

Radiative scattering properties of an ensemble of variously shaped small particles

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This paper presents a rigorous solution to the scattering of a monochromatic plane wave by an arbitrary configuration of wavelength-sized small particles that can be of different shape, structure, size, and composition. A T -matrix formulation is developed for the calculation of optical cross sections and the asymmetry parameter of such an ensemble of scatterers in both fixed and random orientations. The solution is based on the T matrix \mathbf{T}^{jl} , that is, the inverse of the coefficient matrix of boundary condition equations. A linear system containing \mathbf{T}^{jl} is derived to efficiently solve the T matrix, which is required in the practical implementation of the solution.

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I. INTRODUCTION

Radiative scattering by multiple particles is a common subject in a wide range of scientific and technical fields stretching from astrophysics to nanoscience and from remote sensing to aerosol medicine. Since the work on addition theorems for vector spherical wave functions (VSWFs) by Stein [1] and Cruzan [2] in the early 1960s, numerous researchers from diverse scientific and technical areas have contributed to a continual progress towards a complete analytical solution to radiative scattering of a plane wave by multiple spheres. Starting with Liang and Lo [3] and Bruning and Lo [4], contributors include Peterson and Ström [5], Borghese *et al.* [6,7], Fuller and Kattawar [8,9], Hamid, Ciric, and Hamid [10], Mackowski [11], and many others. As an extension of the Lorenz-Mie solution for single homogeneous spheres [12,13] to the multisphere case, the multipole superposition solution to multisphere scattering has been well established to date. Following the pioneer work by Lo and his colleagues [3,4], two solution approaches have been reported to the multisphere scattering. The first is the cluster T matrix (CTM) approach developed initially by Peterson and Ström [5]. Representative work on CTM for the scattering by an ensemble of homogeneous spheres in random orientations includes those by Mackowski [14] and Mackowski and Mishchenko [15]. The main idea of the CTM approach is to construct a single-particle type T matrix for an ensemble of spheres as a whole. A requirement of this approach is the translation of radiative fields between displaced reference systems through the use of Stein and Cruzan's general addition theorems for VSWFs. With the cluster T matrix of single-particle type determined, an ensemble of spheres can be treated as an equivalent single scatterer. In this way, all scattering solutions derived for single particles remain valid and all formulations for single-body scattering can be used directly to solve multiparticle scattering. Though rigorous in principle, CTM has an intrinsic weakness in practical implementations. Its applicability is rather limited regarding the overall size of an ensemble because the truncation of multi-

pole field expansions in CTM depends on the overall dimension of an ensemble rather than the size of individual spheres. The second is a far-field approach, which leads to the development of the generalized multiparticle Mie solution (GMM) [16–22]. It avoids altogether the use of the general addition theorems for VSWFs in field translations [17]. Field-expansion truncation in GMM depends solely on the size of individual particles and is not concerned with the overall dimension of an ensemble. Thus, GMM is completely exempted from the overall size restriction that CTM suffers from in practical applications.

The GMM has been extended to the general case of an arbitrary mixture of spherical and nonspherical scatterers. When the proper T matrices of a group of particles (i.e., T matrices of the particles in single-body scattering) are precisely known or can be computed accurately, the scattering by an arbitrary configuration of these particles can be solved completely for both cases of fixed and random orientations. The following section describes such a general solution to cross sections for extinction, scattering, and radiation pressure, as well as the asymmetry parameter. The solution has been implemented in several computer codes [31]. A couple of practical examples are given in Sec. III to demonstrate the numerical solutions obtained from the public domain GMM codes and to illustrate the significant difference between GMM and CTM.

II. FORMULATION

Under study here is the scattering characteristics of a collection of spherical and/or nonspherical particles that are illuminated by a monochromatic plane wave with an arbitrary linear polarization state. In the so-called “incident reference frame,” in which the incident plane wave propagates in the positive z direction, the polarization state of the incident radiation, i.e., the linear polarization angle β_p , is defined by the angle between the incident electric vector and the positive x direction.

Since the development of a random-orientation scattering formulation builds on the scattering solutions for fixed orientations, this section starts with the discussion of fixed-orientation scattering. It then addresses the calculation of the

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T matrix \mathbf{T}^l , the key quantity in the T -matrix formulations of GMM. Finally, solutions to the random-orientation cross sections are derived.

A. Solution of fixed-orientation scattering

Based on the Mie-type multipole superposition solution method, the incident electric field \mathbf{E}^{inc} and the total scattered field \mathbf{E}^{sca} of an ensemble of L particles are expanded in terms of VSWFs in an arbitrarily chosen primary reference system,

$$\mathbf{E}^{\text{inc}} = -i \sum_{n=1}^{N_{\text{max}}} \sum_{m=-n}^n \sum_{p=1}^2 E_{mn} p_{mnp} \mathbf{N}_{mnp}^{(1)}(\mathbf{r}), \quad (1a)$$

$$\mathbf{E}^{\text{sca}} = i \sum_{n=1}^{N_{\text{max}}} \sum_{m=-n}^n \sum_{p=1}^2 E_{mn} a_{mnp} \mathbf{N}_{mnp}^{(3)}(\mathbf{r}), \quad (1b)$$

where $\mathbf{N}_{mnp}^{(1)}$ and $\mathbf{N}_{mnp}^{(3)}$ denote the VSWFs for incoming and outgoing waves, which are associated with the spherical Bessel and Hankel functions of the first kind, respectively, $i = \sqrt{-1}$, $E_{mn} = E_0 i^n C_{mn}$, and

$$C_{mn} = \left[\frac{(2n+1)(n-m)!}{n(n+1)(n+m)!} \right]^{1/2}. \quad (2)$$

Linear dimensions appearing in all equations in this work are normalized by the wave number $k = 2\pi/\lambda$, where λ is the incident wavelength. Note that the normalization factor E_{mn} in the field expansions defined above is different from what the author used before, which was $E_0 i^n (2n+1)(n-m)!/(n+m)!$. Note also that, to save space, an additional index “ p ” is used in field expansions [15]: $p=1$ stands for the TM mode of electric fields and $p=2$ for the TE mode. In the incident reference frame, the primary incident coefficients p_{mnp} in Eq. (1a) are specifically

$$p_{mnp} = 0 \quad (|m| \neq 1), \quad (3a)$$

$$p_{1np} = \frac{\sqrt{2n+1}}{2} \exp(-i\beta_p), \quad (3b)$$

$$p_{-1np} = (-1)^p p_{1np}^*, \quad (3c)$$

where the superscript asterisk represents complex conjugate. In solving multiparticle scattering, the partial scattered fields \mathbf{E}^{sca} of component particles l must be solved in respective particle-centered reference systems in order to appropriately apply boundary conditions at each particle. Similar to Eqs. (1), the incident and the partial scattered fields of particle l are expanded in the reference system centered inside particle l ,

