–(130), the multi-index $\nu = (\eta, \xi)$ is such that ν takes the values $\nu = 1, 2, 3, 4$ for $(\eta, \xi) = (\theta, \theta), (\theta, \varphi), (\varphi, \theta), (\varphi, \varphi)$, respectively.

Some comments can be made here.

1. For $f \ll 1$, we can approximate $x_{+n}^{1,2} \approx 1$ in Eq. (42). Consequently, we obtain

$$K = k_1 - j \frac{\pi n_0}{k_1^2} \sum_n (2n+1)(T_n^1 + T_n^2), \quad (131)$$

and from the relations

$$S(0) = S_{0\theta\theta}(\hat{\mathbf{s}}, \hat{\mathbf{s}}) = S_{0\varphi\varphi}(\hat{\mathbf{s}}, \hat{\mathbf{s}}) = -\frac{j}{2k_1} \sum_n (2n+1)(T_n^1 + T_n^2), \quad (132)$$

and $C_{ext} = (4\pi/k_1) \text{Im}[S(0)]$, we get

$$\kappa = -j(K - K^*) = n_0 C_{ext}, \quad (133)$$

where $S(\hat{\mathbf{s}}, \hat{\mathbf{s}})$ is the amplitude matrix in the forward direction and C_{ext} is the extinction cross section.

2. For a sparse medium, we have $\bar{X}_L(z) = 0$ implying $J_c(z) = 0$. As a result, we are led to the standard form representation for the vector radiative transfer equation. Alternative derivations of this equation for sparse media are given in Appendix C.
3. In the present approach we considered spherical particles. For a sparse medium consisting of non-spherical particles in arbitrary orientations, the extinction matrix and the phase matrix are averaged over the particle orientations [6,7]. Similarly, for a sparse medium consisting of clusters of particles, the extinction cross section and the phase matrix are averaged over the positions of the particles in the cluster. Several methods for modeling the radiative transfer in a sparse medium consisting of clusters of particles are presented in Appendix D.
4. A backward Monte Carlo method for modeling the radiative transfer in a dense medium is discussed in Appendix E. This model relies on the solution of the integral equation (61) and the computation of the diffuse ladder specific coherency dyadic from Eq. (106), and employs essentially the same assumptions as those used in the derivation of the vector radiative transfer equation (120).

5.2. Reflection and transmission matrices of a layer

The vector radiative transfer equation (126) has been derived by using the integral representation (109) for the diffuse ladder specific coherency dyadic, and the simplified version (111) of the integral equation (61) for the ladder correlation matrix of the exciting

field coefficients. In principle, the reflection and transmission matrices of the layer $R_{JL}(\hat{\mathbf{r}}, \hat{\mathbf{s}})$ and $T_{JL}(\hat{\mathbf{r}}, \hat{\mathbf{s}})$, defined by

$$J_{dL}(0, \hat{\mathbf{r}}) = \cos \theta_0 R_{JL}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) J_c(0), \quad (134)$$

and

$$J_{dL}(H, \hat{\mathbf{r}}) = \cos \theta_0 T_{JL}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) J_c(0), \quad (135)$$

respectively, where $\hat{\mathbf{r}}$ is the scattering direction, can be obtained by solving the vector radiative transfer equation for specific polarizations of the incident wave. However, the above approach can also be used to derive analytical expressions for $R_{JL}(\hat{\mathbf{r}}, \hat{\mathbf{s}})$ and $T_{JL}(\hat{\mathbf{r}}, \hat{\mathbf{s}})$.

To find these expressions, we begin with a result characterizing the solution of the polarized integral equation (61): for $\mathbf{e}_0 = \sum_{\eta} \mathcal{E}_{0\eta} \mathbf{e}_{0\eta}$ with $\mathbf{e}_{0\eta} = 4\pi \mathbf{x}_{\eta}^*(\hat{\mathbf{s}})$, the relation

$$\mathbf{E}_{L0} = \mathbf{e}_0 \mathbf{e}_0^\dagger = \sum_{\eta, \xi = \theta, \varphi} \mathcal{E}_{0\eta} \mathcal{E}_{0\xi}^* \mathbf{e}_{0\eta} \mathbf{e}_{0\xi}^\dagger \quad (136)$$

and the linearity of the integral equation (61) imply that the solution $X_{L\eta\xi}(z_i)$ of the polarized integral equation

$$X_{L\eta\xi}(z_i) = e^{-\kappa_0 z_i} \mathbf{E}_{L0\eta\xi} + n_0 \int_{D-D_{2a}(z_i)} e^{-\kappa R_{ji}} Q(-k_1 \mathbf{R}_{ji}) X_{L\eta\xi}(z_j) \times Q^\dagger(-k_1 \mathbf{R}_{ji}) g(R_{ji}) d^3 \mathbf{R}_{ji}, \quad (137)$$

where $\mathbf{E}_{L0\eta\xi} = \mathbf{e}_{0\eta} \mathbf{e}_{0\xi}^\dagger$, is related to the solution $X_L(z_i)$ of the integral equation (61) via

$$X_L(z_i) = \sum_{\eta, \xi = \theta, \varphi} \mathcal{E}_{0\eta} \mathcal{E}_{0\xi}^* X_{L\eta\xi}(z_i). \quad (138)$$

Now, in Eq. (109), we consider the downward direction $\hat{\mathbf{k}}^- = \hat{\mathbf{r}}$ with $\hat{\mathbf{r}} = \hat{\mathbf{r}}(\theta, \varphi)$, set $z = 0$, and use the representation (138) together with the relation $\mathbf{x}(\hat{\mathbf{r}}) = \sum_{\eta = \theta, \varphi} \mathbf{x}_{\eta}(\hat{\mathbf{r}}) \hat{\eta}(\hat{\mathbf{r}})$, to derive

$$\Sigma_{dL\eta\xi}(0, \hat{\mathbf{r}}) = \sum_{\eta', \xi' = \theta, \varphi} \left\{ \frac{n_0}{k_1^2} \mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} \left[\frac{1}{|\cos \theta|} \right] \times \int_0^H e^{-\frac{\kappa}{|\cos \theta|} z_i} X_{L\eta'\xi'}(z_i) dz_i \right\} \mathbf{T}^\dagger \mathbf{x}_{\xi}^*(\hat{\mathbf{r}}) \mathcal{E}_{0\eta'} \mathcal{E}_{0\xi}^*. \quad (139)$$

Then, from Eq. (139), we find that the elements of the reflection matrix

$$R_{JL}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = [R_{JL(\eta, \xi)(\eta', \xi')}(\hat{\mathbf{r}}, \hat{\mathbf{s}})]$$

are given by

$$R_{JL(\eta, \xi)(\eta', \xi')}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = \frac{n_0}{k_1^2} \mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} \left[\frac{1}{\cos \theta_0 |\cos \theta|} \right] \times \int_0^H e^{-\frac{\kappa}{|\cos \theta|} z_i} X_{L\eta'\xi'}(z_i) dz_i \mathbf{T}^\dagger \mathbf{x}_{\xi}^*(\hat{\mathbf{r}}). \quad (140)$$

For the transmission matrix we proceed similarly. Considering the upward direction $\hat{\mathbf{k}}^+ = \hat{\mathbf{r}}$ with $\hat{\mathbf{r}} = \hat{\mathbf{r}}(\theta, \varphi)$, and setting $z = H$ in Eq. (109), we infer that the elements of the transmission matrix

$$T_{JL}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = [T_{JL(\eta, \xi)(\eta', \xi')}(\hat{\mathbf{r}}, \hat{\mathbf{s}})]$$

are given by

$$T_{JL(\eta, \xi)(\eta', \xi')}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = \frac{n_0}{k_1^2} \mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} \left[\frac{1}{\cos \theta_0 |\cos \theta|} \right] \times \int_0^H e^{-\frac{\kappa}{|\cos \theta|} (H-z_i)} X_{L\eta'\xi'}(z_i) dz_i \mathbf{T}^\dagger \mathbf{x}_{\xi}^*(\hat{\mathbf{r}}). \quad (141)$$

In a subsequent paper we will find exactly the same expressions for the reflection and transmission matrices when the observation point is outside the discrete random medium, i.e., when we approach the boundaries from the exterior of the particulate medium. This agreement certifies somehow the validity of the present approach.

Table 1

The maximum of the relative errors over the scattering angles $\varepsilon_{\max R}$ and $\varepsilon_{\max T}$. Columns 1, 2, and 3 correspond to $f = 0.02$, 0.04, and 0.06, respectively. The unspecified parameters of the calculation are as in Fig. 2.

$k_1 a$	N_{rank}	τ			$\varepsilon_{\max R} [\%]$			$\varepsilon_{\max T} [\%]$		
		1	2	3	1	2	3	1	2	3
5	8	1.62	3.36	5.21	0.79	3.63	7.52	0.62	3.36	9.02
7	10	1.69	3.57	5.62	0.74	3.18	6.02	0.66	3.48	9.11
10	14	1.03	2.11	3.23	0.31	1.45	3.72	0.22	1.18	4.16

5.3. Iterative scheme

For a discrete set of points $\{z_i\}_{i=1}^{N_z}$ in the altitude interval $[0, H]$, $J_{\text{dl}}(z, \hat{\mathbf{k}})$ and $X_L(z)$ can be computed by means of the following iterative scheme: given $\bar{X}_L^{(N-1)}(z_i)$ and $J_{\text{dns}}^{(N-1)}(z_i, \hat{\mathbf{k}})$, at the iteration step N ,

1. solve the vector radiative transfer equation

$$\cos \theta \frac{dJ_{\text{dl}}^{(N)}(z, \hat{\mathbf{k}})}{dz} = -\kappa J_{\text{dl}}^{(N)}(z, \hat{\mathbf{k}}) + n_0 Z_{\text{JL}}(\hat{\mathbf{k}}, \hat{\mathbf{s}}) J_c(z) + n_0 J_{\text{dns}}^{(N-1)}(z, \hat{\mathbf{k}}) + n_0 \int Z_{\text{JL}}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') J_{\text{dl}}^{(N)}(z, \hat{\mathbf{k}}') d^2 \hat{\mathbf{k}}' \quad (142)$$

for $J_{\text{dl}}^{(N)}(z_i, \hat{\mathbf{k}})$;

2. compute the matrix $X_L(z_i)$ as

$$X_L(z_i) = e^{-\kappa_0 z_i} E_{L0} + \bar{X}_L^{(N-1)}(z_i) + 32\pi^2 \sqrt{\frac{\mu_0}{\varepsilon_1}} \sum_{\eta, \xi=\theta, \varphi} \int J_{\text{dl}}^{(N)}(z_i, \hat{\mathbf{k}}) x_{\eta}^* (\hat{\mathbf{k}}) x_{\xi}^T (\hat{\mathbf{k}}) d^2 \hat{\mathbf{k}}; \quad (143)$$

3. update the dense-medium matrix $\bar{X}_L(z_i)$ by computing the elements of the matrix

$$\bar{X}_L^{(N)}(z_i) = (\mathcal{L}_L X_L^{(N)})(z_i) = [\bar{X}_{Lmn, m'n'}^{pq(N)}(z_i)]$$

as (cf. Eq. (88))

$$\bar{X}_{Lmn, m'n'}^{pq(N)}(z_i) = n_0 \sum K_{m_1 n_1 m_2 n_2 n'' n'''}^{pqrt} L_{Lm_1 - mn'' m_2 - m' n'''} \times X_{Lm_1 n_1, m_2 n_2}^{rt}(z_i), \quad p, q = 1, 2; \quad (144)$$

4. update the diffuse coherency column vector for a dense medium $J_{\text{dns}}(z_i, \hat{\mathbf{k}})$ by computing the elements of the vector $J_{\text{dns}}^{(N)}(z_i, \hat{\mathbf{k}})$ as (cf. Eqs. (123) and (129))

$$J_{\text{dns}}^{(N)}(z_i, \hat{\mathbf{k}}) = \frac{1}{2k_1^2} \sqrt{\frac{\varepsilon_1}{\mu_0}} x_{\eta}^T (\hat{\mathbf{k}}) T \bar{X}_L^{(N)}(z_i) T^{\dagger} x_{\xi}^* (\hat{\mathbf{k}}). \quad (145)$$

The iterations are initialized with $\bar{X}_L^{(0)} = 0$ and $J_{\text{dns}}^{(0)}(z_i, \hat{\mathbf{k}}) = 0$, and so, at the first iteration, the pair $J_{\text{dl}}^{(1)}(z_i, \hat{\mathbf{k}})$ and $X_L(z_i)$ corresponds to the sparse-medium solution. At the subsequent iterations, we solve the vector radiative transfer equation for sparse media with a source term accounting for the correlation between the particles.

We may also solve the vector radiative transfer equation (142) by the method of Picard iterations, that is, we may consider the iterative scheme

$$\cos \theta \frac{dJ_{\text{dl}}^{(N)}(z, \hat{\mathbf{k}})}{dz} = -\kappa J_{\text{dl}}^{(N)}(z, \hat{\mathbf{k}}) + n_0 Z_{\text{JL}}(\hat{\mathbf{k}}, \hat{\mathbf{s}}) J_c(z) + n_0 J_{\text{dns}}^{(N-1)}(z, \hat{\mathbf{k}}) + n_0 \int Z_{\text{JL}}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') J_{\text{dl}}^{(N-1)}(z, \hat{\mathbf{k}}') d^2 \hat{\mathbf{k}}' \quad (146)$$

or, equivalently, its integral form

$$J_{\text{dl}}^{(N)}(z, \hat{\mathbf{k}}^b) = n_0 \frac{1}{|\cos \theta|} \int_0^H \delta_{b, \text{sgn}(z-z_i)} e^{-b\kappa \left| \frac{z-z_i}{|\cos \theta|} \right|} \left[Z_{\text{JL}}(\hat{\mathbf{k}}^b, \hat{\mathbf{s}}) J_c(z_i) + J_{\text{dns}}^{(N-1)}(z_i, \hat{\mathbf{k}}^b) + \int Z_{\text{JL}}(\hat{\mathbf{k}}^b, \hat{\mathbf{k}}') J_{\text{dl}}^{(N-1)}(z_i, \hat{\mathbf{k}}') d^2 \hat{\mathbf{k}}' \right] \times dz_i. \quad (147)$$

These iterations are initialized with $J_{\text{dl}}^{(0)}(z, \hat{\mathbf{k}}) = 0$, $\bar{X}_L^{(0)} = 0$, and $J_{\text{dns}}^{(0)}(z_i, \hat{\mathbf{k}}) = 0$. An algorithm based on Eq. (147) and the discrete ordinate method is described in Appendix F.

