Chapter 6

T-Matrix Method and Its Applications

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I. INTRODUCTION

The T-matrix method was initially introduced by Waterman (1965, 1971) as a technique for computing electromagnetic scattering by single, homogeneous nonspherical particles based on the Huygens principle (otherwise known as the extended boundary condition, Schelkunoff equivalent current method, Ewald–Oseen extinction theorem, and null-field method). However, the meant-to-be auxiliary concept of expanding the incident and the scattered waves in vector spherical wave functions (VSWFs) and relating these expansions by means of a T matrix has proved to be extremely powerful by itself and has dramatically expanded the realm of the T-matrix approach. The latter now includes electromagnetic, acoustic, and elastodynamic wave scattering by single and compounded scatterers, multiple scattering in discrete random media, and scattering by gratings and periodically rough surfaces (Varadan and Varadan, 1980; Tsang *et al.*, 1985; Varadan *et al.*, 1988).

At present, the T-matrix approach is one of the most powerful and widely used tools for rigorously computing electromagnetic scattering by single and compounded nonspherical particles. In many applications it compares favorably with other frequently used techniques in terms of efficiency, accuracy, and size parameter range and is the only method that has been used in systematic surveys of nonspherical scattering based on calculations for thousands of particles in random orientation. Recent improvements have made this method applicable to size parameters exceeding 100 and, therefore, suitable for checking the accuracy of the geometric optics approximation and its modifications at lower frequencies.

In this chapter, we review the current status of the T-matrix approach and its various applications. The chapter is composed of seven sections. The following section introduces the general concept of the T-matrix approach in application to an arbitrary nonspherical particle, either single or composite. Section III describes an efficient analytical method for computing orientation-averaged scattering characteristics for ensembles of nonspherical particles based on exploiting the rotational properties of VSWFs. In Section IV we consider the standard scheme for computing the T matrix for single scatterers, either homogeneous or layered, and discuss special techniques for improving the numerical stability of T-matrix computations for particles that are much larger than a wavelength and/or have large aspect ratios. Section V introduces the superposition T-matrix method for computing electromagnetic scattering by aggregated particles based on the translation addition theorem for VSWFs. Section VI briefly describes public-domain T-matrix codes available on the World Wide Web and discusses their ranges of applicability. The concluding section reviews multiple practical applications of the T-matrix approach.

II. THE *T*-MATRIX APPROACH

Consider scattering of a plane electromagnetic wave by a single particle, as discussed in Section IV of Chapter 1, and expand the incident and scattered fields in VSWFs as follows:

$$\mathbf{E}^{\text{inc}}(\mathbf{R}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[a_{mn} \operatorname{Rg} \mathbf{M}_{mn}(k\mathbf{R}) + b_{mn} \operatorname{Rg} \mathbf{N}_{mn}(k\mathbf{R})\right], \tag{1}$$

$$\mathbf{E}^{\text{sca}}(\mathbf{R}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[p_{mn} \mathbf{M}_{mn}(k\mathbf{R}) + q_{mn} \mathbf{N}_{mn}(k\mathbf{R})\right], \qquad R > R_{>}, \tag{2}$$

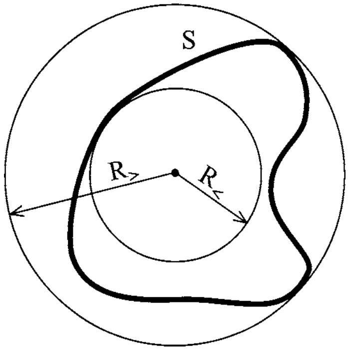

Figure 1 Cross section of a general scattering object bounded by a closed surface S. $R_>$ is the radius of the smallest circumscribed sphere and $R_<$ is the radius of a concentric inscribed sphere.

where

$$\mathbf{M}_{mn}(k\mathbf{R}) = (-1)^m d_n h_n^{(1)}(kR)\mathbf{C}_{mn}(\vartheta)\exp(im\varphi), \tag{3}$$

$$\mathbf{N}_{mn}(k\mathbf{R}) = (-1)^m d_n \left\{ \frac{n(n+1)}{kR} h_n^{(1)}(kR)\mathbf{P}_{mn}(\vartheta) + \frac{1}{kR}\left[kRh_n^{(1)}(kR)\right]'\mathbf{B}_{mn}(\vartheta) \right\} \exp(im\varphi), \tag{4}$$

$$\mathbf{B}_{mn}(\vartheta) = \boldsymbol{\vartheta}\frac{d}{d\vartheta}d_{0m}^n(\vartheta) + \boldsymbol{\varphi}\frac{im}{\sin\vartheta}d_{0m}^n(\vartheta), \tag{5}$$

$$\mathbf{C}_{mn}(\vartheta) = \boldsymbol{\vartheta}\frac{im}{\sin\vartheta}d_{0m}^n(\vartheta) - \boldsymbol{\varphi}\frac{d}{d\vartheta}d_{0m}^n(\vartheta), \tag{6}$$

$$\mathbf{P}_{mn}(\vartheta) = \mathbf{R}\frac{d_{0m}^n(\vartheta)}{R}, \tag{7}$$

$$d_n = \left[\frac{2n+1}{4\pi n(n+1)}\right]^{1/2}, \tag{8}$$

$k = 2\pi/\lambda$ is the wavenumber, λ is the wavelength in the surrounding medium, $R_>$ is the radius of the smallest circumscribing sphere of the scattering particle centered at the origin of the coordinate system (Fig. 1), and $d_{lm}^n(\vartheta)$ are Wigner d functions (Varshalovich *et al.*, 1988) given by

$$d_{lm}^n(\vartheta) = A_{lm}^n(1-\cos\vartheta)^{(l-m)/2}(1+\cos\vartheta)^{-(l+m)/2} \times \frac{d^{n-m}}{(d\cos\vartheta)^{n-m}}\left[(1-\cos\vartheta)^{n-l}(1+\cos\vartheta)^{n+l}\right] \tag{9}$$

for $n \geq n_* = \max(|l|, |m|)$ and by $d^n_{lm}(\vartheta) = 0$ for $n < n_*$. In Eq. (9),

$$A^n_{lm} = \frac{(-1)^{n-m}}{2^n}\left[\frac{(n+m)!}{(n-l)!(n+l)!(n-m)!}\right]^{1/2}. \tag{10}$$