$$\mathbf{E}^{\text{inc}} = -i \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^l) \sum_{n=1}^{N_{\text{max}}^l} \sum_{m=-n}^n \sum_{p=1}^2 E_{mn} p_{mnp}^l \mathbf{N}_{mnp}^{(1)}(\mathbf{r}^l), \quad (4a)$$

$$\mathbf{E}^{\text{sca}} = i \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^l) \sum_{n=1}^{N_{\text{max}}^l} \sum_{m=-n}^n \sum_{p=1}^2 E_{mn} a_{mnp}^l \mathbf{N}_{mnp}^{(3)}(\mathbf{r}^l), \quad (4b)$$

where N_{max}^l is determined by the size of particle l , $\hat{\mathbf{k}}$ is unit vector along the incident direction, \mathbf{d}^l is the position vector of particle center l in the primary reference system,

$$\mathbf{d}^l = \hat{\mathbf{e}}_x X^l + \hat{\mathbf{e}}_y Y^l + \hat{\mathbf{e}}_z Z^l, \quad (5)$$

(X^l, Y^l, Z^l) are the dimensionless (normalized by k) Cartesian coordinates of particle center l , and ($\hat{\mathbf{e}}_x, \hat{\mathbf{e}}_y, \hat{\mathbf{e}}_z$) are Cartesian basis unit vectors. Note the appearance of the incident phase term $\exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^l)$ in Eqs. (4). By the introduction of the incident phase shift, the incident coefficients in Eq. (4a) remain the same as the primary incident coefficients. In the incident reference frame, $p_{mnp}^l \equiv p_{mnp}$ that are given by Eqs. (3).

In formulating fixed-orientation scattering, GMM uses the incident frame so that in Eqs. (4)

$$\hat{\mathbf{k}} = \hat{\mathbf{e}}_z, \quad \hat{\mathbf{k}} \cdot \mathbf{d}^l = Z^l. \quad (6)$$

When particle l is a homogeneous sphere, the scattering coefficients a_{mnp}^l in Eq. (4b) can be expressed as [16]

$$a_{mnp}^l = \bar{a}_{np}^l P_{mnp}^l, \quad (7)$$

where \bar{a}_{np}^l is the Mie scattering coefficients of sphere l and P_{mnp}^l denotes the expansion coefficients of the total incident field for particle l , which includes the exciting plane wave and scattered waves from all other particles in an ensemble. In the incident reference frame, the total incident coefficients P_{mnp}^l are given by [16]

$$P_{mnp}^l = p_{mnp} + (\delta_{ll'} - 1) \exp(iZ^{ll'}) A_{mnm'n'}^{l'lp p'} a_{m'n'p'}^{l'}, \quad (8)$$

where $Z^{ll'} = Z^{l'} - Z^l$, $\delta_{ll'}$ is the Kronecker delta symbol, and $A_{mnm'n'}^{l'lp p'}$ are vector translation coefficients [1,2] characterizing the transformation of scattered waves from particle l' into incident waves for particle l , which are associated with the spherical Hankel function of the first kind. To suppress continual summation signs in equations, a tensorial convention [15] is used in Eq. (8) and hereafter. No summation sign in an equation implies summation over all superscript and/or subscript indices in lower case italics not appearing on the left-hand side of the equation. The linear system of boundary condition equations of Eq. (7) valid for spheres can easily be extended to the case of nonspherical particles [23,24],

$$a_{mnp}^l = \bar{T}_{mn\mu\nu}^{lpq} P_{\mu\nu q}^l, \quad (9)$$

i.e.,

$$a_{mnp}^l = \bar{T}_{mn\mu\nu}^{lpq} [P_{\mu\nu q} + (\delta_{ll'} - 1) \exp(iZ^{ll'}) A_{\mu\nu m'n'}^{l'lp p'} a_{m'n'p'}^{l'}], \quad (10)$$

where $\bar{T}_{mn\mu\nu}^{lpq}$ represents the elements of $\bar{\mathbf{T}}^l$, the proper T matrix of particle l . It is easy to see that Eqs. (8) and (10) involve relative particle positions only, which are determined by the configuration of an ensemble and independent of the choice of the primary reference system. Also, the linear system of Eq. (10) places no restriction on particle shape and structure. The only requirement is that $\bar{\mathbf{T}}^l$ of all component particles in an ensemble be known accurately. With the scattering coefficients a_{mnp}^l solved through the linear system of Eq. (10), all fundamental scattering parameters can be readily calculated, using the existing a_{mnp}^l -based scattering formulations of GMM [17,18]. In addition, a_{mnp}^l can also be expressed in terms of the T matrix \mathbf{T}^{jl} , that is, the formal inverse of the linear system of Eq. (10), which is of the form [21]

$$a_{mnp}^l = \exp(iZ^l) T_{mn\mu\nu}^{jlpq} p_{\mu\nu q}, \quad (11)$$

i.e.,

$$a_{mnp}^l = \frac{\sqrt{2\nu+1}}{2} \exp(iZ^l) [T_{mn1\nu}^{jlpq} \exp(-i\beta_p) + (-1)^q T_{mn,-1,\nu}^{jlpq} \exp(i\beta_p)]. \quad (12)$$

This shows that, in the incident reference frame, the solution of the scattering coefficients a_{mnp}^l involves the determination of $T_{mn\mu\nu}^{jlpq}$ for $\mu = \pm 1$ only.

Through the use of Eq. (11) that relates a_{mnp}^l with the T matrix \mathbf{T}^{jl} , the a_{mnp}^l -based fixed-orientation scattering solution of GMM has been converted to a \mathbf{T}^{jl} -based T -matrix formulation [21]. The T matrix \mathbf{T}^{jl} is also the pivotal quantity in the T -matrix formulation of GMM derived here for random-orientation scattering. Although \mathbf{T}^{jl} is formally the inverse of the coefficient matrix of boundary condition equations, the method of direct matrix inversion is infeasible in most circumstances unless the total number and the size of particles in an ensemble are both sufficiently small. It is thus of critical importance to have a general means of solving \mathbf{T}^{jl} .