We applied the iterative scheme (147) with the boundary conditions $J_{\text{dl}}(z=0, \hat{\mathbf{k}}^+) = 0$ and $J_{\text{dl}}(z=H, \hat{\mathbf{k}}^-) = 0$ to some test examples. To ensure that the iteration method converges, we considered weakly absorbing particles with the relative refractive index $m = 1.33 + 0.01j$. The layer is discretized into $N_{\text{lay}} = \tau / \Delta \tau$ sublayers, where $\tau = \kappa H$ is the optical thickness of the layer and $\Delta \tau$ is chosen to be $\Delta \tau = 0.2$. In Fig. 2 we illustrate the specific intensities $I(z=0, \theta_i^-, \varphi=0)$ and $I(z=H, \theta_i^+, \varphi=0)$ at the scattering angles $\theta_i^{\pm} = \arccos(\pm \mu_i)$, where $\{\mu_i\}_{i=1}^{N_{\mu}}$ is a set of N_{μ} Gauss-Legendre quadrature nodes on the interval $[0, 1]$. Note that the specific intensity $I(z, \hat{\mathbf{k}})$ is the first element of the (diffuse ladder) specific intensity column vector $\mathbf{l}_{\text{dl}}(z, \hat{\mathbf{k}})$, defined by $\mathbf{l}_{\text{dl}}(z, \hat{\mathbf{k}}) = \mathbf{D} J_{\text{dl}}(z, \hat{\mathbf{k}})$, where

$$\mathbf{D} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 0 \\ 0 & -j & j & 0 \end{bmatrix}. \quad (148)$$

The discrepancies between the specific intensities are visible. In fact, as it can be seen in Table 1, the maximum of the relative error over the scattering angles $\varepsilon_{\max R}$ between the specific intensities $I(z=0, \theta_i^-, \varphi=0)$ with and without the dense-media source term, as well as the similar maximum error $\varepsilon_{\max T}$ corresponding to the specific intensities $I(z=H, \theta_i^+, \varphi=0)$, increases with the particle volume concentration.

6. Conclusion

Following closely the approach described in Refs. [3,5] we derived a vector radiative transfer equation with an additional source term typical of dense media. This equation is valid at interior points of the discrete random medium. To reach this goal we were forced to employ a series of approximations that are typical of sparse media. These are:

1. the representation of the total field inside the particulate medium as a superposition of the incident field and all scattered fields,
2. the sparse-medium approximation for the integration domain, and
3. the far-field approximation.

The first two approximations are not very restrictive. The far-field approximation has been used

1. in Section 3.2, to simplify the integral equation for the ladder correlation matrix of the exciting field coefficients, and
2. in Section 4, to compute the diffuse ladder specific coherency dyadic.

It should be pointed out that if in Section 4, the far-field approximation is not used, the diffuse ladder specific coherency dyadic is not a transverse dyadic and consequently, a radiative transfer equation valid at interior points cannot be derived.

Because of the approximations employed, our feeling is that the model can be used to compute the diffuse ladder specific coherency dyadic at interior points for rather low values of the particle volume concentration f . This is the reason why our simulations correspond to a low value of f . For exterior points, i.e., when the scattering is described by the reflection and transmission matrices of the layer, the model can be applied to higher values of the particle volume concentration.

Future work should focus on the design of a validation method for our model. This is not a trivial task because a benchmark model, based on the solution of the multiple scattering equations for the exciting field coefficients, is restricted to a domain of finite size. At the present time, we do not see how such a model can be endowed with periodic boundary conditions as it is done in three-dimensional radiative transfer modeling.

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Appendix A

The integral $M_{Lmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L)$ has been computed by means of the following approach: in Eq. (48) we used the representation (43) for $Q(KR_{ij})$ in terms of $Q(k_1R_{ij})$, and then, by taking into account the relation $Q(k_1R_{ij}) = T_{31}^T(k_1R_{ij})T$, as well as Eqs. (67) and (69), we employed the far-field approximation (91) for $u_{mn}^3(k_1R_{ij})$ in Eqs. (70) and (71). Now, in Eq. (48) we do not use the representation (43) for $Q(KR_{ij})$ and the far-field approximation for $u_{mn}^3(k_1R_{ij})$. Instead, we apply the relation $Q(KR_{ij}) = T_{31}^T(KR_{ij})T$, express $T_{31}(KR_{ij})$ in terms of $u_{mn}^3(KR_{ij})$, and utilize the integral representation of $u_{mn}^3(KR_{ij})$ in terms of plane waves

$$u_{mn}^3(KR_{ij}) = \frac{1}{2\pi j^n} \int Y_{mn}(\hat{\mathbf{k}}^b) e^{j\mathbf{k}_\perp \cdot \mathbf{R}_{ji\perp}} e^{jK_z(\mathbf{k}_\perp)(z_j - z_i)} \frac{d^2\mathbf{k}_\perp}{KK_z(\mathbf{k}_\perp)}, \quad (149)$$

with $\mathbf{R}_{ji} = \mathbf{R}_{ji\perp} + (z_j - z_i)\hat{\mathbf{z}}$, and

$$\mathbf{k}^b = \mathbf{k}_\perp + bK_z(\mathbf{k}_\perp)\hat{\mathbf{z}}, \quad (150)$$

$$K_z(\mathbf{k}_\perp) = \sqrt{K^2 - k_\perp^2}, \quad (151)$$

$$b = \begin{cases} +, & z_j > z_i \\ -, & z_j < z_i \end{cases} \quad (152)$$

Computing the integral over the particle positions in the sense of Cauchy's principal value, we obtain

$$\begin{aligned} M_{Lmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L) &= j^{n'-n} \frac{1}{|K|^2} \sum_{b=\pm} \int Y_{mn}(\hat{\mathbf{k}}^b) Y_{m'n'}^*(\hat{\mathbf{k}}^b) \left[\int_0^H \delta_{b,\text{sgn}(z_j - z_i)} \right. \\ &\quad \times e^{-2bK_z'(\mathbf{k}_\perp)(z_j - z_i)} X_{Lm_1n_1,m_2n_2}^{rt}(z_j) dz_j \left. \right] \frac{d^2\mathbf{k}_\perp}{|K_z(\mathbf{k}_\perp)|^2}, \end{aligned} \quad (153)$$

with $K_z'(\mathbf{k}_\perp) = \text{Im}(K_z(\mathbf{k}_\perp))$.

Next, we assume that $K'' \ll K'$ yielding $K \approx K'$, neglect the evanescent waves, i.e., $|\mathbf{k}_\perp| = k_\perp < K'$, and define the real upward ($b = +$) and downward ($b = -$) vectors for propagating waves by (compare with Eqs. (150) and (151))

$$\mathbf{k}^b = \mathbf{k}_\perp + bK_z'(\mathbf{k}_\perp)\hat{\mathbf{z}}, \quad (154)$$

$$K_z'(\mathbf{k}_\perp) = \sqrt{K'^2 - k_\perp^2}. \quad (155)$$

The upward and downward vectors $\hat{\mathbf{k}}^b$ are described through the propagation direction $\hat{\mathbf{k}} = \hat{\mathbf{k}}(\theta_{ji}, \varphi_{ji})$ as (compare with Eqs. (107) and (108))

$$\hat{\mathbf{k}}^+ = \hat{\mathbf{k}}(\theta_{ji}, \varphi_{ji}), \quad \theta_{ji} \in [0, \pi/2], \quad \varphi_{ji} \in [0, 2\pi], \quad (156)$$

$$\hat{\mathbf{k}}^- = \hat{\mathbf{k}}(\theta_{ji}, \varphi_{ji}), \quad \theta_{ji} \in (\pi/2, \pi], \quad \varphi_{ji} \in [0, 2\pi]. \quad (157)$$

Then, using the relations

$$K_z'(\mathbf{k}_\perp) = K' |\cos \theta_{ji}|, \quad (158)$$

$$d^2\mathbf{k}_\perp = K'^2 \sin \theta_{ji} |\cos \theta_{ji}| d\theta_{ji} d\varphi_{ji} \quad (159)$$

and the approximations $K_z(\mathbf{k}_\perp) \approx K_z'(\mathbf{k}_\perp)$ and

$$K_z''(\mathbf{k}_\perp) \approx \frac{K'K''}{K_z'(\mathbf{k}_\perp)} = \frac{K''}{|\cos \theta_{ji}|}, \quad (160)$$

we obtain

$$\begin{aligned} M_{Lmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L) &= \frac{2\pi}{K'^2} j^{n'-n} \delta_{mm'} \sum_{b=\pm} \int_{\Theta_b} P_n^{(m)}(\cos \theta_{ji}) P_{n'}^{(m')}(\cos \theta_{ji}) \\ &\quad \times \left[\frac{1}{|\cos \theta_{ji}|} \int_0^H \delta_{b,\text{sgn}(z_j - z_i)} e^{-bK \frac{z_j - z_i}{|\cos \theta_{ji}|}} X_{Lm_1n_1,m_2n_2}^{rt}(z_j) dz_j \right] \\ &\quad \times \sin \theta_{ji} d\theta_{ji}, \end{aligned} \quad (161)$$

where κ is defined by Eq. (59), Θ_+ and Θ_- are the intervals $[0, \pi/2]$ and $(\pi/2, \pi]$, respectively, and $\delta_{b,\text{sgn}(z_j - z_i)}$ is given by Eq. (93). Finally, approximating $K' \approx k_1$, making the change of variables $\theta_{ij} = \pi - \theta_{ji}$, and applying the symmetry relation

$$P_n^{(m)}(-\cos \theta) = (-1)^{n-|m|} P_n^{(m)}(\cos \theta),$$

we obtain the representation (92) for $M_{Lmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L)$.

In fact, the neglect of the evanescent waves, which decay far from the sources and boundaries, but can be significant in the near field, is equivalent to the far-field approximation for the fields. Therefore, the two methods for computing the integral $M_{Lmm'n'}^{rtm_1n_1m_2n_2}(z_i; X_L)$ are completely equivalent.

Appendix B

The expression for the diffuse ladder specific coherency dyadic $\bar{\Sigma}_{dl}(z, \hat{\mathbf{k}}^b)$ has been computed as follows: in Eq. (103) we used the representation (102) for $\mathbf{X}_3(-K\mathbf{p})$ in terms of $\mathbf{X}_3(-k_1\mathbf{p})$, and then, the far-field approximation for $\mathbf{X}_3(-k_1\mathbf{p})$. Here, we do not use the representation (102) for $\mathbf{X}_3(-K\mathbf{p})$ and the far-field approximation for $\mathbf{X}_3(-k_1\mathbf{p})$. We first use the integral representation for the vector spherical wave functions in terms of plane electromagnetic waves:

$$\mathbf{X}_3(-K\mathbf{p}) = \frac{1}{2\pi} \int \mathbf{x}(\hat{\mathbf{k}}^b) e^{-j\mathbf{k}_\perp \cdot \mathbf{p}_\perp} e^{jK_z(\mathbf{k}_\perp)(z - z_i)} \frac{d^2\mathbf{k}_\perp}{KK_z(\mathbf{k}_\perp)}, \quad (162)$$

with $\mathbf{p} = \mathbf{p}_\perp + (z_i - z)\hat{\mathbf{z}}$, $\mathbf{k}^b = \mathbf{k}_\perp + bK_z(\mathbf{k}_\perp)\hat{\mathbf{z}}$, $K_z(\mathbf{k}_\perp) = \sqrt{K^2 - k_\perp^2}$, and

$$b = \begin{cases} +, & z > z_i \\ -, & z < z_i \end{cases} \quad (163)$$

Performing the calculation, we find that the diffuse ladder coherency dyadic $\overline{\mathcal{C}}_{\text{dL}}(z)$ can be written as

$$\overline{\mathcal{C}}_{\text{dL}}(z) = \sum_{b=\pm} \int \overline{\mathcal{C}}^b(z, \mathbf{k}_\perp) d^2\mathbf{k}_\perp, \quad (164)$$

where $\overline{\mathcal{C}}^b$ is defined by

$$\begin{aligned} \overline{\mathcal{C}}^b(z, \mathbf{k}_\perp) &= \frac{n_0}{|K|^2 |K_z(\mathbf{k}_\perp)|^2} \mathbf{x}^T(\hat{\mathbf{k}}^b) \mathbf{T} \\ &\times \left[\int_0^H \delta_{b, \text{sgn}(z-z_i)} e^{-2bK_z''(\mathbf{k}_\perp)(z-z_i)} \chi_L(z_i) dz_i \right] \\ &\times \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{k}}^b), \end{aligned} \quad (165)$$

with

$$\delta_{b, \text{sgn}(z-z_i)} = \begin{cases} 1, & b = \text{sgn}(z-z_i) \\ 0, & b \neq \text{sgn}(z-z_i) \end{cases} \quad (166)$$

The next step is to neglect the evanescent waves, define the real upward and downward vectors for propagating waves $\hat{\mathbf{k}}^b$ as in Eqs. (154) and (155), and set (cf. Eqs. (107) and (108)) $\hat{\mathbf{k}}^+ = \hat{\mathbf{k}}(\theta, \varphi)$ for $\theta \in [0, \pi/2]$ and $\varphi \in [0, 2\pi]$, and $\hat{\mathbf{k}}^- = \hat{\mathbf{k}}(\theta, \varphi)$ for $\theta \in (\pi/2, \pi]$ and $\varphi \in [0, 2\pi]$. Then, using the approximations $K \approx K'$, $K_z(\mathbf{k}_\perp) \approx K'_z(\mathbf{k}_\perp)$, (158), and (160), we find that the diffuse ladder specific coherency dyadic $\overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}}^b)$, defined through the relation

$$\overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}}^b) = \overline{\mathcal{C}}^b(z, \mathbf{k}_\perp) K' K'_z(\mathbf{k}_\perp), \quad (167)$$

is given by

$$\begin{aligned} \overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}}^b) &= \frac{n_0}{K'^2} \mathbf{x}^T(\hat{\mathbf{k}}^b) \mathbf{T} \left[\frac{1}{|\cos \theta|} \int_0^H \delta_{b, \text{sgn}(z-z_i)} e^{-bK' \frac{z-z_i}{|\cos \theta|}} \right. \\ &\times \chi_L(z_i) dz_i \left. \right] \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{k}}^b). \end{aligned} \quad (168)$$

Finally, approximating $K' \approx k_1$, yields the representation (109) for $\overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}}^b)$.