The d functions can be expressed in terms of generalized spherical functions as follows (Hovenier and van der Mee, 1983):

$$d^n_{lm}(\vartheta) = i^{m-l} P^n_{lm}(\cos\vartheta). \tag{11}$$

The expressions for the functions $\mathrm{Rg}\,\mathbf{M}_{mn}$ and $\mathrm{Rg}\,\mathbf{N}_{mn}$ can be obtained from Eqs. (3) and (4) by replacing spherical Hankel functions $h^{(1)}_n$ by spherical Bessel functions j_n. Note that the functions $\mathrm{Rg}\,\mathbf{M}_{mn}$ and $\mathrm{Rg}\,\mathbf{N}_{mn}$ are regular at the origin, while the use of the outgoing functions $\mathbf{M}_{mn}$ and $\mathbf{N}_{mn}$ in the expansion of Eq. (2) ensures that the scattered field satisfies the radiation condition at infinity (i.e., the transverse component of the scattered electric field decays as $1/R$, whereas the radial component decays faster than $1/R$ with $R \to \infty$). The requirement $R > R_>$ in Eq. (2) means that the scattered field is considered only outside the smallest circumscribing sphere of the scatterer (Fig. 1). The so-called Rayleigh hypothesis (e.g., Bates, 1975; Paulick, 1990) assumes that the scattered field can be expanded in outgoing waves not only in the outside region, but also in the region between the particle surface and the circumscribing sphere (Fig. 1). Because the range of applicability of this hypothesis is still unknown and is in fact questionable, as recent results by Videen *et al.* (1996) and Ngo *et al.* (1997) seem to indicate, the requirement $R > R_>$ in Eq. (2) is important in order to make sure that the Rayleigh hypothesis is not implicitly used (Lewin, 1970).

The expansion coefficients of the plane incident wave are given by the following simple analytical formulas (Tsang *et al.*, 1985, Chapter 3; Eq. (1) of Chapter 1):

$$a_{mn} = 4\pi(-1)^m i^n d_n \mathbf{C}^*_{mn}(\vartheta^{\mathrm{inc}})\mathbf{E}^{\mathrm{inc}}_0 \exp(-im\varphi^{\mathrm{inc}}), \tag{12}$$

$$b_{mn} = 4\pi(-1)^m i^{n-1} d_n \mathbf{B}^*_{mn}(\vartheta^{\mathrm{inc}})\mathbf{E}^{\mathrm{inc}}_0 \exp(-im\varphi^{\mathrm{inc}}), \tag{13}$$

where an asterisk indicates complex conjugation. Owing to the linearity of Maxwell's equations and boundary conditions, the relation between the scattered field coefficients p_{mn} and q_{mn} on the one hand and the incident field coefficients a_{mn} and b_{mn} on the other hand must be linear and is given by a transition (or T matrix) $\mathbf{T}$ as follows (Waterman, 1971; Tsang *et al.*, 1985, Chapter 3):

$$p_{mn} = \sum_{n'=1}^{\infty}\sum_{m'=-n'}^{n'}\left[T^{11}_{mnm'n'}a_{m'n'} + T^{12}_{mnm'n'}b_{m'n'}\right], \tag{14}$$

$$q_{mn} = \sum_{n'=1}^{\infty}\sum_{m'=-n'}^{n'}\left[T^{21}_{mnm'n'}a_{m'n'} + T^{22}_{mnm'n'}b_{m'n'}\right]. \tag{15}$$

In compact matrix notation, Eqs. (14) and (15) can be rewritten as

$$\begin{bmatrix} \mathbf{p} \\ \mathbf{q} \end{bmatrix} = \mathbf{T} \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} = \begin{bmatrix} \mathbf{T}^{11} & \mathbf{T}^{12} \\ \mathbf{T}^{21} & \mathbf{T}^{22} \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}. \tag{16}$$

Equation (16) forms the basis of the T-matrix approach. Indeed, if the T matrix for a given scatterer is known, Eqs. (14), (15), (12), (13), and (2) give the scattered field and, thus, the amplitude matrix appearing in Eq. (4) of Chapter 1. Specifically, making use of the large argument asymptotic for spherical Hankel functions,

$$h_n^{(1)}(kR) \simeq \frac{(-1)^{n+1}\exp(ikR)}{kR}, \qquad kR \gg n^2, \tag{17}$$

we easily derive in dyadic notation

$$\begin{aligned} &\mathbf{S}\left(\mathbf{n}^{\text{sca}}, \mathbf{n}^{\text{inc}}\right) \\ &\quad = \frac{4\pi}{k} \sum_{nmn'm'} i^{n'-n-1}(-1)^{m+m'} d_n d_{n'} \exp\left[i\left(m\varphi^{\text{sca}} - m'\varphi^{\text{inc}}\right)\right] \\ &\qquad \times \Big\{\left[T^{11}_{mnm'n'}\mathbf{C}_{mn}\left(\vartheta^{\text{sca}}\right) + T^{21}_{mnm'n'} i\mathbf{B}_{mn}\left(\vartheta^{\text{sca}}\right)\right]\mathbf{C}^*_{m'n'}\left(\vartheta^{\text{inc}}\right) \\ &\qquad\quad + \left[T^{12}_{mnm'n'}\mathbf{C}_{mn}\left(\vartheta^{\text{sca}}\right) + T^{22}_{mnm'n'} i\mathbf{B}_{mn}\left(\vartheta^{\text{sca}}\right)\right]\mathbf{B}^*_{m'n'}\left(\vartheta^{\text{inc}}\right)/i\Big\}. \end{aligned} \tag{18}$$

Knowledge of the amplitude matrix allows one to compute any scattering characteristic introduced in Chapter 1.

A fundamental feature of the T-matrix approach is that the T matrix depends only on the physical and geometrical characteristics of the scattering particle (refractive index, size, shape, and orientation with respect to the reference frame) and is completely independent of the incident and scattered fields. This means that the T matrix need be computed only once and then can be used in calculations for any directions of incidence and scattering and for any polarization state of the incident field.

Using Eq. (18) and the reciprocity relation for the amplitude matrix [Eq. (44) of Chapter 1], we derive the following general symmetry relation for the T-matrix elements:

$$T^{kl}_{mnm'n'} = (-1)^{m+m'} T^{lk}_{-m'n'-mn}, \qquad k, l = 1, 2. \tag{19}$$

Energy conservation leads to another important property of the T matrix:

$$\sum_{ln_1m_1} \left(T^{lp}_{m_1n_1mn}\right)^* T^{lq}_{m_1n_1m'n'} \le -\frac{1}{2}\left[\left(T^{qp}_{m'n'mn}\right)^* + T^{pq}_{mnm'n'}\right]. \tag{20}$$

The equality holds only for nonabsorbing particles and is called the unitarity property (Tsang *et al.*, 1985, Chapter 3). These relations are helpful in practice for checking the numerical accuracy of computing the T matrix.