B. Solution of the T matrix \mathbf{T}^{jl}

To solve \mathbf{T}^{jl} , the general case of an arbitrary direction of incidence needs to be considered. An arbitrary direction of incidence can be described by the rotation of the z -pointing plane wave vector ($\hat{\mathbf{k}} = \hat{\mathbf{e}}_z$) in terms of three Euler angles (α, β, γ) and the unit incident vector after rotation becomes

$$\hat{\mathbf{k}} = \hat{\mathbf{e}}_x \sin \beta \cos \alpha + \hat{\mathbf{e}}_y \sin \beta \sin \alpha + \hat{\mathbf{e}}_z \cos \beta. \quad (13)$$

While the incident phase shift in Eqs. (4) is simply Z^l in the incident reference frame, it will be denoted by \check{Z}^l for the off- z -direction incidence,

$$\check{Z}^l = \hat{\mathbf{k}} \cdot \mathbf{d}^l. \quad (14)$$

When $\alpha = \beta = \gamma = 0$, $\check{Z}^l = Z^l$. In spherical polar coordinate system, $\check{Z}^l = d^l \cos \eta^l(\beta, \alpha)$ and

$$\cos \eta^l(\beta, \alpha) = \sin \beta \sin \vartheta^l \cos(\alpha - \varphi^l) + \cos \beta \cos \vartheta^l, \quad (15)$$

where $(d^l, \vartheta^l, \varphi^l)$ are the spherical coordinates of origin l in the primary coordinate system. For off- z -direction incidence, the incident coefficients in Eqs. (1a) and (4a) will be denoted by $\check{p}_{mnp}^l \equiv \check{p}_{mnp}$ and

$$\check{p}_{mnp} = (-1)^{m+1} \exp(im\gamma) [\tilde{\tau}_{mnp}(\beta) \cos(\alpha - \beta_p) + i \tilde{\tau}_{mn3-p}(\beta) \sin(\alpha - \beta_p)], \quad (16)$$

where $\tilde{\tau}_{mnp}$ are the normalized angular function

$$\tilde{\tau}_{mnp} = C_{mn} \tau_{mnp}, \quad (17)$$

and the regular angular function τ_{mnp} are defined by

$$\tau_{mn1}(\theta) = \frac{d}{d\theta} P_n^m(\cos \theta), \quad (18a)$$

$$\tau_{mn2}(\theta) = \frac{m}{\sin \theta} P_n^m(\cos \theta), \quad (18b)$$

with P_n^m being the associated Legendre function of the first kind. When $\alpha = \beta = \gamma = 0$, $\check{p}_{mnp} = p_{mnp}$, i.e., Eq. (16) reduces to Eqs. (3). Extended to the general case of off- z -direction incidence, Eq. (10) becomes

$$\check{a}_{mnp}^l = \bar{T}_{mn\mu\nu}^{lpq} [\check{p}_{\mu\nu q} + (\delta_{ll'} - 1) \times \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{ll'}) A_{\mu\nu m' n'}^{l' l q p'} \check{a}_{m' n' p'}^l], \quad (19)$$

where $\mathbf{d}^{ll'} = \mathbf{d}^{l'} - \mathbf{d}^l$ is the position vector extended from origin l to origin l' ,

$$\hat{\mathbf{k}} \cdot \mathbf{d}^{ll'} = \check{Z}^{ll'} = d^{ll'} \cos \eta^{ll'}(\beta, \alpha), \quad (20)$$

and $\cos \eta^{ll'}$ is similarly defined by Eq. (15). Accordingly, Eq. (11) becomes

$$\check{a}_{mnp}^l = \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{lj}) T_{mn\mu\nu}^{jlpq} \check{p}_{\mu\nu q}. \quad (21)$$

Using Eq. (21) in Eq. (19) for both \check{a}_{mnp}^l and $\check{a}_{m' n' p'}^l$, leads to

$$T_{mn\mu\nu}^{jlpq} = (\delta_{jj'} - 1) \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{jj'}) T_{mn\mu\nu}^{j'lpq} + \bar{T}_{mn\mu\nu}^{lpq} \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{jl}) + (\delta_{ll'} - 1) \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{jl'}) \bar{T}_{mn\mu\nu}^{l'p'q'} A_{\mu' \nu' m' n'}^{l' l q' p'} T_{m' n' p' q}^{j' l' p' q}. \quad (22)$$

All quantities in Eq. (22) are independent of the direction of incidence except for the incident phase terms. Averaging over all possible directions of incidence, Eq. (22) becomes

$$T_{mn\mu\nu}^{jlpq} = (\delta_{jj'} - 1) j_0(d^{jj'}) T_{mn\mu\nu}^{j'lpq} + j_0(d^{jl}) \bar{T}_{mn\mu\nu}^{lpq} + (\delta_{ll'} - 1) j_0(d^{jj'}) \bar{T}_{mn\mu\nu}^{l'p'q'} A_{\mu' \nu' m' n'}^{l' l q' p'} T_{m' n' p' q}^{j' l' p' q}, \quad (23)$$

where j_0 is the zero-order spherical Bessel function of the first kind, which results from the integration over the three Euler angles,

$$\begin{aligned} j_0(d^{jl}) &= \frac{1}{8\pi^2} \int_{\varpi} \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{jl}) d\varpi \\ &= \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} \exp(id^{jl} \cos \eta^{jl}) (\sin \beta) d\beta d\alpha. \end{aligned} \quad (24)$$

Here, $d\varpi$ represents $(\sin \beta) d\beta d\alpha d\gamma$. Because both j_0 and $A_{\mu' \nu' m' n'}^{l' q' p'}$ drop steeply when separation distance between particles increases, interactions between the scattered waves from particle l and the particles not in its vicinity are insignificant. Therefore, Eq. (23) includes in fact only particles that are sufficiently close to particle l . When particle l is a sphere, Eq. (23) reduces to

$$\begin{aligned} T_{mn\mu\nu}^{jlpq} &= (\delta_{jj'} - 1) j_0(d^{jj'}) T_{mn\mu\nu}^{j'lpq} + \bar{a}_{np}^l [j_0(d^{jl}) \delta_{m\mu} \delta_{n\nu} \delta_{pq} \\ &\quad + (\delta_{l'l} - 1) j_0(d^{jj'}) A_{mm'm'n'}^{l'lpq} T_{m'n'\mu\nu}^{j'l'p'q}]. \end{aligned} \quad (25)$$

With the proper T matrices $\bar{\mathbf{T}}^l$ of all individual particles provided, \mathbf{T}^{jl} of an ensemble can be efficiently solved from the linear system of Eq. (23) successively for each set of (μ, ν, q) .