Note that in view of Eq. (159), which implies $d^2\mathbf{k}_\perp = K' K'_z(\mathbf{k}_\perp) d^2\hat{\mathbf{k}}$, and Eq. (167), we deduce that the representation (164) is equivalent to the definition (31) of the diffuse ladder specific coherency dyadic, i.e.,

$$\overline{\mathcal{C}}_{\text{dL}}(z) = \sum_{b=\pm} \int_{\Omega_b} \overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}}^b) d^2\hat{\mathbf{k}} = \int \overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}}) d^2\hat{\mathbf{k}}.$$

As in Appendix A, the neglect of the evanescent waves, which is equivalent to the far-field approximation for the fields, implies that the two methods for computing the diffuse ladder specific coherency dyadic are also equivalent.

Appendix C

Two methods other than that described in Section 5 can be used to derive the vector radiative transfer equation for sparse media. These are described below.

Method 1. For a sparse medium, the integral equation for χ_L reads as (cf. Eq. (61) with $Q(-K\mathbf{R}_{ji})$ in place of $Q(-k_1\mathbf{R}_{ji})$)

$$\chi_L(z_i) = e^{-K_0 z_i} E_{L0} + n_0 \int_D Q(-K\mathbf{R}_{ji}) \chi_L(z_j) Q^\dagger(-K\mathbf{R}_{ji}) d^3\mathbf{R}_{ji}. \quad (169)$$

In the above equation, we employ the relation $Q(-K\mathbf{R}_{ji}) = \mathcal{T}_{31}^T(-K\mathbf{R}_{ji})\mathbf{T}$ in conjunction with the plane-wave representation of

the translation matrix

$$\begin{aligned} \mathcal{T}_{31}(-K\mathbf{R}_{ji}) &= 2 \int \mathbf{x}(\hat{\mathbf{k}}^c) \cdot \mathbf{x}^\dagger(\hat{\mathbf{k}}^c) e^{-i\mathbf{k}_\perp \cdot \mathbf{R}_{ji\perp}} \\ &\times e^{icK_z(\mathbf{k}_\perp)(z_i-z_j)} \frac{d^2\mathbf{k}_\perp}{KK_z(\mathbf{k}_\perp)}, \end{aligned} \quad (170)$$

with $\mathbf{k}^c = \mathbf{k}_\perp + cK_z(\mathbf{k}_\perp)\hat{\mathbf{z}}$, $K_z(\mathbf{k}_\perp) = \sqrt{K^2 - k_\perp^2}$, and

$$c = \begin{cases} +, & z_i > z_j \\ -, & z_i < z_j \end{cases}, \quad (171)$$

and integrate over $\mathbf{R}_{ji\perp}$. Then, accounting for Eqs. (165) and (167), and the relation $d^2\mathbf{k}_\perp = K' K'_z(\mathbf{k}_\perp) d^2\hat{\mathbf{k}}$, we obtain (compare with Eq. (111))

$$\chi_L(z_i) = e^{-K_0 z_i} E_{L0} + (4\pi)^2 \sum_{c=\pm} \int \mathbf{x}^*(\hat{\mathbf{k}}^c) \cdot \overline{\mathcal{S}}_{\text{dL}}(z_i, \hat{\mathbf{k}}^c) \cdot \mathbf{x}^T(\hat{\mathbf{k}}^c) d^2\hat{\mathbf{k}}. \quad (172)$$

In view of the representation (109), we multiply Eq. (172) by

$$\frac{n_0}{K'^2} \mathbf{x}^T(\hat{\mathbf{k}}^b) \mathbf{T} \left[\frac{1}{|\cos \theta|} \int_0^H \delta_{b, \text{sgn}(z-z_i)} e^{-\frac{bK'}{|\cos \theta|} (z-z_i)} (\cdot) dz_i \right] \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{k}}^b)$$

and integrate, where, as usual, $\hat{\mathbf{k}}^+ = \hat{\mathbf{k}}(\theta, \varphi)$ for $\theta \in [0, \pi/2]$ and $\varphi \in [0, 2\pi]$, and $\hat{\mathbf{k}}^- = \hat{\mathbf{k}}(\theta, \varphi)$ for $\theta \in (\pi/2, \pi]$ and $\varphi \in [0, 2\pi]$. The result is

$$\begin{aligned} \overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}}^b) &= \frac{n_0}{K'^2} \frac{1}{|\cos \theta|} \\ &\times \int_0^H \delta_{b, \text{sgn}(z-z_i)} e^{-bK' \frac{z-z_i}{|\cos \theta|}} \mathbf{x}^T(\hat{\mathbf{k}}^b) \mathbf{T} e^{-K_0 z_i} E_{L0} \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{k}}^b) dz_i \\ &+ (4\pi)^2 \frac{n_0}{K'^2} \frac{1}{|\cos \theta|} \int_0^H \delta_{b, \text{sgn}(z-z_i)} e^{-bK' \frac{z-z_i}{|\cos \theta|}} \\ &\times \left[\sum_{c=\pm} \int_{\Omega_c} \mathbf{x}^T(\hat{\mathbf{k}}^b) \mathbf{T} \mathbf{x}^*(\hat{\mathbf{k}}^c) \cdot \overline{\mathcal{S}}_{\text{dL}}(z_i, \hat{\mathbf{k}}^c) \cdot \mathbf{x}^T(\hat{\mathbf{k}}^c) \mathbf{T}^\dagger \mathbf{x}^*(\hat{\mathbf{k}}^b) d^2\hat{\mathbf{k}} \right] dz_i. \end{aligned} \quad (173)$$

In Eq. (173), we approximate $K' \approx k_1$ and employ the relations $E_{L0} = e_0 e_0^\dagger$ and $e_0 = 4\pi \mathbf{x}^*(\hat{\mathbf{s}}) \cdot \mathcal{E}_0(\hat{\mathbf{s}})$, as well as Eqs. (112) and (114). We obtain the integral form of the vector radiative transfer equation:

$$\begin{aligned} \overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}}^b) &= \frac{n_0}{|\cos \theta|} \int_0^H \delta_{b, \text{sgn}(z-z_i)} e^{-bK' \frac{z-z_i}{|\cos \theta|}} \left[\overline{\mathbf{A}}(\hat{\mathbf{k}}^b, \hat{\mathbf{s}}) \cdot \overline{\mathbf{C}}_c(z_i) \cdot \overline{\mathbf{A}}^\dagger(\hat{\mathbf{k}}^b, \hat{\mathbf{s}}) \right. \\ &\left. + \int \overline{\mathbf{A}}(\hat{\mathbf{k}}^b, \hat{\mathbf{k}}') \cdot \overline{\mathcal{S}}_{\text{dL}}(z_i, \hat{\mathbf{k}}') \cdot \overline{\mathbf{A}}^\dagger(\hat{\mathbf{k}}^b, \hat{\mathbf{k}}') d^2\hat{\mathbf{k}}' \right] dz_i, \end{aligned} \quad (174)$$

so that after differentiating with respect to z and using the differentiation rule (119), we are led to the differential form of the vector radiative transfer equation:

$$\begin{aligned} \cos \theta \frac{d\overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}})}{dz} &= -\kappa \overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}}) + n_0 \overline{\mathbf{A}}(\hat{\mathbf{k}}, \hat{\mathbf{s}}) \cdot \overline{\mathbf{C}}_c(z) \cdot \overline{\mathbf{A}}^\dagger(\hat{\mathbf{k}}, \hat{\mathbf{s}}) \\ &+ n_0 \int \overline{\mathbf{A}}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') \cdot \overline{\mathcal{S}}_{\text{dL}}(z, \hat{\mathbf{k}}') \cdot \overline{\mathbf{A}}^\dagger(\hat{\mathbf{k}}, \hat{\mathbf{k}}') d^2\hat{\mathbf{k}}'. \end{aligned} \quad (175)$$

Method 2. Inserting the iterated solution of $\langle e_i e_i^\dagger \rangle_i$ as given by Eq. (49) with $g(R_{ij}) = 1$ in Eq. (29) and accounting of Eq. (33),

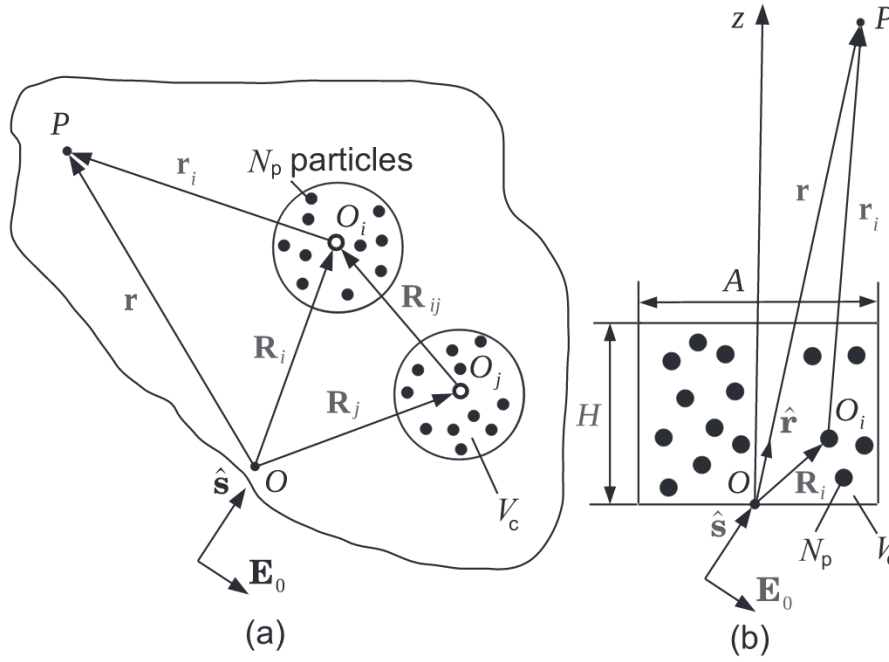


Fig. 4. (a) Scattering by clusters of particles, and (b) the volume element V_c containing N_p randomly distributed particles.

radiative transfer model for dense media assumes that the clusters are situated in the far-field region of each other and so, that their positions are uncorrelated. Inside a cluster, the positions of the particles (i) can be described by the pair correlation function $g(\mathbf{R}_{ij}) = g(R_{ij})$, or (ii) can be randomly generated by a stochastic model. Note that only for $V \approx N_c V_c$, we can approximate $n_0 \approx n_p$, i.e., only when the clusters are close together, the particle distribution in the volume element V_c is approximately equal to the particle distribution in the volume V .

In the following we present several methods for computing the configuration-averaged quantities of a cluster, i.e., the configuration-averaged coherency phase matrix $\langle Z_{JL,c} \rangle$ and the configuration-averaged extinction cross section $\langle C_{ext,c} \rangle$.

Method 1. In Ref. [8], the configuration-averaged quantities of a cluster are computed analytically by means of the quasi-crystalline approximation and the distorted Born approximation.

To explain this method, we consider a group of N_p particles randomly distributed within the volume V_c . The volume element is a cylinder with cross section A and height H (Fig. 4(b)). The observation point is situated in the far-field region of the cluster, and therefore, the representation of the field scattered by particle i , (cf. Eq. (23)) $\mathbf{E}_{scti}(\mathbf{r}) = \mathbf{X}_3^T(k_1 \mathbf{r}_i) \mathbf{T} e_i$ with $\mathbf{r} = \mathbf{R}_i + \mathbf{r}_i$, is used in conjunction with the far-field approximation of the radiating spherical vector wave functions (cf. Eq. (11) of Ref. [1]). The far-field pattern $\mathcal{E}_{sct}^\infty(\hat{\mathbf{r}})$ of the diffuse scattered field $\mathcal{E}_{sct}(\mathbf{r}) = \mathbf{E}_{sct}(\mathbf{r}) - \langle \mathbf{E}_{sct}(\mathbf{r}) \rangle$, defined through the relation $\mathcal{E}_{sct}(\mathbf{r}) = g_0(r) \mathcal{E}_{sct}^\infty(\hat{\mathbf{r}})$ with $g_0(r) = \exp(jk_1 r)/r$, is characterized by the elements of amplitude matrix for the diffuse radiation $\mathcal{S}_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}})$. More precisely, for $\mathcal{E}_{sct}^\infty(\hat{\mathbf{r}}) = \sum_{\eta=\theta,\varphi} \mathcal{E}_{sct\eta}^\infty(\hat{\mathbf{r}}) \hat{\boldsymbol{\eta}}(\hat{\mathbf{r}})$, the $\mathcal{S}_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}})$ are defined through the relation

$$\mathcal{E}_{sct\eta}^\infty(\hat{\mathbf{r}}) = \sum_{\xi=\theta,\varphi} \mathcal{S}_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \mathcal{E}_{0\xi}, \quad (190)$$

and are computed as [19]

$$\mathcal{S}_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = S_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) - \langle S_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle, \quad (191)$$

where

$$S_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = \sum_i S_{i\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \quad (192)$$

are the elements of the amplitude matrix of the cluster,

$$S_{i\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = -\frac{j}{k_1} e^{-jk_1 \hat{\mathbf{r}} \cdot \mathbf{R}_i} \mathbf{X}_{\eta}^T(\hat{\mathbf{r}}) \mathbf{T} e_{i\xi}, \quad (193)$$

are the elements of the amplitude matrix of particle i , and for $e_i = \sum_{\xi=\theta,\varphi} \mathcal{E}_{0\xi} e_{i\xi}$ and $e_0 = \sum_{\xi=\theta,\varphi} \mathcal{E}_{0\xi} e_{0\xi}$, $e_{i\xi}$ satisfies the ξ -polarized equation (34), i.e.,

$$e_{i\xi} = e^{jk_1 \hat{\mathbf{s}} \cdot \mathbf{R}_i} e_{0\xi} + \sum_{j \neq i} Q(k_1 \mathbf{R}_{ij}) e_{j\xi}. \quad (194)$$

In Eqs. (192) and (194), the summations run implicitly from 1 to N_p .