It is useful to note that the VSWFs defined by Eqs. (3) and (4) are not the only possible class of expansion functions. Other classes of expansion functions resulting in somewhat different T matrices have been used (e.g., Waterman, 1971; Barber and Yeh, 1975; Ström and Zheng, 1987). We use the VSWFs defined by Eqs. (3) and (4) because their convenient analytical properties greatly simplify mathematical derivations. Note also that Eqs. (5)–(7) are often written in terms of associated Legendre functions $P_n^m(\cos\vartheta) = (-1)^m[(n+m)!/(n-m)!]^{1/2} d_{0m}^n(\vartheta)$ (e.g., Tsang *et al.*, 1985, Chapter 3). It is well known, however, that the numerical computation of associated Legendre functions via recurrence formulas becomes highly unstable for large n and m, whereas recurrence formulas for Wigner d functions (e.g., Varshalovich *et al.*, 1988) remain quite stable and provide accurate results.

III. ANALYTICAL AVERAGING OVER ORIENTATIONS

An essential feature of the T-matrix approach is analyticity of its mathematical formulation. Indeed, the analytical properties of the special functions involved are well known and can be used to derive general properties of the T matrix and also to analytically average scattering characteristics over particle orientations. The latter feature is particularly important because, in most practical circumstances, particles are distributed over a range of orientations rather than being perfectly aligned.

To derive the rotation transformation rule for the T matrix, consider a laboratory (L) and a particle (P) coordinate system having a common origin inside the scattering particle. Let α, β, and γ be Euler angles of rotation that transform the laboratory coordinate system into the particle coordinate system (Section III of Chapter 1) and let $(kR, \vartheta_L, \varphi_L)$ and $(kR, \vartheta_P, \varphi_P)$ be the spherical coordinates of the same radius vector $k\mathbf{R}$ in the two coordinate systems, respectively. We then have

$$\mathbf{M}_{mn}(kR, \vartheta_P, \varphi_P) = \sum_{m'=-n}^{n} D_{m'm}^n(\alpha, \beta, \gamma)\mathbf{M}_{m'n}(kR, \vartheta_L, \varphi_L), \qquad (21)$$

$$\mathbf{M}_{mn}(kR, \vartheta_L, \varphi_L) = \sum_{m'=-n}^{n} \left[D_{mm'}^n(\alpha, \beta, \gamma)\right]^* \mathbf{M}_{m'n}(kR, \vartheta_P, \varphi_P), \qquad (22)$$

where

$$D^n_{m'm}(\alpha, \beta, \gamma) = \exp(-im'\alpha) d^n_{m'm}(\beta) \exp(-im\gamma) \tag{23}$$

are Wigner D functions (Varshalovich *et al.*, 1988). Analogous expansions hold for the functions $\mathbf{N}_{mn}$, Rg $\mathbf{M}_{mn}$, and Rg $\mathbf{N}_{mn}$. Let $\mathbf{T}(P)$ and $\mathbf{T}(L)$ be the T matrices of the particle with respect to the coordinate systems P and L, respectively. Taking into account Eqs. (1), (2), (14), (15), (21), and (22), we derive (Varadan, 1980)

$$T^{kl}_{mnm'n'}(L) = \sum_{m_1=-n}^{n} \sum_{m_2=-n'}^{n'} \left[D^{n'}_{m'm_2}(\alpha, \beta, \gamma)\right]^* T^{kl}_{m_1 n m_2 n'}(P) D^n_{mm_1}(\alpha, \beta, \gamma), \quad k, l = 1, 2. \tag{24}$$

If we now assume that the T matrix $\mathbf{T}(P)$ is already known and use the Euler angles of rotation α, β, and γ to specify the orientation of the particle with respect to the laboratory coordinate system, then Eq. (24) gives the particle T matrix in the laboratory coordinate system. Therefore, Eqs. (18) and (24) are ideally suited for computing orientationally averaged scattering characteristics using a single precalculated $\mathbf{T}(P)$ matrix (Tsang *et al.*, 1985, Chapter 3).

Note that for particles with special symmetries, a proper choice of the particle coordinate system can substantially simplify the T-matrix calculations. For example, for rotationally symmetric particles, it is convenient to direct the z axis of the particle coordinate system along the axis of symmetry. In this case, the $\mathbf{T}(P)$ matrix becomes diagonal with respect to azimuthal indices m and m',

$$T^{kl}_{mnm'n'}(P) = \delta_{mm'} T^{kl}_{mnmn'}(P), \tag{25}$$

where $\delta_{mm'}$ is the Kronecker delta, and also has the property

$$T^{kl}_{mnmn'}(P) = (-1)^{k+l} T^{kl}_{-mn-mn'}(P). \tag{26}$$

Other possible symmetries of the T matrix are discussed by Schulz *et al.* (1999a). The T matrix becomes especially simple for spherically symmetric particles, in which case we have for any coordinate system:

$$T^{11}_{mnm'n'} = -\delta_{nn'} b_n, \tag{27}$$

$$T^{22}_{mnm'n'} = -\delta_{nn'} a_n, \tag{28}$$

$$T^{12}_{mnm'n'} = T^{21}_{mnm'n'} \equiv 0, \tag{29}$$

where a_n and b_n are the well-known Lorenz–Mie coefficients for homogeneous spheres or their analogs for radially inhomogeneous spheres (Bohren and Huffman, 1983, Chapters 4 and 8). Moreover, in the case of spherically symmetric particles all formulas of the T-matrix approach become identical to the corresponding Lorenz–Mie formulas. Therefore, the T-matrix approach can be considered an extension of the Lorenz–Mie theory to particles without spherical symmetry.

Equation (24) can be used to develop analytical procedures for averaging scattering characteristics over particle orientations. In the practically important case of randomly oriented particles, all particle orientations are equiprobable, and the orientation distribution function $p_o(\alpha, \beta, \gamma)$ is equal to $(8\pi^2)^{-1}$ [Eq. (54) of Chapter 1]. Therefore, using Eq. (24) and the orthogonality property of Wigner D functions (Varshalovich *et al.*, 1988),

$$\begin{aligned}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma\, D^n_{mm'}(\alpha, \beta, \gamma)\big[D^{n'}_{m_1 m'_1}(\alpha, \beta, \gamma)\big]^* \\ = \frac{8\pi^2}{2n+1}\delta_{nn'}\delta_{mm_1}\delta_{m'm'_1}, \qquad (30)\end{aligned}$$

we derive for the orientation-averaged T matrix

$$\begin{aligned}\big\langle T^{kl}_{mnm'n'}\big\rangle &= \frac{1}{8\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma\, T^{kl}_{mnm'n'}(L) \\ &= \frac{1}{2n+1}\delta_{mm'}\delta_{nn'} \sum_{m_1=-n}^{n} T^{kl}_{m_1 n m_1 n}(P), \qquad k, l = 1, 2. \qquad (31)\end{aligned}$$