C. Integral representation of vector translational addition coefficients

In formulating multiparticle scattering for fixed orientations, the following integral expression for vector translation coefficients (that are associated with the spherical Bessel function of the first kind) obtained in GMM [18] plays an important role,

$$\begin{aligned} \bar{A}_{\omega\nu sn}^{ljqp} &= \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} (\sin \theta) d\theta d\phi \exp(i\hat{\mathbf{r}} \cdot \mathbf{d}^{lj}) \exp[i(s - \omega)\phi] \\ &\quad \times [\tilde{\tau}_{snp}(\theta) \tilde{\tau}_{\omega\nu q}(\theta) + \tilde{\tau}_{sn3-p}(\theta) \tilde{\tau}_{\omega\nu 3-q}(\theta)], \end{aligned} \quad (26)$$

where $\hat{\mathbf{r}} \cdot \mathbf{d}^{lj} = d^{lj} \cos \eta^{lj}(\theta, \phi)$ is the scattered phase shift and $\hat{\mathbf{r}} = \hat{\mathbf{e}}_x \sin \theta \cos \phi + \hat{\mathbf{e}}_y \sin \theta \sin \phi + \hat{\mathbf{e}}_z \cos \theta$ is unit position vector. The above equation for $\bar{A}_{\omega\nu sn}^{ljqp}$ has an alternative form in terms of the reduced rotation matrix elements in quantum mechanics [25]. Based on rotational addition theorems [1,25], the primary incident coefficients for an arbitrary direction of incidence [see Eq. (16)] can also be expressed in terms of those in the incident reference frame [see Eqs. (3)]

$$\check{p}_{mnp} = \mathfrak{D}_{sm}^{(n)}(\varpi) p_{snp}, \quad (27)$$

where [25,26]

$$\mathfrak{D}_{sm}^{(n)}(\varpi) = \exp(is\alpha) d_{sm}^{(n)}(\beta) \exp(im\gamma), \quad (28)$$

and $d_{sm}^{(n)}$ is the reduced rotation matrix elements [25]. Inserting Eqs. (3) and (28) into Eq. (27) leads to

$$\begin{aligned} \check{p}_{mnp} &= \frac{\sqrt{2n+1}}{2} \exp(im\gamma) \{ [d_{1m}^{(n)}(\beta) \\ &\quad + (-1)^p d_{-1m}^{(n)}(\beta)] \cos(\alpha - \beta_p) + i [d_{1m}^{(n)}(\beta) \\ &\quad + (-1)^{p+1} d_{-1m}^{(n)}(\beta)] \sin(\alpha - \beta_p) \}. \end{aligned} \quad (29)$$

Comparing Eq. (29) with Eq. (16) reveals that

$$\tilde{\tau}_{mnp} = \frac{\sqrt{2n+1}}{2} [d_{m1}^{(n)} + (-1)^p d_{m,-1}^{(n)}]. \quad (30)$$

A similar relation has been given for rotation functions by Mackowski and Mishchenko [see Eq. (31) in Ref. [15]]. It follows from Eq. (30) that

$$\begin{aligned} \tilde{\tau}_{snp}(\beta) \tilde{\tau}_{\omega\nu q}(\beta) + \tilde{\tau}_{sn3-p}(\beta) \tilde{\tau}_{\omega\nu 3-q}(\beta) \\ = \frac{\sqrt{(2n+1)(2\nu+1)}}{2} [d_{s1}^{(n)}(\beta) d_{\omega 1}^{(\nu)}(\beta) \\ + (-1)^{p+q} d_{s,-1}^{(n)}(\beta) d_{\omega,-1}^{(\nu)}(\beta)]. \end{aligned} \quad (31)$$

This shows that Eq. (26) can alternatively be written as

$$\begin{aligned} \bar{A}_{\omega\nu sn}^{ljqp} &= \frac{\sqrt{(2n+1)(2\nu+1)}}{8\pi} \int_0^{2\pi} \int_0^{\pi} (\sin \beta) d\beta d\alpha \\ &\quad \times \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{lj}) \exp[i(s - \omega)\alpha] [d_{s1}^{(n)}(\beta) d_{\omega 1}^{(\nu)}(\beta) \\ &\quad + (-1)^{p+q} d_{s,-1}^{(n)}(\beta) d_{\omega,-1}^{(\nu)}(\beta)], \end{aligned} \quad (32)$$

where $\hat{\mathbf{k}} \cdot \mathbf{d}^{lj} = d^{lj} \cos \eta^{lj}(\beta, \alpha)$ [see Eq. (20)]. Both Eqs. (26) and (32) are useful in the derivation of the analytical expressions for orientation-averaged scattering parameters.

D. Solution of random-orientation scattering

Orientation-averaged cross sections for extinction $\langle C_{\text{ext}} \rangle$, scattering $\langle C_{\text{sca}} \rangle$, and radiation pressure $\langle C_{\text{pr}} \rangle$ have a simple relation

$$\langle C_{\text{pr}} \rangle = \langle C_{\text{ext}} \rangle - \langle C_{\text{sca}} \rangle \overline{\langle \cos \theta \rangle}, \quad (33)$$

where a pair of “ $\langle \rangle$ ” indicates an average over all possible particle orientations, $\overline{\langle \cos \theta \rangle}$ is the orientation-averaged asymmetry parameter, defined as $\langle C_{\text{sca}} \overline{\langle \cos \theta \rangle} \rangle / \langle C_{\text{sca}} \rangle$. With \mathbf{T}^{jl} determined, $\langle C_{\text{ext}} \rangle$, $\langle C_{\text{sca}} \rangle$, $\langle C_{\text{pr}} \rangle$, and $\langle \cos \theta \rangle$ can be accurately calculated through the analytical solutions derived here. Explicit expressions for these orientation-averaged scattering quantities are obtained by integrating over three Euler angles that completely determine particle orientations. This method for obtaining an orientational average by the integration over the Euler angles was first used by Mishchenko [27] in scattering calculations for the special case of a single axially symmetric particle and by Khlebtsov [28] for a general scatterer. It has also been used by Mackowski [14]

and Mackowski and Mishchenko [15] in the derivation of a CTM random-orientation scattering formulation for an ensemble of spheres.

Based on the result for fixed-orientation scattering [11,16,17], the orientation-averaged extinction cross section is given in the incident reference frame by

$$\langle C_{\text{ext}} \rangle = \frac{4\pi}{k^2} \text{Re} \langle p_{mnp}^{l*} a_{mnp}^l \rangle, \quad (34)$$

where p_{mnp}^{l*} and a_{mnp}^l should be expressed for an arbitrary orientation of an ensemble in the incident reference frame. After the rotation of an ensemble by (α, β, γ) in the incident reference frame, a_{mnp}^l of the component particles can be expressed as

$$a_{mnp}^l = \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^j) \mathcal{D}_{sm}^{(n)}(\boldsymbol{\omega}) \mathcal{D}_{\omega\mu}^{(v)*}(\boldsymbol{\omega}) T_{sn\omega\nu}^{jlpq} p_{\mu\nu q}, \quad (35)$$

where $T_{sn\omega\nu}^{jlpq}$ are the T -matrix elements of \mathbf{T}^{jl} at the orientation of $\alpha = \beta = \gamma = 0$ and $\hat{\mathbf{k}}$ is given by Eq. (13). Also, $p_{mnp}^{l*} = p_{mnp}^*$. These show that

$$\begin{aligned} \langle p_{mnp}^{l*} a_{mnp}^l \rangle &= \frac{\sqrt{(2n+1)(2\nu+1)}}{16\pi} T_{sn\omega\nu}^{jlpq} \int_0^{2\pi} \int_0^\pi \sin\beta d\beta d\alpha \\ &\times \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^j) \exp[i(s-\omega)\alpha] [d_{s1}^{(n)}(\beta) d_{\omega 1}^{(v)}(\beta) \\ &+ (-1)^{p+q} d_{s,-1}^{(n)}(\beta) d_{\omega,-1}^{(v)}(\beta)]. \end{aligned} \quad (36)$$