As in Section 3.1, for a large geometrical thickness H , we approximate the conditional configuration average of the exciting field coefficients $\langle e_{i\xi} \rangle_i$ by that of a dense semi-infinite medium. In this case, $\langle e_{i\xi} \rangle_i$ is given by (cf. Eq. (37)) $\langle e_{i\xi} \rangle_i = \exp(j\mathbf{K} \cdot \mathbf{R}_i) e_\xi$, \mathbf{K} is given by Eq. (38), and both K and e_ξ are computed from the generalized Lorentz-Lorenz law and the generalized Ewald-Oseen extinction theorem for a dense semi-infinite discrete random medium [1]. To compute the effective coherency phase matrix, the quasi-crystalline approximation is used in conjunction with the distorted Born approximation. Because the quasi-crystalline approximation combined with the distorted Born approximation may not conserve energy, the computational process is organized as follows:

1. compute $K' = \text{Re}(K)$ from the Lorentz-Lorenz law,
2. compute the effective coherency phase matrix \bar{Z}_{JL} from the distorted Born approximation,
3. integrate the elements of the effective coherency phase matrix over the unit sphere to determine the effective scattering cross section \bar{C}_{sct} ,
4. compute the effective absorption cross section \bar{C}_{abs} from the coherent exciting field, and finally,
5. calculate the extinction cross section by adding the effective absorption and scattering cross sections, i.e., $\bar{C}_{ext} = \bar{C}_{abs} + \bar{C}_{sct}$.

These steps are outlined below.

Effective coherency phase matrix. The elements of the configuration-averaged coherency phase matrix of the cluster $\langle Z_{JL,c} \rangle$

are expressed in terms of the configuration-averaged products $\langle \mathcal{S}_{\eta\xi} \mathcal{S}_{\eta'\xi'}^* \rangle$ via

$$\langle Z_{\text{JL}(\eta,\eta')(\xi,\xi')}(\hat{\mathbf{r}},\hat{\mathbf{s}}) \rangle = \langle \mathcal{S}_{\eta\xi}(\hat{\mathbf{r}},\hat{\mathbf{s}}) \mathcal{S}_{\eta'\xi'}^*(\hat{\mathbf{r}},\hat{\mathbf{s}}) \rangle := \mathcal{S}_{\text{d}\eta\xi\eta'\xi'}(\hat{\mathbf{r}},\hat{\mathbf{s}}). \quad (195)$$

In this regard and in view of Eq. (188), we define

$$\overline{\mathcal{S}}_{\text{d}\eta\xi\eta'\xi'}(\hat{\mathbf{r}},\hat{\mathbf{s}}) = \frac{1}{n_p V_c} \mathcal{S}_{\text{d}\eta\xi\eta'\xi'}(\hat{\mathbf{r}},\hat{\mathbf{s}}), \quad (196)$$

in which case, the elements of the effective coherency phase matrix are

$$\overline{Z}_{\text{JL}(\eta,\eta')(\xi,\xi')}(\hat{\mathbf{r}},\hat{\mathbf{s}}) = \overline{\mathcal{S}}_{\text{d}\eta\xi\eta'\xi'}(\hat{\mathbf{r}},\hat{\mathbf{s}}). \quad (197)$$

The quantity $\mathcal{S}_{\text{d}\eta\xi\eta'\xi'}$ is given by [19]

$$\begin{aligned} \mathcal{S}_{\text{d}\eta\xi\eta'\xi'}(\hat{\mathbf{r}},\hat{\mathbf{s}}) &= n_p \int \langle S_{\eta\xi} S_{\eta'\xi'}^* \rangle_i d^3 \mathbf{R}_i + n_p^2 \int [\langle S_{\eta\xi} S_{\eta'\xi'}^* \rangle_{ij} g(\mathbf{R}_{ij}) \\ &\quad - \langle S_{\eta\xi} \rangle_i \langle S_{\eta'\xi'}^* \rangle_j] d^3 \mathbf{R}_j d^3 \mathbf{R}_i, \end{aligned} \quad (198)$$

so that by means of the distorted Born approximation,

$$\langle S_{\eta\xi} S_{\eta'\xi'}^* \rangle_{ij} = \langle S_{\eta\xi} \rangle_i \langle S_{\eta'\xi'}^* \rangle_j, \quad (199)$$

we obtain

$$\begin{aligned} \mathcal{S}_{\text{d}\eta\xi\eta'\xi'}(\hat{\mathbf{r}},\hat{\mathbf{s}}) &= n_p \int \langle S_{\eta\xi} \rangle_i \langle S_{\eta'\xi'}^* \rangle_i d^3 \mathbf{R}_i \\ &\quad + n_p^2 \int [g(\mathbf{R}_{ij}) - 1] \langle S_{\eta\xi} \rangle_i \langle S_{\eta'\xi'}^* \rangle_j d^3 \mathbf{R}_j d^3 \mathbf{R}_i. \end{aligned} \quad (200)$$

Taking the configuration average of $S_{\eta\xi}$ given by Eq. (193) with the position of particle i held fixed, using $\langle e_{i\xi} \rangle_i = \exp(j\mathbf{K} \cdot \mathbf{R}_i) e_\xi$, making the change of variables $\mathbf{R}_j = \mathbf{R}_i + \mathbf{R}_{ji}$, and neglecting boundary effects, we obtain

$$\begin{aligned} \mathcal{S}_{\text{d}\eta\xi\eta'\xi'}(\hat{\mathbf{r}},\hat{\mathbf{s}}) &= \frac{n_p A}{k_1^2} \left\{ \int_0^H e^{-\kappa_z z_i} dz_i + n_p \int e^{-\kappa_z z_i} \right. \\ &\quad \times \left[\int e^{-j\mathbf{K} \cdot \mathbf{R}_{ji}} e^{j\mathbf{K} \cdot \mathbf{R}_{ji}} h(\mathbf{R}_{ji}) d^3 \mathbf{R}_{ji} \right] dz_i \Big\} \\ &\quad \times [\mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} e_\xi][\mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} e_{\xi'}]^*, \end{aligned} \quad (201)$$

where (cf. Eq. (101)) $\kappa_z = 2K_z''$ and $h(\mathbf{R}_{ji}) = g(\mathbf{R}_{ji}) - 1$. To compute the integral over \mathbf{R}_{ji} we choose the origin of a local coordinate system at the center of particle i , and since $h(\mathbf{R}_{ji})$ decreases very rapidly to zero, we let $\mathbf{R}_{ji} \in \mathbb{R}^3$. Consequently, the integral will not depend on the position of particle i , and we get

$$\begin{aligned} \mathcal{S}_{\text{d}\eta\xi\eta'\xi'}(\hat{\mathbf{r}},\hat{\mathbf{s}}) &= \frac{n_p V_c}{k_1^2} \frac{1 - e^{-\kappa_z H}}{\kappa_z H} [1 + n_p h_p(|\text{Re}(\mathbf{K}) - k_1 \hat{\mathbf{r}}|)] \\ &\quad \times [\mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} e_\xi][\mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} e_{\xi'}]^*. \end{aligned} \quad (202)$$

In Eq. (202), $h_p(\mathbf{p})$ is the Fourier transform of the total distribution function $h(\mathbf{r}) = g(\mathbf{r}) - 1$, i.e.,

$$h_p(\mathbf{p}) = \int h(\mathbf{r}) e^{-j\mathbf{p} \cdot \mathbf{r}} d^3 \mathbf{r}, \quad (203)$$

and for spherical symmetry, i.e., $h_p(\mathbf{p}) = h_p(p)$, we approximate

$$h_p(\mathbf{K}^* - k\hat{\mathbf{r}}) = h_p(|\mathbf{K}^* - k\hat{\mathbf{r}}|) \approx h_p(|\text{Re}(\mathbf{K}) - k\hat{\mathbf{r}}|).$$

Note that $h_p(p)$ solving the Ornstein-Zernike equation has a closed-form representation in terms of $p = |\text{Re}(\mathbf{K}) - k\hat{\mathbf{r}}|$ and the volume concentration of the particles $f = n_p V_0$ [1]. In the limit of small $\kappa_z H$, we use

$$\lim_{\kappa_z H \rightarrow 0} \frac{1 - e^{-\kappa_z H}}{\kappa_z H} = 1, \quad (204)$$

and we end up with

$$\overline{\mathcal{S}}_{\text{d}\eta\xi\eta'\xi'}(\hat{\mathbf{r}},\hat{\mathbf{s}}) = \frac{1}{k_1^2} F(\hat{\mathbf{r}}) [\mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} e_\xi][\mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} e_{\xi'}]^*, \quad (205)$$

where

$$F(\hat{\mathbf{r}}) = 1 + n_p h_p(|\text{Re}(\mathbf{K}) - k_1 \hat{\mathbf{r}}|). \quad (206)$$

It should be pointed out that for a sparse medium, we have $F(\hat{\mathbf{r}}) = 1$ and $e_\xi \approx e_{0\xi} = 4\pi \mathbf{x}_\xi^*(\hat{\mathbf{s}})$ (the exciting field is approximately equal to the incident field). In this case, Eq. (205) becomes

$$\begin{aligned} \overline{\mathcal{S}}_{\text{d}\eta\xi\eta'\xi'}(\hat{\mathbf{r}},\hat{\mathbf{s}}) &= S_{0\eta\xi}(\hat{\mathbf{r}},\hat{\mathbf{s}}) S_{0\eta'\xi'}^*(\hat{\mathbf{r}},\hat{\mathbf{s}}) \\ &= \frac{1}{k_1^2} [\mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} e_{0\xi}][\mathbf{x}_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} e_{0\xi'}]^* \\ &= Z_{\text{JL}(\eta,\eta')(\xi,\xi')}(\hat{\mathbf{r}},\hat{\mathbf{s}}), \end{aligned}$$

where $S_{0\eta\xi}$ are the elements of the single-particle amplitude matrix in the particle-centered coordinate system. Thus, $\overline{Z}_{\text{JL}} = Z_{\text{JL}}$ as it should be.

Effective scattering cross section. The configuration average of the scattering cross section of the cluster is given by

$$\langle C_{\text{sct},c} \rangle = \frac{1}{2} \sum_{\eta,\xi=\theta,\varphi} \int |\mathcal{S}_{\eta\xi}(\hat{\mathbf{r}},\hat{\mathbf{s}})|^2 d^2 \hat{\mathbf{r}}; \quad (207)$$

whence in view of Eq. (188), it follows that the effective scattering cross section can be computed as

$$\overline{C}_{\text{sct}} = \frac{1}{n_p V_c} \langle C_{\text{sct},c} \rangle = \frac{1}{2} \sum_{\eta,\xi=\theta,\varphi} \int \overline{\mathcal{S}}_{\text{d}\eta\xi\eta\xi}(\hat{\mathbf{r}},\hat{\mathbf{s}}) d^2 \hat{\mathbf{r}}, \quad (208)$$

where $\overline{\mathcal{S}}_{\text{d}\eta\xi\eta\xi}(\hat{\mathbf{r}},\hat{\mathbf{s}})$ is given by Eq. (205).

Effective absorption cross section. For a ξ -polarized incident field, the configuration average of the field exciting particle i in the local coordinate system attached to particle i (the coherent exciting field) is

$$\langle \mathbf{E}_{\text{exci}}^{(i)}(\mathbf{r}_i) \rangle_i = \mathbf{X}_1^T(k\mathbf{r}_i) \langle e_{i\xi} \rangle_i. \quad (209)$$

Then, using again $\langle e_{i\xi} \rangle_i = \exp(j\mathbf{K} \cdot \mathbf{R}_i) e_\xi$ with $e_\xi = [e_{\xi mn}^1 \quad e_{\xi mn}^2]^T$, we find that the absorption cross section of particle i is

$$\begin{aligned} \langle C_{\text{absi}} \rangle_i &= -\frac{1}{k_1^2} e^{j(\mathbf{K}-\mathbf{K}^*) \cdot \mathbf{R}_i} \sum_{mn} \{ [\text{Re}(T_n^1) + |T_n^1|^2] |e_{\xi mn}^1|^2 \\ &\quad + [\text{Re}(T_n^2) + |T_n^2|^2] |e_{\xi mn}^2|^2 \}. \end{aligned} \quad (210)$$

The configuration average of the absorption cross section of the cluster reads

$$\langle C_{\text{abs},c} \rangle = \sum_i \langle C_{\text{absi}} \rangle = n_p \int \langle C_{\text{absi}} \rangle_i d^3 \mathbf{R}_i, \quad (211)$$

so that by means of the result

$$\int e^{j(\mathbf{K}-\mathbf{K}^*) \cdot \mathbf{R}_i} d^3 \mathbf{R}_i = V_c \frac{1 - e^{-\kappa_z H}}{\kappa_z H} \rightarrow V_c \text{ as } \kappa_z H \rightarrow 0,$$

we obtain

$$\begin{aligned} \overline{C}_{\text{abs}} &= \frac{1}{n_p V_c} \langle C_{\text{abs},c} \rangle \\ &= -\frac{1}{k_1^2} \sum_{mn} \{ [\text{Re}(T_n^1) + |T_n^1|^2] |e_{\xi mn}^1|^2 \\ &\quad + [\text{Re}(T_n^2) + |T_n^2|^2] |e_{\xi mn}^2|^2 \}. \end{aligned} \quad (212)$$

To simplify the analysis it is convenient to consider a plane electromagnetic wave at *normal incidence*, i.e., $\hat{\mathbf{s}} = \hat{\mathbf{z}}$. In this case, the generalized Ewald-Oseen extinction theorem for computing e_ξ (which determines the conditional configuration average of the exciting field coefficients $\langle e_{i\xi} \rangle_i = \exp(j\mathbf{K} \cdot \mathbf{R}_i) e_\xi$) is polarization independent [2], and moreover, only the azimuthal modes $m = 1$ and $m = -1$ are involved in the summation (212). Choosing the xz -plane as the scattering plane we find that for $\hat{\mathbf{r}} = \hat{\mathbf{r}}(\theta = \Theta, \varphi = 0)$, the non-zero configuration-averaged

products $\langle \mathcal{S}_{\eta\xi}(\Theta) \mathcal{S}_{\eta'\xi'}^*(\Theta) \rangle$ are $\langle |\mathcal{S}_{\theta\theta}(\Theta)|^2 \rangle$, $\langle \mathcal{S}_{\theta\theta}(\Theta) \mathcal{S}_{\varphi\varphi}^*(\Theta) \rangle$, $\langle \mathcal{S}_{\varphi\varphi}(\Theta) \mathcal{S}_{\theta\theta}^*(\Theta) \rangle$, and $\langle |\mathcal{S}_{\varphi\varphi}(\Theta)|^2 \rangle$. These four quantities are the diagonal elements of the configuration-averaged coherency scattering matrix $\langle \mathbf{F}_{\text{JL},c}(\Theta) \rangle$. This matrix determines the configuration-averaged coherency phase matrix for the directions $\hat{\mathbf{r}} = \hat{\mathbf{r}}(\theta, \varphi)$ and $\hat{\mathbf{s}} = \hat{\mathbf{s}}(\theta_0, \varphi_0)$ via

$$\langle \mathbf{Z}_{\text{JL},c}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle = \mathbf{D}^{-1} \mathbf{L}(-\sigma_2) \mathbf{D} \langle \mathbf{F}_{\text{JL},c}(\Theta) \rangle \mathbf{D}^{-1} \mathbf{L}(\pi - \sigma_1) \mathbf{D},$$

with $\mathbf{D}^{-1} = (1/2)\mathbf{D}^\dagger$. For the definitions of the rotation matrix \mathbf{L} and the angles σ_1 and σ_2 we refer, for example, to Ref. [6].