As a result, we obtain the following general formula for the extinction cross section of randomly oriented particles (Mishchenko, 1991b):

$$\begin{aligned}\langle C_{\mathrm{ext}}\rangle &= \frac{2\pi}{k}\,\mathrm{Im}\big[\langle S_{11}(\mathbf{n}, \mathbf{n})\rangle + \langle S_{22}(\mathbf{n}, \mathbf{n})\rangle\big] \\ &= -\frac{2\pi}{k^2}\,\mathrm{Re}\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\sum_{k=1}^{2} T^{kk}_{mnmn}(P). \qquad (32)\end{aligned}$$

A similar but less simple formula was derived by Borghese *et al.* (1984). Because the choice of the particle coordinate system is arbitrary, we can conclude that the orientation-averaged extinction cross section is proportional to the real part of the trace of the T matrix computed in an arbitrary reference frame. An equally simple formula can be derived for the scattering cross section of randomly oriented particles (Mishchenko, 1991a; Khlebtsov, 1992):

$$\langle C_{\mathrm{sca}}\rangle = \frac{2\pi}{k^2}\sum_{n=1}^{\infty}\sum_{n'=1}^{\infty}\sum_{m=-n}^{n}\sum_{m'=-n'}^{n'}\sum_{k=1}^{2}\sum_{l=1}^{2}\big|T^{kl}_{mnm'n'}(P)\big|^2. \qquad (33)$$

The orientation-averaged extinction and scattering cross sections must be invariant with respect to the choice of the coordinate system. And indeed, using

Eq. (24) and the unitarity property of Wigner D functions (Varshalovich *et al.*, 1988),

$$\sum_{m''=-n}^{n} \left[D^{n}_{m''m}(\alpha,\beta,\gamma)\right]^{*} D^{n}_{m''m'}(\alpha,\beta,\gamma) = \delta_{mm'}, \tag{34}$$

we derive the following two general invariants:

$$\sum_{m} T^{kl}_{mnmn}(L) = \sum_{m} T^{kl}_{mnmn}(P), \tag{35}$$

$$\sum_{mm'} \left|T^{kl}_{mnm'n'}(L)\right|^{2} = \sum_{mm'} \left|T^{kl}_{mnm'n'}(P)\right|^{2}, \qquad k,l = 1,2. \tag{36}$$

Energy conservation requires that the orientation-averaged extinction cross section always be larger than or equal to the orientation-averaged scattering cross section. Therefore, the elements of the T matrix computed in an arbitrary reference frame must satisfy the partial inequality [cf. Eqs. (32), (33), (35), and (36)]

$$\sum_{nn'mm'kl} \left|T^{kl}_{mnm'n'}(P)\right|^{2} \le -\mathrm{Re} \sum_{nmk} T^{kk}_{mnmn}(P), \tag{37}$$

where the equality holds only for lossless particles. It is easy to show that this partial inequality is consistent with Eq. (20).

Computation of the elements of the scattering matrix given by Eq. (61) of Chapter 1 requires orientation averaging of products of amplitude matrix elements. This problem was addressed by Mishchenko (1991a) for the case of rotationally symmetric particles, that is, when Eqs. (25) and (26) apply. His approach is based on exploiting the Clebsch–Gordan expansion

$$d^{n}_{mm'}(\beta) d^{n'}_{m_1m'_1}(\beta) = \sum_{n_1=|n-n'|}^{n+n'} C^{n_1 m+m_1}_{nmn'm_1} C^{n_1 m'+m'_1}_{nm'n'm'_1} d^{n_1}_{m+m_1,\, m'+m'_1}(\beta) \tag{38}$$

and the orthogonality relation

$$\int_0^{\pi} d\beta \sin\beta \, d^{n}_{mm'}(\beta) d^{n'}_{mm'}(\beta) = \delta_{nn'} \frac{2}{2n+1}, \tag{39}$$

where C^{ij}_{klmn} are the well-known Clebsch–Gordan coefficients, which can be efficiently computed using the recurrence formulas listed by Varshalovich *et al.* (1988). Furthermore, instead of directly computing the scattering matrix elements, Mishchenko (1991a) first computed the expansion coefficients appearing in Eqs. (72)–(77) of Chapter 1. Because both the expansion coefficients and the $\mathbf{T}(P)$ matrix elements are independent of the directions and polarization states of the incident and scattered beams, one may expect a direct relationship between these two sets of quantities that does not involve any angular variables. And indeed, Mishchenko (1991a) derived simple analytical formulas directly expressing the expansion coefficients of Eqs. (72)–(77) of Chapter 1 in the elements of the $\mathbf{T}(P)$ matrix. As a result, the computation of the highly complicated angular structure of light scattered by a nonspherical particle in a fixed orientation (Section V of Chapter 2) with further numerical integration over orientations is avoided, thereby making the analytical averaging method very accurate and fast. The most time-consuming part in any computations based on the T-matrix method is evaluation of multiple nested summations, and an important advantage of the analytical approach is that the maximal order of nested summations involved is only three. This makes the analytical approach ideally suited to developing an efficient computer code (Section VI). Direct comparisons of the analytical method and the straightforward averaging procedure using numerical angular integrations over particle orientations (Wiscombe and Mugnai, 1986; Barber and Hill, 1990; Sid'ko *et al.*, 1990) have shown that the former is faster by a factor of several tens (Mishchenko, 1991a; W. M. F. Wauben, personal communication).

Mackowski and Mishchenko (1996) extended the analytical approach to randomly oriented particles lacking rotational symmetry. Khlebtsov (1992) and Fucile *et al.* (1993) studied the same problem but did not use the idea of expanding the scattering matrix elements in generalized spherical functions.

Mishchenko (1991b, 1992a) considered the problem of computing the extinction matrix for nonspherical particles axially oriented by an external force. An orientation distribution function symmetric with respect to the z axis of the laboratory reference frame is given by Eq. (55) of Chapter 1, which, along with Eqs. (24) and (38), leads to a simple formula for the orientationally averaged T matrix in the laboratory frame:

$$\begin{aligned}
&\left\langle T^{kl}_{mnm'n'}(L)\right\rangle \\
&\quad = \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta\, \sin\beta \int_0^{2\pi} d\gamma\, T^{kl}_{mnm'n'}(L;\alpha,\beta,\gamma)\, p_{\mathrm{o}}(\alpha,\beta,\gamma) \\
&\quad = \delta_{mm'} \sum_{m_1=-M}^{M} \sum_{n_1=|n-n'|}^{n+n'} (-1)^{m+m_1} p_{n_1} C^{n_1 0}_{nmn'-m} C^{n_1 0}_{nm_1n'-m_1} T^{kl}_{m_1nm_1n'}(P), \quad (40)
\end{aligned}$$

where $M = \min(n, n')$ and

$$p_n = \int_0^{\pi} d\beta \sin\beta\; p(\beta) d^n_{00}(\beta) \quad (41)$$

are coefficients in the expansion of the function $p(\beta)$ in Legendre polynomials:

$$p(\beta) = \sum_{n=0}^{\infty} \frac{2n+1}{2} p_n P_n(\cos\beta). \quad (42)$$

Equations (18) and (40) along with the optical theorem, Eqs. (35)–(41) of Chapter 1, provide a fast and accurate method for computing the ensemble-averaged extinction matrix with respect to the laboratory frame. Equation (40) was later rederived by Fucile *et al.* (1995).