It follows readily from Eqs. (36) and (32) that

$$\langle p_{mnp}^{l*} a_{mnp}^l \rangle = \frac{1}{2} \tilde{T}_{\omega\nu\omega\nu}^{(jj)qq}, \quad (37)$$

and

$$\langle C_{\text{ext}} \rangle = \frac{2\pi}{k^2} \text{Re} \tilde{T}_{\omega\nu\omega\nu}^{(jj)qq}, \quad (38)$$

where

$$\tilde{T}_{\omega\nu\omega\nu}^{(jj)qq} = \tilde{A}_{\omega\nu sn}^{ljqp} T_{sn\omega\nu}^{jlpq}. \quad (39)$$

The expression for the scattering cross section of an ensemble of particles in fixed orientations [18] shows that random-orientation averaged scattering cross section can be written in the form

$$\begin{aligned} \langle C_{\text{sca}} \rangle &= \frac{1}{8\pi^2 k^2} \text{Re} \int_{\Omega} \int_{\boldsymbol{\omega}} d\boldsymbol{\omega} d\Omega \tilde{a}_{mnp}^{l*} \tilde{a}_{m'n'p'}^l \exp(i\hat{\mathbf{r}} \cdot \mathbf{d}^{l'l}) \\ &\times \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{l'l}) \exp[i(m'-m)\phi] \\ &\times [\tilde{\tau}_{mnp}(\theta) \tilde{\tau}_{m'n'p'}(\theta) + \tilde{\tau}_{mn3-p}(\theta) \tilde{\tau}_{m'n'3-p'}(\theta)], \end{aligned} \quad (40)$$

where $d\Omega = (\sin\theta)d\theta d\phi$ and

$$\begin{aligned} \tilde{a}_{mnp}^{l*} \tilde{a}_{m'n'p'}^l &= \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{l'j}) \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{l'l}) T_{mn\mu'\nu'}^{j'lpq*} T_{m'n'\mu\nu}^{jl'p'q} \\ &\times \mathcal{D}_{\omega'\mu'}^{(v')*}(\boldsymbol{\omega}) \mathcal{D}_{\omega\mu}^{(v)}(\boldsymbol{\omega}) p_{\omega'\nu'q'}^* p_{\omega\nu q}. \end{aligned} \quad (41)$$

By using Eqs. (3), (26), (32), and (41) in Eq. (40), it is straightforward to show that

$$\langle C_{\text{sca}} \rangle = \frac{2\pi}{k^2} \text{Re} [\tilde{\mathcal{T}}_{mn\mu\nu}^{(jl)pq*} \tilde{T}_{mn\mu\nu}^{(jl)pq}], \quad (42)$$

where

$$\tilde{T}_{mn\mu\nu}^{(jl)pq} = \tilde{A}_{mnm'n'}^{l'lp'q} T_{m'n'\mu\nu}^{jl'p'q}, \quad (43a)$$

$$\tilde{\mathcal{T}}_{mn\mu\nu}^{(jl)pq} = T_{mn\mu'\nu'}^{j'lpq*} \tilde{A}_{\mu'\nu'\mu\nu}^{j'q'q}. \quad (43b)$$

Similarly, the orientation-averaged asymmetry parameter can be obtained from the equation

$$\begin{aligned} \langle C_{\text{sca}} \overline{\cos\theta} \rangle &= \frac{1}{8\pi^2 k^2} \text{Re} \int_{\Omega} \int_{\boldsymbol{\omega}} d\boldsymbol{\omega} d\Omega \hat{\mathbf{k}} \cdot \hat{\mathbf{r}} \tilde{a}_{mnp}^{l*} \tilde{a}_{m'n'p'}^l \\ &\times \exp(i\hat{\mathbf{r}} \cdot \mathbf{d}^{l'l}) \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{l'l}) \exp[i(m'-m)\phi] \\ &\times [\tilde{\tau}_{mnp}(\theta) \tilde{\tau}_{m'n'p'}(\theta) \\ &+ \tilde{\tau}_{mn3-p}(\theta) \tilde{\tau}_{m'n'3-p'}(\theta)], \end{aligned} \quad (44)$$

where

$$\begin{aligned} \hat{\mathbf{k}} \cdot \hat{\mathbf{r}} &= \sin\beta \cos\alpha \sin\theta \cos\phi + \sin\beta \sin\alpha \sin\theta \sin\phi \\ &+ \cos\beta \cos\theta. \end{aligned} \quad (45)$$

Along the same line described above, it can be shown that the final result of $\langle \overline{\cos\theta} \rangle$ is

$$\langle \overline{\cos\theta} \rangle = \frac{2\pi}{k^2 \langle C_{\text{sca}} \rangle} \text{Re} [\tilde{\mathcal{F}}_{mn\mu\nu}^{(jl)pq} + \tilde{\mathcal{G}}_{mn\mu\nu}^{(jl)pq} + \tilde{\mathcal{H}}_{mn\mu\nu}^{(jl)pq}], \quad (46)$$

where

$$\begin{aligned} \tilde{\mathcal{F}}_{mn\mu\nu}^{(jl)pq} &= [f_1(m, n) \tilde{T}_{mn\mu\nu}^{(jl)3-pq} + f_2(m, n) \tilde{T}_{mn+1\mu\nu}^{(jl)pq} \\ &+ f_3(m, n) \tilde{T}_{mn-1\mu\nu}^{(jl)pq}] [f_1(\mu, \nu) \tilde{\mathcal{T}}_{mn\mu\nu}^{(jl)p3-q*} \\ &+ f_2(\mu, \nu) \tilde{\mathcal{T}}_{mn\mu\nu+1}^{(jl)pq*} + f_3(\mu, \nu) \tilde{\mathcal{T}}_{mn\mu\nu-1}^{(jl)pq*}], \end{aligned} \quad (47a)$$

$$\begin{aligned} \tilde{\mathcal{G}}_{mn\mu\nu}^{(jl)pq} &= \frac{1}{2} [f_4(m, n) \tilde{T}_{m+1n\mu\nu}^{(jl)3-pq} + f_5(m, n) \tilde{T}_{m+1n+1\mu\nu}^{(jl)pq} \\ &+ f_6(m, n) \tilde{T}_{m+1n-1\mu\nu}^{(jl)pq}] [f_4(-\mu, \nu) \tilde{\mathcal{T}}_{mn\mu-1\nu}^{(jl)p3-q*} \\ &- f_5(-\mu, \nu) \tilde{\mathcal{T}}_{mn\mu-1\nu+1}^{(jl)pq*} - f_6(-\mu, \nu) \tilde{\mathcal{T}}_{mn\mu-1\nu-1}^{(jl)pq*}], \end{aligned} \quad (47b)$$