Method 2. A numerical method for computing the configuration-averaged quantities of a cluster by simulating the multiple scattering of waves by volumes of discrete random media consisting of spherical particles was described by Tse et al. [9]. The effective optical properties are computed by simulating random positions of particles inside a spherical cluster (by random shuffling and bonding) and by averaging over a number of realizations. For L realizations of the particle positions inside a cluster, the computational process is organized as follows:

1. solve the multiple scattering equations for the exciting field coefficients

$$\mathbf{e}_{i\xi}^{(l)} = \mathbf{e}^{jk_1 \hat{\mathbf{s}} \mathbf{R}_i^{(l)}} \mathbf{e}_{0\xi} + \sum_{j \neq i} \mathbf{Q}(k_1 \mathbf{R}_{ij}^{(l)}) \mathbf{e}_{j\xi}^{(l)}, \quad (213)$$

i.e., determine $\mathbf{e}_{i\xi}^{(l)}$, $i = 1, \dots, N_p$, for each configuration l ;

2. for each configuration l , compute the elements of the amplitude matrix of particle i (cf. Eq. (193))

$$S_{i\eta\xi}^{(l)}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = -\frac{j}{k_1} \mathbf{e}^{-jk_1 \hat{\mathbf{r}} \mathbf{R}_i^{(l)}} \mathbf{x}_{\eta}^T(\hat{\mathbf{r}}) \mathbf{T} \mathbf{e}_{i\xi}^{(l)} \quad (214)$$

and the elements of the amplitude matrix of the cluster (cf. Eq. (191))

$$S_{\eta\xi}^{(l)}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = \sum_i S_{i\eta\xi}^{(l)}(\hat{\mathbf{r}}, \hat{\mathbf{s}}); \quad (215)$$

3. calculate the configuration average of the elements of the amplitude matrix of the cluster

$$\langle S_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle = \frac{1}{L} \sum_{l=1}^L S_{\eta\xi}^{(l)}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \quad (216)$$

and for each configuration l , the elements of the amplitude matrix of the cluster for the diffuse radiation (cf. Eq. (191))

$$\mathcal{S}_{\eta\xi}^{(l)}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = S_{\eta\xi}^{(l)}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) - \langle S_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle; \quad (217)$$

4. compute the configuration-averaged coherency phase matrix of the cluster (cf. Eq. (195))

$$\langle \mathbf{Z}_{\text{JL},c(\eta,\eta')(\xi,\xi')}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle = \frac{1}{L} \sum_{l=1}^L \mathcal{S}_{\eta\xi}^{(l)}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \mathcal{S}_{\eta'\xi'}^{(l)*}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \quad (218)$$

and the configuration-averaged scattering cross section of the cluster $\langle C_{\text{sct},c} \rangle$ (cf. Eq. (207))

$$\begin{aligned} \langle C_{\text{sct},c} \rangle &= \frac{1}{L} \sum_{l=1}^L \left[\frac{1}{2} \sum_{\eta,\xi=\theta,\varphi} \int |\mathcal{S}_{\eta\xi}^{(l)}(\hat{\mathbf{r}}, \hat{\mathbf{s}})|^2 d^2\hat{\mathbf{r}} \right] \\ &= \frac{1}{2} \sum_{\eta,\xi=\theta,\varphi} \int \langle \mathbf{Z}_{\text{JL},c(\eta,\eta)(\xi,\xi)}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle d^2\hat{\mathbf{r}}; \end{aligned} \quad (219)$$

5. for each configuration l , compute the absorption cross section of particle i (for the exciting field $\mathbf{E}_{\text{exci}}^{(l)(i)}(\mathbf{r}_i) = \mathbf{X}_1^T(k\mathbf{r}_i) \mathbf{e}_{i\xi}^{(l)}$ and a given polarization state ξ of the incident field)

$$\begin{aligned} C_{\text{absi}}^{(l)} &= -\frac{1}{k_1^2} \sum_{mn} \{ [\text{Re}(T_n^1) + |T_n^1|^2] |e_{i\xi mn}^{(l)1}|^2 \\ &\quad + [\text{Re}(T_n^2) + |T_n^2|^2] |e_{i\xi mn}^{(l)2}|^2 \}, \end{aligned} \quad (220)$$

where $\mathbf{e}_{i\xi}^{(l)} = [e_{i\xi mn}^{(l)1} \ e_{i\xi mn}^{(l)2}]^T$, and then, the configuration-averaged absorption cross section of the cluster

$$\langle C_{\text{abs},c} \rangle = \frac{1}{L} \sum_{l=1}^L \sum_i C_{\text{absi}}^{(l)}. \quad (221)$$

The multiple scattering equation (213) can be solved iteratively, e.g., by the generalized minimum residual method, whereby the matrix-vector multiplication, required in each iteration step, can be accelerated by the fast multipole method [10,11]. Note that in iterative methods, the matrix resulting from Eq. (213) needs to be well conditioned. Actually, the multiple scattering equation (213) can be reformulated in terms of the scattered field coefficients $\mathbf{s}_{i\xi}^{(l)} = \mathbf{T} \mathbf{e}_{i\xi}^{(l)}$, or the internal field coefficients $\mathbf{c}_{i\xi}^{(l)} = \mathbf{T}_{\text{int}} \mathbf{e}_{i\xi}^{(l)}$, where \mathbf{T}_{int} is the particle-centered “transition matrix” relating the expansion coefficients of the internal field to those of the exciting field. In Ref. [12] it has been shown that the condition number of the matrix equation with internal field coefficients is better thus, this approach is recommended.

In this numerical approach, the configuration-averaged quantities of a cluster are computed by solving the multiple scattering equation (213) without any approximation as, for example, the quasi-crystalline approximation or the distorted Born approximation. Thus, the scattering by the particles in the cluster is accurately described in the sense that all interference effects between different types of scattered waves are taken into account.

Method 3. In Ref. [13], the configuration-averaged quantities of a cluster are computed by considering the first-order approximation for the exciting field coefficients \mathbf{e}_i satisfying Eq. (34), i.e., $\mathbf{e}_i = \exp(jk_1 \hat{\mathbf{s}} \cdot \mathbf{R}_i) \mathbf{e}_0$. As a result, the field scattered by particle i is

$$\mathbf{E}_{\text{scti}}(\mathbf{r}) = \mathbf{X}_3^T(k_1 \mathbf{r}_i) \mathbf{T} \mathbf{e}_i = \mathbf{e}^{jk_1 \hat{\mathbf{s}} \mathbf{R}_i} \mathbf{X}_3^T(k_1 \mathbf{r}_i) \mathbf{T} \mathbf{e}_0, \quad (222)$$

where $\mathbf{r} = \mathbf{R}_i + \mathbf{r}_i$, the elements of the amplitude matrix of particle i are

$$S_{i\eta\mu}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = -\frac{j}{k_1} \mathbf{e}^{jk_1 (\hat{\mathbf{s}} - \hat{\mathbf{r}}) \cdot \mathbf{R}_i} \mathbf{x}_{\eta}^T(\hat{\mathbf{r}}) \mathbf{T} \mathbf{e}_{0\mu}, \quad (223)$$

and the elements of the amplitude matrix of the cluster become

$$S_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = \sum_i S_{i\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) = -\frac{j}{k_1} \mathbf{x}_{\eta}^T(\hat{\mathbf{r}}) \mathbf{T} \mathbf{e}_{0\xi} \sum_i \mathbf{e}^{jk_1 (\hat{\mathbf{s}} - \hat{\mathbf{r}}) \cdot \mathbf{R}_i}. \quad (224)$$

By means of Eq. (191) it follows that

$$\begin{aligned} \langle \mathbf{Z}_{\text{JL},c(\eta,\eta')(\xi,\xi')}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle &= \langle \mathcal{S}_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \mathcal{S}_{\eta'\xi'}^*(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle \\ &= \langle S_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) S_{\eta'\xi'}^*(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle - \langle S_{\eta\xi}(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle \langle S_{\eta'\xi'}^*(\hat{\mathbf{r}}, \hat{\mathbf{s}}) \rangle. \end{aligned} \quad (225)$$

The configuration-averaged quantities $\langle S_{\eta\xi} \rangle \langle S_{\eta'\xi'}^* \rangle$ and $\langle S_{\eta\xi} S_{\eta'\xi'}^* \rangle$ are computed by simulating random positions of particles inside a cluster and by averaging over a number of realizations. However, in order to improve the convergence of the configuration averaging, an analytical averaging over orientations is performed. This approach is described below.

Assuming spherical symmetry, the probability density $p(\mathbf{R}_i)$ can be written as

$$p(\mathbf{R}_i) = p(R_i) p(\hat{\mathbf{R}}_i) = \frac{1}{4\pi} p(R_i), \quad (226)$$

For more details on the derivation of Eq. (242) we refer to Ref. [19]. The final result is

$$\Sigma_{\text{dL}\eta\xi}(\mathbf{r}, -\hat{\mathbf{p}}) = h_{\eta} h_{\xi} \sum_{\eta', \xi'=\theta, \varphi} h_{\eta'} h_{\xi'} \Psi_{\eta\xi\eta'\xi'}(\mathbf{r}, -\hat{\mathbf{p}}) \mathcal{E}_{0\eta'} \mathcal{E}_{0\xi'}^* \quad (243)$$

In Eq. (243),

$$\Psi_{\eta\xi\eta'\xi'}(\mathbf{r}, -\hat{\mathbf{p}}) = \sum_{k=0}^{\infty} \Psi_{\eta\xi\eta'\xi'}^{(k)}(\mathbf{r}, -\hat{\mathbf{p}}), \quad (244)$$

where

$$\begin{aligned} \Psi_{\eta\xi\eta'\xi'}^{(k)}(\mathbf{r}, -\hat{\mathbf{p}}) &= \int_{D-D_{2a}(\mathbf{R}_{k-1})} \cdots \left[\int_{D-D_{2a}(\mathbf{R}_0)} \left[\int_D \right. \right. \\ &\quad \times F_{k\eta\xi\eta'\xi'}(\mathbf{R}_k, \dots, \mathbf{R}_1, \mathbf{R}_0) d^3\mathbf{R}_0 \left. \right] d^3\mathbf{R}_1 \left. \right] \cdots d^3\mathbf{R}_k \end{aligned} \quad (245)$$

and

$$\begin{aligned} F_{k\eta\xi\eta'\xi'}(\mathbf{R}_k, \dots, \mathbf{R}_1, \mathbf{R}_0) &= \frac{n_0}{k_1^2} t_k(\mathbf{R}_k, \dots, \mathbf{R}_1, \mathbf{R}_0) \\ &\quad \times e^{-K_0 \mathbf{R}_k \cdot \hat{\mathbf{z}}} [\mathbf{x}_{\eta'}^T(-\hat{\mathbf{s}}) \mathbf{T} \mathbf{Q}_k(\mathbf{R}_k, \dots, \mathbf{R}_1, \mathbf{R}_0) \mathbf{e}_{0\eta}(\hat{\mathbf{p}})] \\ &\quad \times [\mathbf{x}_{\xi'}^T(-\hat{\mathbf{s}}) \mathbf{T} \mathbf{Q}_k(\mathbf{R}_k, \dots, \mathbf{R}_1, \mathbf{R}_0) \mathbf{e}_{0\xi}(\hat{\mathbf{p}})]^* e^{-K R_{0p}} \\ &\quad \times \frac{1}{R_{0p}^2} \delta(\hat{\mathbf{R}}_{0p} - \hat{\mathbf{p}}), \quad k \geq 0, \end{aligned} \quad (246)$$

with $t_0 = 1$ and $\mathbf{Q}_0 = \mathbf{I}$. For $k \geq 1$, the quantities $t_k(\cdot)$ and $\mathbf{Q}_k(\cdot)$ in Eq. (246) are computed recursively as

$$t_k(\mathbf{R}_k, \mathbf{R}_{k-1}, \dots, \mathbf{R}_0) = n_0 e^{-K R_{k,k-1}} g(\mathbf{R}_{k,k-1}) \times t_{k-1}(\mathbf{R}_{k-1}, \dots, \mathbf{R}_0) \quad (247)$$

and

$$\mathbf{Q}_k(\mathbf{R}_k, \mathbf{R}_{k-1}, \dots, \mathbf{R}_0) = \mathbf{Q}(k_1 \mathbf{R}_{k,k-1}) \mathbf{Q}_{k-1}(\mathbf{R}_{k-1}, \dots, \mathbf{R}_0), \quad (248)$$

where, as before, $t_0 = 1$ and $\mathbf{Q}_0 = \mathbf{I}$.