The analytical orientation-averaging approach for randomly and axially oriented nonspherical particles was straightforwardly extended by Paramonov (1995) to arbitrary quadratically integrable orientation distribution functions. Unfortunately, the resulting formulas involve highly nested summations, and their efficient numerical implementation may be problematic. In this case, the standard averaging approach employing numerical integrations over orientation angles may prove to be more efficient. This approach was described by Wiscombe and Mugnai (1986), Barber and Hill (1990), and Vivekanandan *et al.* (1991) and is based on the equivalence of averaging over particle orientations and averaging over directions of light incidence and scattering and the fact that knowledge of the $\mathbf{T}(P)$ matrix enables computations of the amplitude matrix for any direction of light incidence and scattering with respect to the particle coordinate system, Eq. (18).

IV. COMPUTATION OF THE T MATRIX FOR SINGLE PARTICLES

The standard scheme for computing the T matrix for single homogeneous scatterers in the particle reference frame is called the extended boundary condition method (EBCM) and is based on the vector Huygens principle (Waterman, 1971). The general problem is to find the field scattered by an object bounded by a closed surface S (Fig. 1). The Huygens principle establishes the following relationship between the incident field $\mathbf{E}^{\mathrm{inc}}(\mathbf{R})$, the total external field $\mathbf{E}(\mathbf{R})$ (i.e., the sum of the incident and the scattered fields), and the surface field on the exterior of S:

$$\left.\begin{matrix}\mathbf{E}(\mathbf{R})\\ 0\end{matrix}\right\} = \mathbf{E}^{\mathrm{inc}}(\mathbf{R}) + \text{ integral over } S, \qquad \mathbf{R}\left\{\begin{matrix}\text{outside } S\\ \text{inside } S,\end{matrix}\right. \tag{43}$$

where the integral term involves the unknown surface field on the exterior of S. The gist of the numerical procedure is to find the surface field on the exterior of S by applying Eq. (43) to points inside S and then to use this surface field to compute the integral term on the right-hand side of Eq. (43) for points outside S, that is, the scattered field.

In more technical terms, the incident and the scattered waves are expanded in regular and outgoing VSWFs, respectively, according to Eqs. (1) and (2). The convergence of the expansion of Eq. (1) is guaranteed inside an inscribed sphere with radius $R_<$, whereas Eq. (2) is strictly valid only for points outside the circumscribing sphere. The internal field can also be expanded in VSWFs regular at the origin:

$$\mathbf{E}^{\text{int}}(\mathbf{R}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[c_{mn} \operatorname{Rg} \mathbf{M}_{mn}(\mathrm{m}k\mathbf{R}) + d_{mn} \operatorname{Rg} \mathbf{N}_{mn}(\mathrm{m}k\mathbf{R}) \right], \quad \mathbf{R} \text{ inside } S, \tag{44}$$

where m is the refractive index of the particle relative to that of the surrounding medium. Via boundary conditions, the surface field on the exterior of S can be expressed in the surface field on the interior of S. The latter is given by Eq. (44). As a result, the application of Eqs. (1), (43), and (44) to points with $R < R_<$ gives a matrix equation

$$\begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} = \begin{bmatrix} \mathbf{Q}^{11} & \mathbf{Q}^{12} \\ \mathbf{Q}^{21} & \mathbf{Q}^{22} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}, \tag{45}$$

in which the elements of the $\mathbf{Q}$ matrix are simple surface integrals of products of VSWFs that depend only on the particle size, shape, and refractive index. Inversion of this matrix equation expresses the unknown expansion coefficients of the internal field $\mathbf{c}$ and $\mathbf{d}$ in the known expansion coefficients of the incident field $\mathbf{a}$ and $\mathbf{b}$. Analogously, the application of boundary conditions and Eq. (44) to the integral term on the right-hand side of Eq. (43) for points with $R > R_>$ and using Eq. (2) gives the following matrix expression:

$$\begin{bmatrix} \mathbf{p} \\ \mathbf{q} \end{bmatrix} = - \begin{bmatrix} \operatorname{Rg} \mathbf{Q}^{11} & \operatorname{Rg} \mathbf{Q}^{12} \\ \operatorname{Rg} \mathbf{Q}^{21} & \operatorname{Rg} \mathbf{Q}^{22} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}, \tag{46}$$

where the elements of the $\operatorname{Rg} \mathbf{Q}$ matrix are also given by simple integrals over the particle surface and depend only on the particle characteristics. By comparing Eqs. (16), (45), and (46), we obtain

$$\mathbf{T} = -\operatorname{Rg} \mathbf{Q}\mathbf{Q}^{-1}. \tag{47}$$

Finally, Eq. (16) gives the expansion coefficients of the scattered field and, thus, the scattered field itself.

General formulas for computing the matrices $\mathbf{Q}$ and $\operatorname{Rg} \mathbf{Q}$ for particles of an arbitrary shape are given by Tsang *et al.* (1985, Chapter 3). These formulas become much simpler for rotationally symmetric particles provided that the z axis of the particle coordinate system coincides with the axis of particle symmetry [pages 187 and 188 of Tsang *et al.* (1985); cf. Eqs. (25) and (26)]. This simplicity explains why nearly all numerical results computed with EBCM pertain to bodies of revolution. However, several successful attempts have been made to apply EBCM to scatterers lacking rotational symmetry such as triaxial ellipsoids (Schneider and Peden, 1988; Schneider *et al.*, 1991) and cubes (Wriedt and Doicu, 1998; Wriedt and Comberg, 1998; Laitinen and Lumme, 1998). Peterson and Ström (1974) (see also Bringi and Seliga, 1977a; Wang and Barber, 1979) extended EBCM to layered scatterers, while Lakhtakia *et al.* (1985b) and Lakhtakia (1991) applied EBCM to light scattering by chiral particles embedded in an achiral isotropic or chiral host medium.