$$\begin{aligned}
\tilde{T}_{mn\mu\nu}^{(j)ppq} = & \frac{1}{2} [f_4(-m, n) \tilde{T}_{m-1n\mu\nu}^{(j)3-pq} - f_5(-m, n) \tilde{T}_{m-1n+1\mu\nu}^{(j)1pq} \\
& - f_6(-m, n) \tilde{T}_{m-1n-1\mu\nu}^{(j)1pq}] [f_4(\mu, \nu) \tilde{\mathcal{X}}_{mn\mu+1\nu}^{(j)1pq*} \\
& + f_5(\mu, \nu) \tilde{\mathcal{X}}_{mn\mu+1\nu+1}^{(j)1pq*} + f_6(\mu, \nu) \tilde{\mathcal{X}}_{mn\mu+1\nu-1}^{(j)1pq*}].
\end{aligned} \quad (47c)$$

The f coefficients in these equations are given by

$$f_1(m, n) = \frac{m}{n(n+1)}, \quad (48a)$$

$$f_2(m, n) = \frac{1}{n+1} \left[\frac{n(n+2)(n-m+1)(n+m+1)}{(2n+1)(2n+3)} \right]^{1/2}, \quad (48b)$$

$$f_3(m, n) = \frac{1}{n} \left[\frac{(n^2-1)(n^2-m^2)}{(2n-1)(2n+1)} \right]^{1/2}, \quad (48c)$$

$$f_4(m, n) = - \frac{[(n-m)(n+m+1)]^{1/2}}{n(n+1)}, \quad (48d)$$

$$\begin{aligned}
f_5(m, n) = & \frac{1}{n+1} \left[\frac{(n+m+1)(n+m+2)}{n(n+2)(2n+1)(2n+3)} \right]^{1/2} \left[m(m+1) \right. \\
& \left. + \frac{(n-m)(n+m+3)}{2} + \frac{(n+m)(n-m+1)}{2} \right],
\end{aligned} \quad (48e)$$

$$\begin{aligned}
f_6(m, n) = & - \frac{1}{n} \left[\frac{(n-m)(n-m-1)}{(n^2-1)(4n^2-1)} \right]^{1/2} \left[m(m+1) \right. \\
& \left. + \frac{(n-m-2)(n+m+1)}{2} + \frac{(n+m)(n-m+1)}{2} \right].
\end{aligned} \quad (48f)$$

When the total particle number $L=1$ in an ensemble, all the results discussed above for both fixed- and random-orientation scatterings reduce to the solution for a single particle. When $L=1$, neither phase shift nor interaction between particles is involved. In this special case, $j \equiv l \equiv 1$, $\tilde{A}_{\omega\nu sn}^{jjqp} = \delta_{\omega s} \delta_{n\nu} \delta_{pq}$ so that $\tilde{T}_{mn\mu\nu}^{(j)1pq} = \tilde{\mathcal{X}}_{mn\mu\nu}^{(j)1pq} = T_{mn\mu\nu}^{pq}$, where $T_{mn\mu\nu}^{pq}$ is the elements of the T matrix \mathbf{T} of a single scatterer. With $\tilde{T}_{mn\mu\nu}^{(j)1pq}$ replaced by $T_{mn\mu\nu}^{pq}$ and $\tilde{\mathcal{X}}_{mn\mu\nu}^{(j)1pq*}$ by $T_{mn\mu\nu}^{pq*}$, Eqs. (38), (42), and (46)–(48) become the formulas for orientation-averaged scattering parameters of a single scatterer. This single-particle solution should be of exactly the same form as the CTM multiparticle solution [5,14,15] with \mathbf{T} understood as the single-particle type cluster T matrix.

III. PUBLIC DOMAIN CODES AND ILLUSTRATIVE EXAMPLES

As the practical implementation of the solution discussed above, several Fortran codes have been developed [31]. These public-domain codes can be used to test the formula-

TABLE I. Comparison of the calculated and measured asymmetry parameters of eight linear chains of identical spheres at a random-orientation average.

L ^a	x ^b	Refractive index	kS ^c	$\langle \cos \theta \rangle$		$\delta\%$ ^d
				Calculated	Measured	
2	2.176	(1.629, 0.0125)	4.352	0.659	0.647	1.8
5	2.176	(1.629, 0.0125)	4.352	0.712	0.677	4.9
2	3.083	(1.610, 0.0040)	6.166	0.689	0.685	0.6
2	3.083	(1.610, 0.0040)	8.030	0.673	0.662	1.6
2	3.083	(1.610, 0.0040)	12.510	0.669	0.658	1.6
3	3.083	(1.610, 0.0040)	6.166	0.725	0.731	0.8
2	4.346	(1.630, 0.0100)	8.692	0.662	0.651	1.7
2	4.346	(1.630, 0.0100)	10.760	0.650	0.619	4.8

^aNumber of spheres in each of the linear chains.

^bSize parameter of a single component sphere.

^c k is the wave number and S is the center-to-center separation distance between each pair of neighboring spheres.

^dRelative deviation calculated by $\delta = |1 - M/C|$, where M is the measured $\langle \cos \theta \rangle$ and C is the calculated $\langle \cos \theta \rangle$.

tions developed here by comparing numerical solutions with laboratory scattering measurements and with numerical solutions obtained from other solution techniques. Practical examples of using the codes and comparison with CTM can be found in Xu and Khlebtsov [22]. A couple of numerical examples are also given below for illustrative purposes.

A. Comparison between theory and experiment

Experimental scrutiny is a powerful means to test scattering solutions. Microwave analog to light scattering measurements are especially suitable for this purpose. As an illustrative example, theoretical predictions for the asymmetry parameter obtained from Eqs. (46)–(48) are compared with laboratory microwave scattering measurements. In the 1980s Wang and Gustafson [29] determined experimentally the orientation-averaged asymmetry parameters of a set of multisphere configurations. Table I lists the physical and geometrical parameters of eight linear sphere chains that Wang and Gustafson measured, each consisting of 2, 3, or 5 identical spheres in various intersphere separations. The scattering by these ensembles of spheres is calculated by using the GMM01TRA.F code [31], which is an implementation of the solution described above. The experimental data and theoretical predictions are also shown in Table I, which indicate that the numerical solutions agree with experimental results. Relative deviations between the theoretical and experimental results are within 5%.