To find an estimate for $\Psi_{\eta\xi\eta'\xi'}(\mathbf{r}, -\hat{\mathbf{p}})$ in Eq. (243), we consider L independent Markov chain paths of lengths $K^{(l)}$, $l = 1, \dots, L$, i.e.,

$$\begin{aligned} \{\mathbf{R}_{0:K^{(l)}}^{(l)}\} : \mathbf{R}_0^{(l)} \rightarrow \mathbf{R}_1^{(l)} \rightarrow \dots \rightarrow \mathbf{R}_k^{(l)} \rightarrow \dots \\ \rightarrow \mathbf{R}_{K^{(l)}-1}^{(l)} \rightarrow \mathbf{R}_{K^{(l)}}^{(l)} = \{\emptyset\} \end{aligned} \quad (249)$$

with the initial probability density function $p(\mathbf{R}_0^{(l)})$ on D , a transition function $p(\mathbf{R}_{k-1}^{(l)} \rightarrow \mathbf{R}_k^{(l)})$ which gives the probability of moving from state $\mathbf{R}_{k-1}^{(l)}$ to state $\mathbf{R}_k^{(l)}$, and the absorbing state $\emptyset \notin D$. The absorption probability at an arbitrary state \mathbf{R}_{k-1} is $1 - \omega$, i.e., $p(\mathbf{R}_{k-1} \rightarrow \{\emptyset\}) = 1 - \omega$, in which case, ω is the survival probability at state \mathbf{R}_{k-1} , i.e.,

$$\int_{D-D_{2a}(\mathbf{R}_{k-1})} p(\mathbf{R}_{k-1} \rightarrow \mathbf{R}_k) d^3\mathbf{R}_k = \omega. \quad (250)$$

The probability of the Markov chain (249), with the initial state $\mathbf{R}_0^{(l)}$ and the absorbing state $\mathbf{R}_{K^{(l)}}^{(l)}$ is

$$\begin{aligned} p_M(\mathbf{R}_0^{(l)}, \mathbf{R}_1^{(l)}, \dots, \mathbf{R}_{K^{(l)}}^{(l)}) &= p(\mathbf{R}_0^{(l)}) p(\mathbf{R}_0^{(l)} \rightarrow \mathbf{R}_1^{(l)}) p(\mathbf{R}_1^{(l)} \rightarrow \mathbf{R}_2^{(l)}) \dots \\ &\quad \times p(\mathbf{R}_{K^{(l)}-1}^{(l)} \rightarrow \mathbf{R}_{K^{(l)}}^{(l)}) p(\mathbf{R}_{K^{(l)}}^{(l)} \rightarrow \{\emptyset\}) \\ &= (1 - \omega) p(\mathbf{R}_0^{(l)}) \prod_{j=1}^{K^{(l)}} p(\mathbf{R}_{j-1}^{(l)} \rightarrow \mathbf{R}_j^{(l)}), \end{aligned} \quad (251)$$

while for $k < K^{(l)}$, we have (the chain does not terminate at $\mathbf{R}_k^{(l)}$)

$$\begin{aligned} p_M(\mathbf{R}_0^{(l)}, \mathbf{R}_1^{(l)}, \dots, \mathbf{R}_k^{(l)}) &= p(\mathbf{R}_0^{(l)}) p(\mathbf{R}_0^{(l)} \rightarrow \mathbf{R}_1^{(l)}) p(\mathbf{R}_1^{(l)} \rightarrow \mathbf{R}_2^{(l)}) \dots \\ &\quad \times p(\mathbf{R}_{k-1}^{(l)} \rightarrow \mathbf{R}_k^{(l)}). \end{aligned} \quad (252)$$

The k -fold integral in Eq. (245) is estimated as

$$\Psi_{\eta\xi\eta'\xi'}^{(k)}(\mathbf{r}, -\hat{\mathbf{p}}) \approx \tilde{\Psi}_{\eta\xi\eta'\xi'}^{(k)}(\mathbf{r}, -\hat{\mathbf{p}}) = \frac{1}{L} \sum_{l=1}^L w_{\eta\xi\eta'\xi'}(\mathbf{R}_{0:k}^{(l)}), \quad (253)$$

where the weights $w_{\eta\xi\eta'\xi'}(\mathbf{R}_{0:k}^{(l)})$ are defined by

$$w_{\eta\xi\eta'\xi'}(\mathbf{R}_{0:k}^{(l)}) = \frac{F_{k\eta\xi\eta'\xi'}(\mathbf{R}_k^{(l)}, \dots, \mathbf{R}_1^{(l)}, \mathbf{R}_0^{(l)})}{p(\mathbf{R}_0^{(l)}) \prod_{j=1}^k p(\mathbf{R}_{j-1}^{(l)} \rightarrow \mathbf{R}_j^{(l)})}. \quad (254)$$

Consequently, an unbiased estimate for $\Psi_{\eta\xi\eta'\xi'}(\mathbf{r}, -\hat{\mathbf{p}})$ is

$$\tilde{\Psi}_{\eta\xi\eta'\xi'}(\mathbf{r}, -\hat{\mathbf{p}}) = \frac{1}{L} \sum_{l=1}^L \sum_{k=0}^{K^{(l)}} w_{\eta\xi\eta'\xi'}(\mathbf{R}_{0:k}^{(l)}). \quad (255)$$

Note that each sample contributes to $K^{(l)}$ trajectories, and strictly speaking, in Eq. (255), the last weights $w_{\eta\xi\eta'\xi'}(\mathbf{R}_{0:K^{(l)}}^{(l)})$ should be multiplied by $1/(1 - \omega)$ because $\mathbf{R}_{K^{(l)}}^{(l)}$ is an absorbing state.

Before proceeding we make a short comment. Consider the product

$$\begin{aligned} f_{k\eta'}^\eta(\mathbf{R}_k, \dots, \mathbf{R}_1, \mathbf{R}_0) &= -\frac{j}{k_1} \mathbf{e}^{i\mathbf{K}_0 \cdot \mathbf{R}_k} \mathbf{x}_{\eta'}^T(-\hat{\mathbf{s}}) \mathbf{T} \\ &\quad \times [\mathbf{e}^{j(K-k_1)R_{k,k-1}} \mathbf{Q}(k_1 \mathbf{R}_{k,k-1})] \dots [\mathbf{e}^{j(K-k_1)R_{10}} \mathbf{Q}(k_1 \mathbf{R}_{10})] \\ &\quad \times \mathbf{e}_{0\eta}(\hat{\mathbf{p}}) \mathbf{e}^{i\mathbf{K}_p \cdot (\mathbf{R}_0 - \mathbf{r})}, \end{aligned}$$

where $(\hat{\mathbf{p}} = (\theta_p, \varphi_p))$

$$\mathbf{K}_p = k_1 \hat{\mathbf{p}} + (K - k_1) \frac{\hat{\mathbf{z}}}{\cos \theta_p}, \quad (256)$$

and the following scattering process: (i) the particle placed at \mathbf{R}_0 is illuminated by the η -polarized plane electromagnetic wave

$$\mathbf{E}_0(\mathbf{r}') = \hat{\boldsymbol{\eta}}(\hat{\mathbf{p}}) e^{i\mathbf{k}_1 \hat{\mathbf{p}} \cdot (\mathbf{r}' - \mathbf{r})} \quad (257)$$

propagating in an effective medium in the direction $\hat{\mathbf{p}}$, (ii) the field scattered by the particle placed at \mathbf{R}_0 propagates in an effective medium and excites the particle placed at \mathbf{R}_1 , (iii) the field scattered by the particle placed at \mathbf{R}_1 propagates in an effective medium and excites the particle placed at \mathbf{R}_2 , and so on (Fig. 5). In a local coordinate system centered at \mathbf{R}_0 ,

$$\mathbf{e}^{i\mathbf{k}_1 \hat{\mathbf{p}} \cdot (\mathbf{R}_0 - \mathbf{r})} \mathbf{e}_{0\eta}(\hat{\mathbf{p}})$$

are the expansion coefficients of the plane electromagnetic wave (257) in terms of regular vector spherical wave functions, and in order to take into account that the incident wave propagates in an effective medium, we replace $k_1 \hat{\mathbf{p}} \rightarrow \mathbf{K}_p$, that is,

$$\mathbf{e}^{i\mathbf{k}_1 \hat{\mathbf{p}} \cdot (\mathbf{R}_0 - \mathbf{r})} \rightarrow \mathbf{e}^{i\mathbf{K}_p \cdot (\mathbf{R}_0 - \mathbf{r})}.$$

In the effective medium, the expansion coefficients of the field exciting particle k (placed at \mathbf{R}_k) due to a η -polarized plane electromagnetic wave illuminating the first particle of the chain are

$$\begin{aligned} \mathbf{e}_k^\eta &= \mathbf{Q}(K \mathbf{R}_{k,k-1}) \dots \mathbf{Q}(K \mathbf{R}_{10}) \mathbf{e}_{0\eta}(\hat{\mathbf{p}}) \mathbf{e}^{i\mathbf{K}_p \cdot (\mathbf{R}_0 - \mathbf{r})} \\ &= [\mathbf{e}^{j(K-k_1)R_{k,k-1}} \mathbf{Q}(k_1 \mathbf{R}_{k,k-1})] \dots [\mathbf{e}^{j(K-k_1)R_{10}} \mathbf{Q}(k_1 \mathbf{R}_{10})] \\ &\quad \times \mathbf{e}_{0\eta}(\hat{\mathbf{p}}) \mathbf{e}^{i\mathbf{K}_p \cdot (\mathbf{R}_0 - \mathbf{r})}. \end{aligned} \quad (258)$$

The far-field pattern $\mathbf{E}_{\text{sctk}}^{\eta\infty}(-\hat{\mathbf{s}})$ of the field scattered by particle k in direction $-\hat{\mathbf{s}}$ is

$$\mathbf{E}_{\text{sctk}}^{\eta\infty}(-\hat{\mathbf{s}}) = \sum_{\eta'=\theta, \varphi} E_{\text{sctk}\eta'}^{\eta\infty}(-\hat{\mathbf{s}}) \hat{\boldsymbol{\eta}}'(-\hat{\mathbf{s}}), \quad (259)$$

$$E_{\text{sctk}\eta'}^{\eta\infty}(-\hat{\mathbf{s}}) = -\frac{j}{k_1} e^{jk_1 \hat{\mathbf{s}} \cdot \mathbf{R}_k} \times_{\eta'}^T(-\hat{\mathbf{s}}) \mathbf{T} e_{k_1}^{\eta}, \quad (260)$$

and as before, to describe the propagation of the scattered wave in an effective medium we make the replacement $k_1 \hat{\mathbf{s}} \rightarrow \mathbf{K}_0$, that is,

$$e^{jk_1 \hat{\mathbf{s}} \cdot \mathbf{R}_k} \rightarrow e^{j\mathbf{K}_0 \cdot \mathbf{R}_k}.$$

Thus, we have $f_{k\eta'}^{\eta}(\cdot) = E_{\text{sctk}\eta'}^{\eta\infty}(-\hat{\mathbf{s}})$, and since $j(\mathbf{K}_p - \mathbf{K}_p^*) \cdot (\mathbf{R}_0 - \mathbf{r}) = -\kappa R_{0p}$, $j(K - K^*) R_{k,k-1} = -\kappa R_{k,k-1}$, and $j(\mathbf{K}_0 - \mathbf{K}_0^*) \cdot \mathbf{R}_k = -\kappa_0 \mathbf{R}_k \cdot \hat{\mathbf{z}}$, we see that $f_{k\eta'}^{\eta}(\cdot) f_{k\xi'}^{\xi*}(\cdot) = E_{\text{sctk}\eta'}^{\eta\infty}(-\hat{\mathbf{s}}) E_{\text{sctk}\xi'}^{\xi\infty*}(-\hat{\mathbf{s}})$ determines $F_{k\eta\xi\eta'\xi'}(\cdot)$ when the correlations between the particles are not taken into account. In importance sampling, the main problem that has to be solved is the choice of the initial probability density $p(\mathbf{R}_0)$ and the probability transition function $p(\mathbf{R}_{k-1} \rightarrow \mathbf{R}_k)$.

1. The probability density $p(\mathbf{R}_0)$ is chosen as

$$p(\mathbf{R}_0) = p(\mathbf{R}_{0p}) = \frac{1}{R_{0p}^2} p(R_{0p}) \delta(\hat{\mathbf{R}}_{0p} - \hat{\mathbf{p}}), \quad (261)$$

where R_{0p} is defined by the probability density

$$p(r) = \kappa e^{-\kappa r}, \quad r \geq 0. \quad (262)$$

Note that if $\hat{\mathbf{R}}_{0p}$ is a realization of R_{0p} , then in Eq. (254), the term $(1/\kappa)p(\mathbf{R}_{0p})$ given by Eq. (261) and the last three terms in the expression of $F_{k\eta\xi\eta'\xi'}(\cdot)$ given by Eq. (246) cancel out.