Alternative derivations and formulations of EBCM are discussed by Ström (1975), Barber and Yeh (1975), Agarwal (1976), Bates and Wall (1977), and Morita (1979). The derivation given by Waterman (1979) is especially simple and makes it quite clear that EBCM is not based on the Rayleigh hypothesis, and that scattering objects need not be convex and close to spherical in order to ensure the validity of EBCM. It is interesting that EBCM can in fact be derived from the Rayleigh hypothesis (Burrows, 1969; Bates, 1975; Chew, 1990, Section 8.5; Schmidt *et al.*, 1998). This does not mean, however, that EBCM is equivalent to the Rayleigh hypothesis or requires it to be valid (Lewin, 1970). The equivalence of the two approaches would follow from a reciprocal derivation of the Rayleigh hypothesis from EBCM, but this has not been done so far.

A serious practical difficulty with EBCM is the poor numerical stability of calculations for particles with very large real and/or imaginary parts of the refractive index, large sizes compared with a wavelength, and/or extreme geometries such as spheroids with large axial ratios. The origin of this problem can be explained as follows. Although the expansions of Eqs. (1) and (2) are, in general, infinite, in practical computer calculations they must be truncated to a finite maximum size. This size depends on the required accuracy of computations and is found by increasing the size of the $\mathbf{Q}$ and $\mathrm{Rg}\,\mathbf{Q}$ matrices in unit steps until an accuracy criterion is satisfied. Unfortunately, different elements of the $\mathbf{Q}$ matrix can differ by many orders of magnitude, thus making the numerical calculation of the inverse matrix $\mathbf{Q}^{-1}$ an ill-conditioned process strongly influenced by round-off errors. The ill-conditionality means that even small numerical errors in the computed elements of the $\mathbf{Q}$ matrix can result in large errors in the elements of the inverse matrix $\mathbf{Q}^{-1}$. The round-off errors become increasingly significant with increasing particle size parameter and/or aspect ratio and rapidly accumulate with increasing size of the $\mathbf{Q}$ matrix. As a result, T-matrix computations for large and/or highly aspherical particles can be slowly convergent or even divergent (Barber, 1977; Varadan and Varadan, 1980; Wiscombe and Mugnai, 1986).

Efficient approaches for overcoming the numerical instability problem in computing the T matrix for highly elongated particles are the so-called iterative EBCM (IEBCM) and a closely related multiple multipole EBCM (Iskander *et al.*, 1983; Lakhtakia *et al.*, 1983; Iskander and Lakhtakia, 1984; Iskander *et al.*, 1989b; Doicu and Wriedt, 1997a, b; Wriedt and Doicu, 1997, 1998). The main idea of IEBCM is to represent the internal field by several subdomain spherical function expansions centered on the major axis of an elongated scatterer. These subdomain expansions are linked to each other by being explicitly matched in the appropriate overlapping zones. IEBCM has been used to compute light scattering and absorption by highly elongated lossy and low-loss dielectric scatterers with aspect ratios as large as 17. In some cases the use of IEBCM instead of the regular EBCM allows one to more than quadruple the maximal convergent size parameter. The disadvantage of IEBCM is that its numerical stability is achieved at the expense of a considerable increase in computer code complexity and required central processing unit (CPU) time.

Another approach to deal with the numerical instability of the regular EBCM exploits the unitarity property of the T matrix for nonabsorbing particles (Waterman, 1973; Lakhtakia *et al.*, 1984, 1985a). This technique is based on iterative orthogonalization of the T matrix, is simple and computationally efficient, and results in numerically stable T matrices for elongated and flattened spheroids with aspect ratios as large as 20. The obvious disadvantage of this approach is that it is applicable only to perfectly conducting or lossless dielectric scatterers. Wielaard *et al.* (1997) demonstrated that a better approach is to invert the $\mathbf{Q}$ matrix using a special form of the lower triangular–upper triangular (LU) factorization method. This technique is applicable not only to nonabsorbing but also to lossy particles and increases the maximum convergent size parameter for lossless and low-loss particles by a factor of several units.

Mishchenko and Travis (1994a) showed that an efficient general method for ameliorating the numerical instability of inverting the $\mathbf{Q}$ matrix is to improve the accuracy with which this matrix is calculated and inverted. Specifically, they calculated the elements of the $\mathbf{Q}$ matrix and performed the matrix inversion using extended-precision (REAL*16 and COMPLEX*32) instead of double-precision (REAL*8 and COMPLEX*16) floating-point variables. Extensive checks have shown that this approach more than doubles the maximum size parameter for which convergence of T-matrix computations can be achieved. Timing tests performed on IBM RISC workstations show that the use of extended-precision arithmetic slows computations down by a factor of only 5 to 6. Other key features of this approach are its simplicity and the fact that little additional programming effort and negligibly small extra memory are required.

An interesting method for computing the T matrix for spheroids was developed by Schulz *et al.* (1998a), who used the separation of variables method to derive the T matrix in spheroidal coordinates and then converted it into the regular T matrix in spherical coordinates.

V. AGGREGATED AND COMPOSITE PARTICLES

According to Eqs. (21) and (22), VSWFs in a rotated reference frame can be expanded in VSWFs in the original reference frame, thereby leading to a simple rotation transformation rule for the T matrix, Eq. (24). Analogously, VSWFs in a translated coordinate system can be expressed in VSWFs in the original coordinate system via the translation addition theorem, resulting in a translation transformation rule for the T matrix. The latter can be used to develop a T-matrix scheme to compute light scattering by aggregated particles. This superposition T-matrix approach was developed by Peterson and Ström (1973) (see also Peterson, 1977) for the general case of a cluster composed of an arbitrary number of nonspherical components.

Consider a cluster consisting of N arbitrarily shaped and arbitrarily oriented particles illuminated by a plane external electromagnetic wave and assume that the T matrices of each of the particles are known with respect to their local coordinate systems with origins inside the particles. Assume also that all these local coordinate systems have the same spatial orientation as the laboratory reference frame and that the smallest circumscribing spheres of the component particles centered at the origins of their respective local coordinate systems do not overlap. [Note that Peterson (1977) discusses weaker restrictions on possible particle configurations.] The total electric field scattered by the entire cluster can be represented as a superposition of individual scattering contributions from each particle:

$$\mathbf{E}^{\text{sca}}(\mathbf{R}) = \sum_{j=1}^{N} \mathbf{E}_j^{\text{sca}}(\mathbf{R}), \tag{48}$$

where $\mathbf{R}$ connects the origin of the laboratory coordinate system and the observation point. Because of electromagnetic interactions between the component particles, the individual scattered fields are interdependent and the total electric field illuminating each particle is the superposition of the external incident field $\mathbf{E}_0^{\text{inc}}$ and the sum of the individual fields scattered by all other component particles:

$$\mathbf{E}_j^{\text{inc}}(\mathbf{R}) = \mathbf{E}_0^{\text{inc}}(\mathbf{R}) + \sum_{l \neq j} \mathbf{E}_l^{\text{sca}}(\mathbf{R}), \qquad j = 1, \ldots, N. \tag{49}$$