B. Configuration-dependence of scattering properties

Scattering characteristics of an ensemble of particles are largely configuration dependent. Figure 1 is such an example, which refers to an ensemble consisting of only two spheres that have the same size parameter of $ka=1$ but different refractive indices of (1.6, 0.1) and (2.5155, 0.0213). The two spheres are gradually pulled apart, which means that

the overall size of the sphere ensemble gradually increases. Figure 1 shows the random-orientation-averaged volume-equivalent extinction efficiencies and asymmetry parameters as function of the separation-to-diameter ratio S/d , where S is the center-to-center separation distance and d is the diameter of the two spheres. The numerical solutions are obtained from two independent codes. One is GMM code GMM01TRA.F. The other is CTM code SCSMTM1.FOR developed by Mackowski [32]. From the figure we see that both codes provide identical theoretical results in their common region of validity. However, the CTM code fails to work when S/d exceeds ~ 32 , which is the maximum overall dimension that the code can handle.

IV. REMARKS

The solution process of GMM is substantially different from that of CTM starting with the treatment of one of the multiple scattering effects—the far-field interference be-

tween scattered waves from different component particles. The far-field interference is caused by both incident and scattered phase differences with regard to different component particles. GMM deals directly with precise phase relations for both incident and scattered waves, while CTM expresses the phase factors in terms of infinite series expansions. Different theoretical treatments lead to significantly different ways for translating the incident and scattered fields between displaced reference systems.

In CTM, for an ensemble of particles in a given orientation, the total scattering coefficients \check{a}_{mnp} in Eq. (1b) for an arbitrary direction of incidence are given by [14]

$$\check{a}_{mnp} = \sum_{\nu=1}^{N_{\max}} \sum_{\mu=-\nu}^{\nu} \sum_{q=1}^2 T_{mn\mu\nu}^{pq} \check{p}_{\mu\nu q}, \quad (49)$$

where $T_{mn\mu\nu}^{pq}$ are the elements of the cluster T matrix \mathbf{T} defined by $\mathbf{T} = \tilde{\mathbf{A}}^{l0} \mathbf{T}^{jl} \tilde{\mathbf{A}}^{0j}$, i.e.,

$$T_{mn\mu\nu}^{pq} = \sum_{l=1}^L \sum_{j=1}^L \sum_{n'=1}^{N_{\max}^j} \sum_{m'=-n'}^{n'} \sum_{\nu'=1}^{N_{\max}^j} \sum_{\mu'=-\nu'}^{\nu'} \sum_{p'=1}^2 \sum_{q'=1}^2 \tilde{A}_{mnm'n'}^{l0pp'} T_{m'n'\mu'\nu'}^{jlp'q'} \tilde{A}_{\mu'\nu'\mu\nu}^{0jq'q}, \quad (50)$$

and thus

$$\check{a}_{mnp} = \sum_{\nu=1}^{N_{\max}} \sum_{\mu=-\nu}^{\nu} \sum_{q=1}^2 \sum_{l=1}^L \sum_{j=1}^L \sum_{n'=1}^{N_{\max}^j} \sum_{m'=-n'}^{n'} \sum_{p'=1}^2 \sum_{\nu'=1}^{N_{\max}^j} \sum_{\mu'=-\nu'}^{\nu'} \sum_{q'=1}^2 \tilde{A}_{mnm'n'}^{l0pp'} T_{m'n'\mu'\nu'}^{jlp'q'} \tilde{A}_{\mu'\nu'\mu\nu}^{0jq'q} \check{p}_{\mu\nu q}. \quad (51)$$

N_{\max} in Eqs. (49) and (51) required in practical calculations is roughly proportional to the overall size of an ensemble. $\tilde{A}_{\mu'\nu'\mu\nu}^{0jq'q}$ on the right-hand side of Eq. (51) is to translate the incident plane wave from the primary into the reference system j and $\tilde{A}_{mnm'n'}^{l0pp'}$ is to translate the partial scattered field of particle l into the primary reference system. CTM does not use \mathbf{T}^{jl} directly and, instead, transform \mathbf{T}^{jl} into the cluster T matrix \mathbf{T} through the use of two large-dimensional translation matrices of $\tilde{\mathbf{A}}^{0j}$ and $\tilde{\mathbf{A}}^{l0}$. In practical scattering calculations, CTM bypasses the calculation of \mathbf{T}^{jl} . To obtain the cluster T matrix \mathbf{T} for ensembles of homogeneous spheres, Mackowski and Mishchenko [15] use the following linear system to directly calculate $\mathbf{T}^l = \mathbf{T}^{jl} \tilde{\mathbf{A}}^{0j}$ and skip the calculation of \mathbf{T}^{jl} [see Eqs. (63) and (64) in Ref. [15]],

$$T_{mn\mu\nu}^{lpq} = \bar{a}_{np}^l \left[\tilde{A}_{mnm'n'}^{0lpq} + \sum_{l'=1}^L \sum_{n'=1}^{N_{\max}^{l'}} \sum_{m'=-n'}^{n'} \sum_{p'=1}^2 (\delta_{l'l} - 1) \times A_{mnm'n'}^{l'lp'p'} T_{m'n'\mu'\nu'}^{l'p'q} \right]. \quad (52)$$

All \mathbf{T}^l of individual spheres are then translated to the primary reference system to form the single-centered cluster T matrix \mathbf{T} ,

$$T_{mn\mu\nu}^{pq} = \sum_{l'=1}^L \sum_{n'=1}^{N_{\max}^{l'}} \sum_{m'=-n'}^{n'} \sum_{p'=1}^2 \tilde{A}_{mnm'n'}^{l'0pp'} T_{m'n'\mu'\nu'}^{l'p'q}. \quad (53)$$

There is another recursive T -matrix algorithm developed by Wang and Chew [30], which uses a successive transformation method to calculate the cluster T matrix \mathbf{T} . When the single-particle type \mathbf{T} is obtained, an ensemble of particles can be treated as an equivalent single particle and all scattering solutions developed for a single scatterer can be simply used to calculate the scattering properties of an ensemble of particles. As mentioned above, a drawback of this CTM approach is that the dimensions of $\tilde{\mathbf{A}}^{0j}$ and $\tilde{\mathbf{A}}^{l0}$ required in practical scattering calculations depend on translation distances and are proportional to the overall dimension of an ensemble. The use of either one or both of $\tilde{\mathbf{A}}^{0j}$ and $\tilde{\mathbf{A}}^{l0}$ sets a ceiling for the overall size of an ensemble that can be handled in practical calculations. This overall size restriction is not related to the availability of computer memory. Accordingly, the choice of the primary coordinate system in the implementation of CTM is not trivial and cannot be arbitrary.