2. The transition function $p(\mathbf{R}_{k-1} \rightarrow \mathbf{R}_k)$ is represented in the standard form

$$p(\mathbf{R}_{k-1} \rightarrow \mathbf{R}_k) = \omega p(\mathbf{R}_{k,k-1}) = \omega \frac{p(R_{k,k-1})}{R_{k,k-1}^2} p(\hat{\mathbf{R}}_{k,k-1}), \quad (263)$$

where ω is the single-scattering albedo of the particle. For $p(R_{k,k-1})$, we use the probability density function

$$p(r) = \frac{g(r)e^{-\kappa r}}{\int_{2a}^{\infty} g(r)e^{-\kappa r} dr}, \quad r \geq 2a. \quad (264)$$

To construct the probability density function $p(\hat{\mathbf{R}}_{k,k-1})$ with $\hat{\mathbf{R}}_{k,k-1} = (\theta_{k,k-1}, \varphi_{k,k-1})$, we consider the scattering by the particles chain $\{\mathbf{R}_0, \dots, \mathbf{R}_K\}$ placed in free space (cf. Fig. 5 with $k=K$) and being illuminated by the plane electromagnetic wave $\mathbf{E}_0(\mathbf{r}') = \mathcal{E}_0(\hat{\mathbf{p}}) \exp[jk_1 \hat{\mathbf{p}} \cdot (\mathbf{r}' - \mathbf{r})]$ with $\mathcal{E}_0(\hat{\mathbf{p}}) = \sum_{\eta=\theta, \varphi} \mathcal{E}_{0\eta}(\hat{\mathbf{p}}) \hat{\boldsymbol{\eta}}(\hat{\mathbf{p}})$. In a local coordinate system centered at \mathbf{R}_0 , $\exp[jk_1 \hat{\mathbf{p}} \cdot (\mathbf{R}_0 - \mathbf{r})] e_0(\hat{\mathbf{p}})$ with $e_0(\hat{\mathbf{p}}) = \sum_{\eta=\theta, \varphi} \mathcal{E}_{0\eta}(\hat{\mathbf{p}}) e_{0\eta}(\hat{\mathbf{p}})$, are the expansion coefficients of the incident plane electromagnetic wave in terms of regular vector spherical wave functions,

$$\begin{aligned} e_{k-1} &= Q(k_1 \mathbf{R}_{k-1,k-2}) \dots Q(k_1 \mathbf{R}_{10}) e_0(\hat{\mathbf{p}}) e^{jk_1 \hat{\mathbf{p}} \cdot (\mathbf{R}_0 - \mathbf{r})} \\ &= Q_{k-1}(\mathbf{R}_{k-1}, \dots, \mathbf{R}_0) e_0(\hat{\mathbf{p}}) e^{jk_1 \hat{\mathbf{p}} \cdot (\mathbf{R}_0 - \mathbf{r})} \end{aligned} \quad (265)$$

are the expansion coefficients of the field exciting particle $k-1$, $\mathbf{E}_{\text{sctk-1}}^{\infty}(\hat{\mathbf{r}})$ with

$$\mathbf{E}_{\text{sctk-1}}^{\infty}(\hat{\mathbf{r}}) = \sum_{\eta'=\theta, \varphi} E_{\text{sctk-1}, \eta'}^{\infty}(\hat{\mathbf{r}}) \hat{\boldsymbol{\eta}}'(\hat{\mathbf{r}}), \quad (266)$$

$$E_{\text{sctk-1}, \eta'}^{\infty}(\hat{\mathbf{r}}) = -\frac{j}{k_1} e^{-jk_1 \hat{\mathbf{r}} \cdot \mathbf{R}_{k-1}} \times_{\eta'}^T(\hat{\mathbf{r}}) \mathbf{T} e_{k-1}, \quad (267)$$

is the far-field pattern of the field scattered by particle $k-1$ in the direction $\hat{\mathbf{r}} = \hat{\mathbf{r}}(\theta, \varphi)$, and $\sum_{\eta'=\theta, \varphi} |E_{\text{sctk-1}, \eta'}^{\infty}(\hat{\mathbf{r}})|^2$ is the differential scattering cross section. Taking these results into account, we construct the probability density function as

$$p(\theta, \varphi) = \frac{\sum_{\eta'=\theta, \varphi} |E_{\text{sctk-1}, \eta'}^{\infty}(\hat{\mathbf{r}})|^2}{\sum_{\eta'=\theta, \varphi} \int |E_{\text{sctk-1}, \eta'}^{\infty}(\hat{\mathbf{r}})|^2 d^2 \hat{\mathbf{r}}}, \quad (268)$$

and sample the polar angle $\tilde{\theta} = \theta_{k,k-1}$ from the marginal probability density

$$p(\theta) = \int_0^{2\pi} p(\theta, \varphi) d\varphi \quad (269)$$

and the azimuth angle $\tilde{\varphi} = \varphi_{k,k-1}$ from the conditional probability

$$p(\varphi|\tilde{\theta}) = \frac{p(\tilde{\theta}, \varphi)}{p(\tilde{\theta})}. \quad (270)$$

Note that this is not the only option for constructing $p(\hat{\mathbf{R}}_{k,k-1})$ and other alternative solutions can be considered.

We conclude this appendix with some comments.

1. To construct the probability density function $p(\hat{\mathbf{R}}_{k,k-1})$ we considered a chain of particles placed in free space whose positions are uncorrelated, and assumed that particle k is situated in the far zone of particle $k-1$. Thus, as the matrix $(\mathcal{M}_L \mathbf{X}_L)(z_i)$ given by Eq. (94), or equivalently, by Eq. (98), the probability density function $p(\hat{\mathbf{R}}_{k,k-1})$ is a characteristic of a sparse medium. On the other hand, in Eq. (264), the probability density function $p(r)$ includes the transmission terms $\exp[j(K-k_1)R_{j,j-1}]$, $j=1, \dots, k$ from Eq. (258) and the pair correlation functions $g(R_{j,j-1})$. Thus, as the matrix $(\mathcal{L}_L \mathbf{X}_L)(z_i)$ given by Eq. (88), the probability density function $p(r)$ is a characteristic of a dense medium.
2. For a sparse medium, we use the far-field approximation

$$Q(k_1 \mathbf{R}_{k,k-1}) = -4\pi j \frac{e^{jk_1 \mathbf{R}_{k,k-1}}}{k_1 R_{k,k-1}} \sum_{\eta} \times_{\eta}^*(\hat{\mathbf{R}}_{k,k-1}) \times_{\eta}^T(\hat{\mathbf{R}}_{k,k-1})^T, \quad (271)$$

the representation of the elements of the single-particle amplitude matrix in the particle-centered coordinate system

$$S_{0\eta_1\eta}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') = -j \frac{4\pi}{k_1} \times_{\eta_1}^T(\hat{\mathbf{k}}) \mathbf{T} \times_{\eta}^*(\hat{\mathbf{k}}'), \quad (272)$$

and the relation giving the components of the ladder coherency phase matrix

$$Z_{\text{JL}(\eta_1, \xi_1)(\eta, \xi)}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') = S_{0\eta_1\eta}(\hat{\mathbf{k}}, \hat{\mathbf{k}}') S_{0\xi_1\xi}^*(\hat{\mathbf{k}}, \hat{\mathbf{k}}'), \quad (273)$$

to obtain

$$\begin{aligned} F_{k\eta\xi\eta'\xi'}(\mathbf{R}_k, \dots, \mathbf{R}_1, \mathbf{R}_0) &= n_0 e^{-\kappa_0 \mathbf{R}_k \cdot \hat{\mathbf{z}}} \left[\prod_{j=1}^k \left(n_0 \frac{e^{-\kappa R_{j,j-1}}}{R_{j,j-1}^2} \right) \right] \\ &\times \sum_{\eta_1, \xi_1=\theta, \varphi} Z_{\text{JL}(\eta', \xi')(\eta_1, \xi_1)}(-\hat{\mathbf{s}}, \hat{\mathbf{R}}_{k,k-1}) \\ &\times Z_{\text{JL}(\eta_1, \xi_1)(\eta, \xi)}(\hat{\mathbf{R}}_{k,k-1}, \hat{\mathbf{R}}_{k-1,k-2}, \dots, \hat{\mathbf{R}}_{10}, \hat{\mathbf{p}}) \\ &\times e^{-\kappa R_{0p}} \frac{1}{R_{0p}^2} \delta(\hat{\mathbf{R}}_{0p} - \hat{\mathbf{p}}), \quad k \geq 1 \end{aligned} \quad (274)$$

with $Z_{\text{JL}}(\hat{\mathbf{R}}_{10}, \hat{\mathbf{p}}) = Z_{\text{JL}}(\hat{\mathbf{R}}_{10}, \hat{\mathbf{p}})$, and

$$\begin{aligned} F_{0\eta\xi\eta'\xi'}(\mathbf{R}_0) &= n_0 e^{-\kappa_0 \mathbf{R}_k \cdot \hat{\mathbf{z}}} Z_{\text{JL}(\eta', \xi')(\eta, \xi)}(-\hat{\mathbf{s}}, \hat{\mathbf{p}}) \\ &\times e^{-\kappa R_{0p}} \frac{1}{R_{0p}^2} \delta(\hat{\mathbf{R}}_{0p} - \hat{\mathbf{p}}), \end{aligned} \quad (275)$$

where

$$\begin{aligned} Z_{\text{JLk}}(\hat{\mathbf{R}}_{k,k-1}, \hat{\mathbf{R}}_{k-1,k-2}, \dots, \hat{\mathbf{R}}_{10}, \hat{\mathbf{p}}) &= Z_{\text{JL}}(\hat{\mathbf{R}}_{k,k-1}, \hat{\mathbf{R}}_{k-1,k-2}) \\ &\times Z_{\text{JLk-1}}(\hat{\mathbf{R}}_{k-1,k-2}, \dots, \hat{\mathbf{R}}_{10}, \hat{\mathbf{p}}), \quad k \geq 2, \end{aligned} \quad (276)$$

and, as before, $Z_{\text{JL1}}(\hat{\mathbf{R}}_{10}, \hat{\mathbf{p}}) = Z_{\text{JL}}(\hat{\mathbf{R}}_{10}, \hat{\mathbf{p}})$. On the other hand, because for sparse media, $g(r) = 1$ and $\int_{2a}^{\infty} dr \rightarrow \int_0^{\infty} dr$, the probability density function $p(r)$ given by Eq. (264) simplifies to that

given by Eq. (262). Furthermore, the exciting field coefficients given by (cf. Eq. (265))

$$e_{k-1} = 4\pi \sum_{\xi=\theta, \varphi} \mathcal{E}_{\xi}(\hat{\mathbf{R}}_{k-1, k-2}) \times_{\xi}^* (\hat{\mathbf{R}}_{k-1, k-2}), \quad (277)$$

$$\begin{aligned} \mathcal{E}_{\xi}(\hat{\mathbf{R}}_{k-1, k-2}) &= \left(\prod_{j=1}^{k-1} \frac{e^{ik_1 R_{j,j-1}}}{R_{j,j-1}} \right) \\ &\times \sum_{\eta} S_{0k-1, \xi \eta}(\hat{\mathbf{R}}_{k-1, k-2}, \hat{\mathbf{R}}_{k-2, k-3}, \dots, \hat{\mathbf{R}}_{10}, \hat{\mathbf{p}}) \\ &\times \mathcal{E}_{0\eta}(\hat{\mathbf{p}}) e^{ik_1 \hat{\mathbf{p}} \cdot (\mathbf{R}_0 - \mathbf{r})}, \quad k \geq 2 \end{aligned} \quad (278)$$

with $S_{01}(\hat{\mathbf{R}}_{10}, \hat{\mathbf{p}}) = S_0(\hat{\mathbf{R}}_{10}, \hat{\mathbf{p}})$, and

$$e_0 = 4\pi \sum_{\xi=\theta, \varphi} \mathcal{E}_{0\xi}(\hat{\mathbf{p}}) \times_{\xi}^* (\hat{\mathbf{p}}) e^{ik_1 \hat{\mathbf{p}} \cdot (\mathbf{R}_0 - \mathbf{r})}, \quad (279)$$

where

$$\begin{aligned} S_{0k-1}(\hat{\mathbf{R}}_{k-1, k-2}, \hat{\mathbf{R}}_{k-2, k-3}, \dots, \hat{\mathbf{R}}_{10}, \hat{\mathbf{p}}) \\ = S_0(\hat{\mathbf{R}}_{k-1, k-2}, \hat{\mathbf{R}}_{k-2, k-3}) \\ \times S_{0k-2}(\hat{\mathbf{R}}_{k-2, k-3}, \dots, \hat{\mathbf{R}}_{10}, \hat{\mathbf{p}}), \quad k \geq 3, \end{aligned} \quad (280)$$

$S_{01}(\hat{\mathbf{R}}_{10}, \hat{\mathbf{p}}) = S_0(\hat{\mathbf{R}}_{10}, \hat{\mathbf{p}})$, and $S_0 = [S_{0\xi\eta}(\hat{\mathbf{k}}, \hat{\mathbf{k}}')]$, are the expansion coefficients of a plane electromagnetic wave with amplitudes $\mathcal{E}_{\xi}(\hat{\mathbf{R}}_{k-1, k-2})$, $\xi = \theta, \varphi$, propagating in the direction $\hat{\mathbf{R}}_{k-1, k-2}$. Consequently,

$$P(\hat{\mathbf{r}}, \hat{\mathbf{R}}_{k-1, k-2}) = 4\pi \frac{\sum_{\eta'=\theta, \varphi} |E_{\text{sctk-1}, \eta'}^{\infty}(\hat{\mathbf{r}})|^2}{\sum_{\eta'=\theta, \varphi} \int |E_{\text{sctk-1}, \eta'}^{\infty}(\hat{\mathbf{r}})|^2 d^2 \hat{\mathbf{r}}} \quad (281)$$

with $E_{\text{sctk-1}, \eta'}^{\infty}(\hat{\mathbf{r}})$ as in Eq. (267), is the phase function for the incident and scattering directions $\hat{\mathbf{R}}_{k-1, k-2}$ and $\hat{\mathbf{r}}$, respectively. Thus, as in the standard Monte Carlo method for solving the radiative transfer equation in a sparse medium, the probability density function $p(\theta, \varphi)$ is proportional to the phase function $P(\hat{\mathbf{r}}, \hat{\mathbf{R}}_{k-1, k-2})$. Note that in Eq. (254), the product $\prod_{j=1}^{k-1} (1/R_{j,j-1}^2)$ in the expression of $F_{k\eta\xi\eta'\xi'}(\cdot)$ and the same product in the expression $\prod_{j=1}^k p(\mathbf{R}_{j-1}^{(l)} \rightarrow \mathbf{R}_j^{(l)})$ (resulting from Eq. (263)) cancel out.