To make use of the information contained in the jth particle T matrix, we must expand the fields incident on and scattered by this particle in VSWFs centered at the origin of the particle's local coordinate system:

$$\begin{aligned}
\mathbf{E}_j^{\text{inc}}(\mathbf{R}) &= \sum_{nm} \left[a_{mn}^{j} \operatorname{Rg} \mathbf{M}_{mn}(k\mathbf{R}_j) + b_{mn}^{j} \operatorname{Rg} \mathbf{N}_{mn}(k\mathbf{R}_j) \right] \\
&= \sum_{nm} \Bigg[\Bigg(a_{mn}^{j0} + \sum_{l \neq j} a_{mn}^{jl} \Bigg) \operatorname{Rg} \mathbf{M}_{mn}(k\mathbf{R}_j) \\
&\qquad + \Bigg(b_{mn}^{j0} + \sum_{l \neq j} b_{mn}^{jl} \Bigg) \operatorname{Rg} \mathbf{N}_{mn}(k\mathbf{R}_j) \Bigg], \qquad j = 1, \ldots, N,
\end{aligned} \tag{50}$$

$$\mathbf{E}_j^{\text{sca}}(\mathbf{R}) = \sum_{nm} \left[p_{mn}^{j} \mathbf{M}_{mn}(k\mathbf{R}_j) + q_{mn}^{j} \mathbf{N}_{mn}(k\mathbf{R}_j) \right], \qquad R_j > R_{>j},$$
$$j = 1, \ldots, N, \tag{51}$$

where the $\mathbf{R}_j$ connects the origin of the jth particle local coordinate system and the observation point $\mathbf{R}$, $R_{>j}$ is the radius of the smallest circumscribing sphere of the jth particle, the expansion coefficients a_{mn}^{j0} and b_{mn}^{j0} describe the external incident field, and the expansion coefficients a_{mn}^{jl} and b_{mn}^{jl} describe the contribution of the lth particle to the field illuminating the jth particle:

$$\mathbf{E}_0^{\text{inc}}(\mathbf{R}) = \sum_{nm} \left[a_{mn}^{j0} \, \mathrm{Rg}\, \mathbf{M}_{mn}(k\mathbf{R}_j) + b_{mn}^{j0} \, \mathrm{Rg}\, \mathbf{N}_{mn}(k\mathbf{R}_j) \right],$$
$$j = 1, \ldots, N, \tag{52}$$

$$\mathbf{E}_l^{\text{sca}}(\mathbf{R}) = \sum_{nm} \left[a_{mn}^{jl} \, \mathrm{Rg}\, \mathbf{M}_{mn}(k\mathbf{R}_j) + b_{mn}^{jl} \, \mathrm{Rg}\, \mathbf{N}_{mn}(k\mathbf{R}_j) \right],$$
$$j, l = 1, \ldots, N. \tag{53}$$

The expansion coefficients of the illuminating and scattered fields are related via the jth particle T matrix $\mathbf{T}^j$:

$$\begin{bmatrix} \mathbf{p}^j \\ \mathbf{q}^j \end{bmatrix} = \mathbf{T}^j \left(\begin{bmatrix} \mathbf{a}^{j0} \\ \mathbf{b}^{j0} \end{bmatrix} + \sum_{l \neq j} \begin{bmatrix} \mathbf{a}^{jl} \\ \mathbf{b}^{jl} \end{bmatrix} \right), \qquad j = 1, \ldots, N. \tag{54}$$

The field scattered by the lth particle can also be expanded in VSWFs centered at the origin of the lth local coordinate system:

$$\mathbf{E}_l^{\text{sca}}(\mathbf{R}) = \sum_{\nu\mu} \left[p_{\mu\nu}^{l} \mathbf{M}_{\mu\nu}(k\mathbf{R}_l) + q_{\mu\nu}^{l} \mathbf{N}_{\mu\nu}(k\mathbf{R}_l) \right], \qquad R_l > R_{>l}, \tag{55}$$

where $\mathbf{R}_l$ connects the origin of the lth particle coordinate system and the observation point $\mathbf{R}$. Using the translation addition theorem (Tsang *et al.*, 1985, Chapter 6), the VSWFs in Eq. (55) can be expanded in regular VSWFs originating inside the jth particle:

$$\mathbf{M}_{\mu\nu}(k\mathbf{R}_l) = \sum_{nm} \left[A_{mn\mu\nu}(k\mathbf{R}_{lj}) \mathrm{Rg}\, \mathbf{M}_{mn}(k\mathbf{R}_j) + B_{mn\mu\nu}(k\mathbf{R}_{lj}) \mathrm{Rg}\, \mathbf{N}_{mn}(k\mathbf{R}_j) \right],$$
$$R_j < R_{lj}, \tag{56}$$

$$\mathbf{N}_{\mu\nu}(k\mathbf{R}_l) = \sum_{nm} \left[B_{mn\mu\nu}(k\mathbf{R}_{lj}) \mathrm{Rg}\, \mathbf{M}_{mn}(k\mathbf{R}_j) + A_{mn\mu\nu}(k\mathbf{R}_{lj}) \mathrm{Rg}\, \mathbf{N}_{mn}(k\mathbf{R}_j) \right],$$
$$R_j < R_{lj}, \tag{57}$$

where the vector $\mathbf{R}_{lj} = \mathbf{R}_l - \mathbf{R}_j$ connects the origins of the local coordinate systems of the lth and the jth particles, and the translation coefficients $A_{mn\mu\nu}(k\mathbf{R}_{lj})$

and $B_{mn\mu\nu}(k\mathbf{R}_{lj})$ are given by the analytical expressions listed on page 449 of Tsang *et al.* (1985). Comparing Eqs. (53)–(57), we finally derive in matrix notation

$$\begin{bmatrix}\mathbf{p}^j\\ \mathbf{q}^j\end{bmatrix} = \mathbf{T}^j\left(\begin{bmatrix}\mathbf{a}^{j0}\\ \mathbf{b}^{j0}\end{bmatrix} + \sum_{l\neq j}\begin{bmatrix}\mathbf{A}(k\mathbf{R}_{lj}) & \mathbf{B}(k\mathbf{R}_{lj})\\ \mathbf{B}(k\mathbf{R}_{lj}) & \mathbf{A}(k\mathbf{R}_{lj})\end{bmatrix}\begin{bmatrix}\mathbf{p}^l\\ \mathbf{q}^l\end{bmatrix}\right),$$
$$j = 1, \ldots, N. \tag{58}$$

Because the expansion coefficients of the external plane electromagnetic wave a_{mn}^{j0} and b_{mn}^{j0} and the translation coefficients $A_{mn\mu\nu}(k\mathbf{R}_{lj})$ and $B_{mn\mu\nu}(k\mathbf{R}_{lj})$ can be computed via closed-form analytical formulas, Eq. (58) can be considered a system of linear algebraic equations that can be solved numerically and yields the expansion coefficients of the individual scattered fields p_{mn}^j and q_{mn}^j for each of the cluster components. When these coefficients are known, Eqs. (51) and (48) give the total field scattered by the cluster.