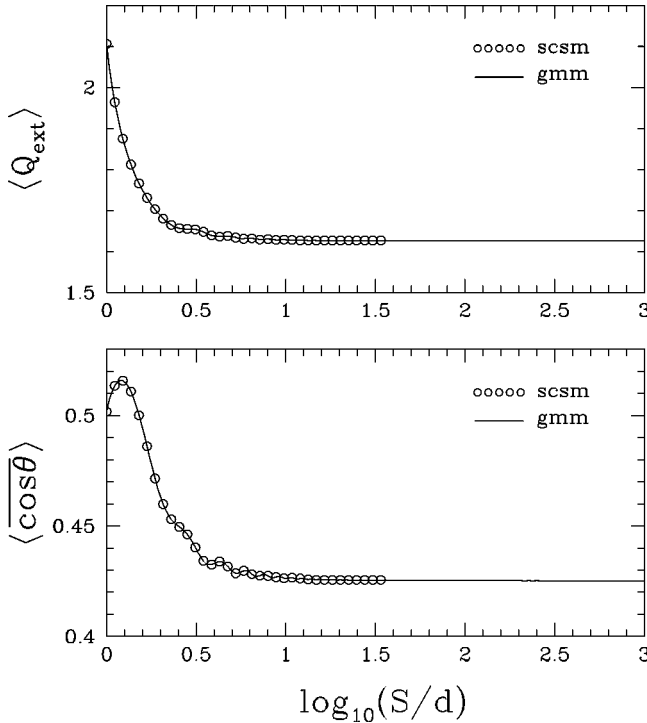


FIG. 1. Variation of random-orientation-averaged extinction efficiency and asymmetry parameter of two spheres of identical size ($ka=1$) with separation-to-diameter ratio S/d (“ S ” is the center-to-center separation distance between spheres and “ d ” is the sphere diameter). Refractive indices of the two spheres are (1.6, 0.1) and (2.5155, 0.0213), respectively. The numerical solutions shown are obtained from two double-precision codes of SCSMTM1.FOR and GMM01TRAF (labeled “scsm” and “gmm”).

It is probably best for CTM to place the primary origin at the geometric center of an ensemble in order to keep the translation distances between the primary and particle centers smallest.

In GMM, the total scattering coefficients \check{a}_{mnp} for far field are given by [17–22]

$$\check{a}_{mnp} = \sum_{l=1}^L \exp[i(\hat{\mathbf{k}} - \hat{\mathbf{r}}) \cdot \mathbf{d}^l] \times \sum_{j=1}^L \sum_{\nu=1}^{N_{\max}^j} \sum_{\mu=-\nu}^{\nu} \sum_{q=1}^2 \exp(i\hat{\mathbf{k}} \cdot \mathbf{d}^{lj}) T_{mn\mu\nu}^{jlpq} \check{p}_{\mu\nu q}, \quad (54)$$

which includes both incident and scattered phase shifts. The incident phase term varies with incident direction and the scattered phase term changes with scattering direction. These phase terms result from the asymptotic spherical Hankel functions valid in the far-field zone, the use of which introduces no approximation to the scattering solutions under discussion [17]. One obvious advantage of this far-field approach is clearly that the primary origin can be arbitrarily placed. The displacement of the primary coordinate system causes no additional computational efforts. Replacing the primary origin does not affect any results and the calculation of the cross sections. Another advantage of GMM is appar-

ently that the field expansion truncations required in practical calculations are associated with individual particle size only and not concerned with the separation distances between particles. In Eq. (54), $T_{mn\mu\nu}^{jlpq} \equiv 0$ whenever $n > N_{\max}^l$ or $\nu > N_{\max}^j$, where N_{\max}^l and N_{\max}^j are determined solely by the sizes of particles l and j , respectively. By comparison between Eqs. (51) and (54) we see that the two large-dimensional translation matrices $\tilde{\mathbf{A}}^{0j}$ and $\tilde{\mathbf{A}}^{l0}$ in Eq. (51) of CTM are, respectively, equivalent to the simple incident and scattered phase terms $\exp[i(\hat{\mathbf{k}} \cdot \mathbf{d}^j)]$ and $\exp[-i(\hat{\mathbf{r}} \cdot \mathbf{d}^l)]$ in Eq. (54) of GMM. In field translations, GMM does not involve the use of the general addition theorems for VSWFs (i.e., the use of either $\tilde{\mathbf{A}}^{0j}$ or $\tilde{\mathbf{A}}^{l0}$). It is thus completely free from CTM’s overall size limitation. GMM expresses all scattering quantities in terms of the T matrix \mathbf{T}^{jl} , unlike CTM that needs to transform \mathbf{T}^{jl} into the cluster T matrix \mathbf{T} . Also, when all separation distances between particles in an ensemble are sufficiently large, all individual particles become independent scattering units and \mathbf{T}^{jl} is block diagonal. In this particular case, GMM automatically reduces to the noninteracting (i.e., independent) scattering solution and requires little computational effort in practical scattering calculations.

It needs to be mentioned that CTM and GMM are both rigorous approaches to the multiparticle scattering in principle. Numerical solutions from both formulations should be identical when both can provide a practical solution. The scattering formulations of GMM should be of exactly the same form of CTM when $L=1$, i.e., for a single particle. Some of the GMM formulations can also be obtained within the framework of CTM. For example, Eqs. (38) and (42) for $\langle C_{\text{ext}} \rangle$ and $\langle C_{\text{sca}} \rangle$ can be derived from CTM by simply applying the identity of $\tilde{A}_{\mu\nu mn}^{ljqp} = \tilde{A}_{\mu\nu m'n'}^{0jqp'}$, $\tilde{A}_{m'n' mn}^{l0p'p}$ and eliminating $\tilde{\mathbf{A}}^{0j}$ and $\tilde{\mathbf{A}}^{l0}$, as shown by Mackowski [14]. However, since the solution processes of CTM and GMM are radically different, CTM is unable to turn all scattering formulas to the GMM type. Also, an important point is that the GMM type of \mathbf{T}^{jl} -based formulations have never been effectively used, because there was no efficient scheme available for obtaining \mathbf{T}^{jl} before. The direct matrix inversion is of limited use in practical scattering calculations. By using the linear system of Eq. (23), \mathbf{T}^{jl} can be solved efficiently and the practical application of the GMM-type \mathbf{T}^{jl} -based formulations becomes generally feasible. With \mathbf{T}^{jl} solved for an arbitrary ensemble of particles, even the cluster T matrix \mathbf{T} can also be easily obtained through Eq. (50).

It also needs to be emphasized that this work concentrates on far-field solution and does not address the near-field calculations, which are beyond the scope of this article.

V. SUMMARY

A far-field solution of GMM has been extended to the general case of an arbitrary mixture of particles of different shapes for either fixed- or random-orientation scattering. This solution places no restriction on the overall dimension for an ensemble of particles in practical applications. It does not require the use of general addition theorems for VSWFs

in field translations. Field-expansion truncations depend on individual particle size only. The choice of the primary reference center can be arbitrary and it does not need to be close to the geometric center of an ensemble. The displacement of

the primary reference system has no effect on scattering calculations. The kernel quantity in the T -matrix formulation of GMM is the T matrix \mathbf{T}^{jl} . An efficient scheme has been devised to solve \mathbf{T}^{jl} effectively.

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