3. In a forward Monte Carlo approach for a sparse medium, the quantity of interest is the diffuse ladder coherency dyadic at point \mathbf{r} in an arbitrary small solid angle $\Delta\Omega(\hat{\mathbf{p}})$ around the direction $\hat{\mathbf{p}}$. This is defined by

$$\mathcal{C}_{\text{dL}\Delta\Omega(\hat{\mathbf{p}}), \eta\xi}(\mathbf{r}) = \int_{\Delta\Omega(\hat{\mathbf{p}})} \Sigma_{\text{dL}\eta\xi}(\mathbf{r}, -\hat{\mathbf{p}}') d^2 \hat{\mathbf{p}}' \quad (282)$$

and is the analog of the local estimate of the radiance in the radiative transfer theory [15]. Using Eq. (239) with $x_{\eta}(-\hat{\mathbf{p}})\delta(\hat{\mathbf{R}}_{0P} - \hat{\mathbf{p}}) = x_{\eta}(-\hat{\mathbf{R}}_{0P})\delta(\hat{\mathbf{R}}_{0P} - \hat{\mathbf{p}})$, and introducing the indicator function

$$\chi(\hat{\mathbf{R}}_{0P}) = \int_{\Delta\Omega(\hat{\mathbf{p}})} \delta(\hat{\mathbf{R}}_{0P} - \hat{\mathbf{p}}') d^2 \hat{\mathbf{p}}' = \begin{cases} 1, & \hat{\mathbf{R}}_{0P} \in \Delta\Omega(\hat{\mathbf{p}}) \\ 0, & \text{otherwise} \end{cases}, \quad (283)$$

we obtain

$$\begin{aligned} \mathcal{C}_{\text{dL}\Delta\Omega(\hat{\mathbf{p}}), \eta\xi}(\mathbf{r}) &= \frac{n_0}{k_1^2} \sum_{\eta', \xi'=\theta, \varphi} \int_D e^{-kR_{0P}} x_{\eta'}^T(-\hat{\mathbf{R}}_{0P}) T x_{L\eta'\xi'}(\mathbf{R}_0) \\ &\times T^{\dagger} x_{\xi}^* (-\hat{\mathbf{R}}_{0P}) \mathcal{E}_{0\eta'} \mathcal{E}_{0\xi'}^* \frac{1}{R_{0P}^2} \chi(\hat{\mathbf{R}}_{0P}) d^3 \mathbf{R}_0. \end{aligned} \quad (284)$$

From Eq. (284) we see that for a Markov chain $\{\mathbf{R}_0; K\}$, only the particles k with $\hat{\mathbf{R}}_{kP} \in \Delta\Omega(\hat{\mathbf{p}})$ will contribute to the estimate of $\mathcal{C}_{\text{dL}\Delta\Omega(\hat{\mathbf{p}}), \eta\xi}(\mathbf{r})$. Thus, if the direction $\hat{\mathbf{p}}$ is specified, a backward

Monte Carlo method seems to be more efficient than a forward Monte Carlo method. From the other side, one trajectory in the forward Monte Carlo approach can yield contributions to the diffuse ladder coherency dyadics $\mathcal{C}_{\text{dL}\Delta\Omega(\hat{\mathbf{p}}_1), \eta\xi}(\mathbf{r})$ corresponding to many directions $\hat{\mathbf{p}}_i$.

4. In Refs. [20–22], the method presented in this appendix has been extended to clusters of particles (actually, a forward Monte Carlo approach has been used to analyze the incoherent part of the scattered radiation at an observation point that is outside the discrete random medium). In this method, the clusters are not situated in the far-field region of each other as in Appendix D, i.e., clusters with large size parameters are allowed to come into contact. Starting with the series representation for the exciting field coefficients (51) and assuming that (i) a chain of clusters is a Markov chain and moreover, (ii) the positions of the clusters are uncorrelated, the integral equation (61), with $g(R_{ij}) = 1$ and the matrix $Q^{\dagger}(k_1 \mathbf{R}_{ij})$ as in Eq. (240) but with the transition matrix of a particle T replaced by the transition matrix of a cluster T_c , is derived. This integral equation is used in conjunction with the integral representation for the diffuse ladder specific coherency dyadic (106) and solved by means of a forward Monte Carlo approach. In the Monte Carlo simulations, the probability density function $p(\theta, \varphi)$ corresponding to the transition function $p(\mathbf{R}_{k-1} \rightarrow \mathbf{R}_k)$ is constructed by assuming that the cluster k is situated in the far zone of the cluster $k-1$. Although, for example, the assumption that a chain of clusters with large size parameters is a Markov chain is very strong, i.e., for the chain, $i \leftarrow j \leftarrow k$, we suppose that $p(\mathbf{R}_k | \mathbf{R}_j, \mathbf{R}_i) = p(\mathbf{R}_k | \mathbf{R}_j)$, meaning that the position of cluster k depends only on the position of cluster j and not on the position of cluster i , the numerical analysis reported in these papers showed that this approach yields accurate results for volume concentrations f beyond its theoretical limit, e.g., for f up to 0.25.

Appendix F

In this appendix we present an iteration algorithm based on Eq. (147) and the discrete ordinate method. As boundary conditions, we impose $J_{\text{dL}}(z=0, \hat{\mathbf{k}}^+) = 0$ and $J_{\text{dL}}(z=H, \hat{\mathbf{k}}^-) = 0$.

Let $\hat{\mathbf{s}} = \hat{\mathbf{s}}(\mu_0, \varphi_0)$ be the incidence direction, and $\{\mu_k, w_{\mu k}\}_{k=1}^{N_{\mu}}$ be a set of N_{μ} Gauss–Legendre quadrature nodes and weights on the interval $[0, 1]$. Furthermore, consider a discrete set of points $\{z_i\}_{i=1}^{N_z}$ in the altitude interval $[0, H]$. For the directions $\hat{\mathbf{k}} = \hat{\mathbf{k}}(\mu, \varphi)$ and $\hat{\mathbf{k}}_1 = \hat{\mathbf{k}}_1(\mu_1, \varphi_1)$, assume the azimuthal expansions

$$J_{\text{dL}}(z, \hat{\mathbf{k}}) = \sum_{m=-M_{\text{rank}}}^{M_{\text{rank}}} J_{\text{dLm}}(z, \mu) e^{im(\varphi - \varphi_0)}, \quad (285)$$

$$J_{\text{dns}}(z, \hat{\mathbf{k}}) = \sum_{m=-M_{\text{rank}}}^{M_{\text{rank}}} J_{\text{dnsm}}(z, \mu) e^{im(\varphi - \varphi_0)}, \quad (286)$$

and

$$Z_{\text{JL}}(\hat{\mathbf{k}}, \hat{\mathbf{k}}_1) = \sum_{m=-M_{\text{rank}}}^{M_{\text{rank}}} Z_{\text{JLm}}(\mu, \mu_1) e^{im(\varphi - \varphi_1)}, \quad (287)$$

where M_{rank} is the maximum azimuthal order, and set

$$x_{\eta}(\mu, \varphi_0) = \begin{bmatrix} x_{\eta mn}^1(\mu, \varphi_0) \\ x_{\eta mn}^2(\mu, \varphi_0) \end{bmatrix}. \quad (288)$$

The algorithm is organized as follows: given $\bar{X}_L^{(N-1)}(z_i)$ and $J_{\text{dnsm}}^{(N-1)}(z_i, \pm\mu_k)$ with $i = 1, \dots, N_z$ and $k = 1, \dots, N_{\mu}$, at the iteration step N

1. set $J_{\text{dLm}}^{(N)}(z_i = 0, \mu_k) = 0$ and $J_{\text{dLm}}^{(N)}(z_i = H, -\mu_k) = 0$, and for all azimuthal modes $m = -M_{\text{rank}}, \dots, M_{\text{rank}}$, compute the remaining $J_{\text{dLm}}^{(N)}(z_i, \pm\mu_k)$ with $i = 1, \dots, N_z$ and $k = 1, \dots, N_\mu$ by using the relations (cf. Eq. (147))

$$\begin{aligned} J_{\text{dLm}}^{(N)}(z_i, \mu_k) &= n_0 \frac{1}{\mu_k} \int_0^{z_i} e^{-\kappa \frac{z_i - z_j}{\mu_k}} \left\{ J_{\text{JLm}}(\mu_k, \mu_0) J_c(z_j) + J_{\text{dLm}}^{(N-1)}(z_j, \mu_k) \right. \\ &\quad + 2\pi \sum_{l=1}^{N_\mu} w_{\mu l} [J_{\text{JLm}}(\mu_k, \mu_l) J_{\text{dLm}}^{(N-1)}(z_j, \mu_l) \\ &\quad \left. + J_{\text{JLm}}(\mu_k, -\mu_l) J_{\text{dLm}}^{(N-1)}(z_j, -\mu_l) \right\} dz_j \end{aligned} \quad (289)$$

and

$$\begin{aligned} J_{\text{dLm}}^{(N)}(z_i, -\mu_k) &= n_0 \frac{1}{\mu_k} \int_{z_i}^H e^{-\kappa \frac{z_i - z_j}{\mu_k}} \left\{ J_{\text{JLm}}(-\mu_k, \mu_0) J_c(z_j) + J_{\text{dLm}}^{(N-1)}(z_j, -\mu_k) \right. \\ &\quad + 2\pi \sum_{l=1}^{N_\mu} w_{\mu l} [J_{\text{JLm}}(-\mu_k, \mu_l) J_{\text{dLm}}^{(N-1)}(z_j, \mu_l) \\ &\quad \left. + J_{\text{JLm}}(-\mu_k, -\mu_l) J_{\text{dLm}}^{(N-1)}(z_j, -\mu_l) \right\} dz_j; \end{aligned} \quad (290)$$

2. compute the elements of the matrix $X_L(z_i)$ as (cf. Eq. (143))

$$\begin{aligned} X_{\text{Lmn}, m' n'}^{pq}(z_i) &= e^{-\kappa_0 z_i} E_{0mn, m' n'}^{pq} + \bar{X}_{\text{Lmn}, m' n'}^{pq(N-1)}(z_i) \\ &\quad + 32\pi^2 \sqrt{\frac{\mu_0}{\varepsilon_1}} U_{mn, m' n'}^{pq(N)}(z_i), \end{aligned} \quad (291)$$

where

$$\begin{aligned} U_{mn, m' n'}^{pq(N)}(z_i) &= 2\pi \sum_{\eta, \xi = \theta, \varphi} \sum_{l=1}^{N_\mu} w_{\mu l} \\ &\quad \times \left[J_{\text{dLm}-m'(\eta, \xi)}^{(N)}(z_i, \mu_l) x_{\eta mn}^{p*}(\mu_l, \varphi_0) x_{\xi m' n'}^q(\mu_l, \varphi_0) \right. \\ &\quad \left. + J_{\text{dLm}-m'(\eta, \xi)}^{(N)}(z_i, -\mu_l) x_{\eta mn}^{p*}(-\mu_l, \varphi_0) x_{\xi m' n'}^q(-\mu_l, \varphi_0) \right]; \end{aligned} \quad (292)$$

3. compute the elements of the dense-medium matrix $\bar{X}_L^{(N)}(z_i)$ as (cf. Eq. (144))

$$\begin{aligned} \bar{X}_{\text{Lmn}, m' n'}^{pq(N)}(z_i) &= n_0 \sum K_{m_1 n_1 m_2 n_2 n' n''}^{pqrt} L_{\text{Lmn}-mn'' m_2 -m' n''} \\ &\quad \times X_{\text{Lmn}_1 n_1 m_2 n_2}^{rt}(z_i), \quad p, q = 1, 2; \end{aligned} \quad (293)$$

4. for all azimuthal modes $m = -M_{\text{rank}}, \dots, M_{\text{rank}}$ compute the elements of the diffuse coherency column vector for dense media $J_{\text{dLm}}^{(N)}(z_i, \pm\mu_k)$ with $i = 1, \dots, N_z$ and $k = 1, \dots, N_\mu$ by using the relation (cf. Eq. (145))

$$\begin{aligned} J_{\text{dLm}}^{(N)}(z_i, \pm\mu_k) &= \frac{1}{2k_1^2} \sqrt{\frac{\varepsilon_1}{\mu_0}} \sum_{p,q=1}^2 \sum_{n=1}^{N_{\text{rank}}} \sum_{n'=1}^{N_{\text{rank}}} \sum_{m'=\max(-n, m-n')}^{\min(n, n'+m)} \\ &\quad \times x_{\eta mn}^p(\pm\mu_k, \varphi_0) T_n^{p*} \bar{X}_{\text{Lmn}, m' -mn'}^{pq(N)}(z_i) T_{n'}^{q*} x_{\xi m' -mn'}^{q*}(\pm\mu_k, \varphi_0). \end{aligned} \quad (294)$$

The integrals over z_j in Eqs. (289) and (290) are calculated by using the following quadrature scheme. Consider the generic integrals

$$I_+ = \int_0^{z_i} g(z) F(z) dz = \sum_{k=1}^{i-1} \int_{z_k}^{z_{k+1}} g(z) F(z) dz = \sum_{k=1}^{i-1} I_k, \quad (295)$$

$$I_- = \int_{z_i}^H g(z) F(z) dz = \sum_{k=i}^{N_z-1} \int_{z_k}^{z_{k+1}} g(z) F(z) dz = \sum_{k=i}^{N_z-1} I_k \quad (296)$$

with

$$I_k = \int_{z_k}^{z_{k+1}} g(z) F(z) dz, \quad (297)$$

and let $\{x_l, w_{xl}\}_{l=1}^{N_x}$ be a set of N_x Gauss-Legendre quadrature points and weights on the interval $[-1, 1]$. For each interval $[z_k, z_{k+1}]$ compute

$$1. \bar{z}_l = \frac{z_{k+1} - z_k}{2} x_l + \frac{z_{k+1} + z_k}{2}, \quad (298)$$

$$2. \bar{w}_{zl} = \frac{z_{k+1} - z_k}{2} w_{xl}, \quad (299)$$

$$3. F_l = \frac{\bar{z}_l - z_k}{z_{k+1} - z_k} F(z_{k+1}) + \frac{z_{k+1} - \bar{z}_l}{z_{k+1} - z_k} F(z_k), \quad (300)$$

$$4. g_l = g(\bar{z}_l), \quad (301)$$

$$5. I_k = \sum_{l=1}^{N_x} \bar{w}_{zl} g_l F_l. \quad (302)$$

Thus, in the interval $[z_k, z_{k+1}]$, the (matrix) function $F(z)$ with the endpoint values $F(z_k)$ and $F(z_{k+1})$ is assumed to vary linearly, while the (scalar) function $g(z)$ is sampled at all quadrature points inside this interval. In Eqs. (289) and (290), the functions $g(z)$ are $\exp[-\kappa(z_i - z)/\mu_k]$ and $\exp[-\kappa(z - z_i)/\mu_k]$, respectively.

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