Equation (58) becomes especially simple for a cluster composed of spherical particles because in this case the individual particle T matrices are diagonal with standard Lorenz–Mie coefficients standing along their main diagonal [Eqs. (27)–(29)]. The resulting equation is identical to that derived using the so-called multisphere superposition formulation or multisphere separation of variables technique (Bruning and Lo, 1971; Borghese *et al.*, 1979, 1984; Hamid *et al.*, 1990; Fuller, 1991; Mackowski, 1991; Ioannidou *et al.*, 1995). In this regard, the latter can be considered a particular case of the superposition T-matrix method. Solutions of Eq. (58) for clusters of spheres have been obtained using different numerical techniques (direct matrix inversion, method of successive orders of scattering, conjugate gradients method, method of iterations, recursive method) and have been extensively reported in the literature (Hamid *et al.*, 1991; Fuller, 1994a, 1995a; de Daran *et al.*, 1995; Xu, 1995; Tishkovets and Litvinov, 1996; Rannou *et al.*, 1997; Videen *et al.*, 1998). Fikioris and Uzunoglu (1979), Borghese *et al.* (1992, 1994), Fuller (1995b), Mackowski and Jones (1995), and Skaropoulos *et al.* (1994, 1996) extended the superposition approach to the case of internal aggregation by solving the problem of light scattering by spherical particles with eccentric spherical inclusions, whereas Videen *et al.* (1995b) considered a more general case of a sphere with an irregular inclusion. It should be noted that particles with single inclusions can also be treated using the standard EBCM for multilayered scatterers (Peterson and Ström, 1974).

Inversion of Eq. (58) gives (Mackowski, 1994)

$$\begin{bmatrix}\mathbf{p}^j\\ \mathbf{q}^j\end{bmatrix} = \sum_{l=1}^{N}\mathbf{T}^{jl}\begin{bmatrix}\mathbf{a}^{l0}\\ \mathbf{b}^{l0}\end{bmatrix}, \qquad j = 1, \ldots, N, \tag{59}$$

where the matrix $\mathbf{T}^{jl}$ transforms the expansion coefficients of the incident field centered at the lth particle into the jth-particle-centered expansion coefficients of the field scattered by the jth particle. The calculation of the $\mathbf{T}^{jl}$ matrices implies numerical inversion of a large matrix and can be a time-consuming process. However, these matrices are independent of the incident field and depend only on the cluster configuration and shapes and orientations of the component particles. Therefore, they need be computed only once and then can be used in computations for any direction and polarization state of the incident field.

Furthermore, in the far-field region the scattered-field expansions from the individual particles can be transformed into a single expansion centered at the origin of the laboratory reference frame. This single origin can represent the average of the component particle positions but in general can be arbitrary. The first step is to expand the incident and total scattered fields in VSWFs centered at the origin of the laboratory reference frame according to Eqs. (1) and (2). We again employ the translation addition theorem given by

$$\begin{aligned} \mathrm{Rg}\,\mathbf{M}_{mn}(k\mathbf{R}) = \sum_{\nu\mu}\big[&\mathrm{Rg}\,A_{\mu\nu mn}(k\mathbf{R}_{0l})\mathrm{Rg}\,\mathbf{M}_{\mu\nu}(k\mathbf{R}_l) \\ &+ \mathrm{Rg}\,B_{\mu\nu mn}(k\mathbf{R}_{0l})\mathrm{Rg}\,\mathbf{N}_{\mu\nu}(k\mathbf{R}_l)\big], \end{aligned} \tag{60}$$

$$\begin{aligned} \mathrm{Rg}\,\mathbf{N}_{mn}(k\mathbf{R}) = \sum_{\nu\mu}\big[&\mathrm{Rg}\,B_{\mu\nu mn}(k\mathbf{R}_{0l})\mathrm{Rg}\,\mathbf{M}_{\mu\nu}(k\mathbf{R}_l) \\ &+ \mathrm{Rg}\,A_{\mu\nu mn}(k\mathbf{R}_{0l})\mathrm{Rg}\,\mathbf{N}_{\mu\nu}(k\mathbf{R}_l)\big] \end{aligned} \tag{61}$$

and by reciprocal formulas

$$\begin{aligned} \mathbf{M}_{mn}(k\mathbf{R}_j) &= \sum_{\nu\mu}\big[\mathrm{Rg}\,A_{\mu\nu mn}(k\mathbf{R}_{j0})\mathbf{M}_{\mu\nu}(k\mathbf{R}) + \mathrm{Rg}\,B_{\mu\nu mn}(k\mathbf{R}_{j0})\mathbf{N}_{\mu\nu}(k\mathbf{R})\big], \\ &\quad R > R_{j0}, \end{aligned} \tag{62}$$

$$\begin{aligned} \mathbf{N}_{mn}(k\mathbf{R}_j) &= \sum_{\nu\mu}\big[\mathrm{Rg}\,B_{\mu\nu mn}(k\mathbf{R}_{j0})\mathbf{M}_{\mu\nu}(k\mathbf{R}) + \mathrm{Rg}\,A_{\mu\nu mn}(k\mathbf{R}_{j0})\mathbf{N}_{\mu\nu}(k\mathbf{R})\big], \\ &\quad R > R_{j0}, \end{aligned} \tag{63}$$

where $\mathbf{R}_{0l} = \mathbf{R} - \mathbf{R}_l$, $\mathbf{R}_{j0} = \mathbf{R}_j - \mathbf{R}$, and the translation coefficients $\mathrm{Rg}\,A_{\mu\nu mn}(k\mathbf{R}_{0l})$ and $\mathrm{Rg}\,B_{\mu\nu mn}(k\mathbf{R}_{0l})$ differ from $A_{\mu\nu mn}(k\mathbf{R}_{0l})$ and $B_{\mu\nu mn}(k\mathbf{R}_{0l})$ in that they are based on spherical Bessel functions rather than on spherical Hankel functions. We then easily derive

$$\begin{bmatrix} \mathbf{a}^{l0} \\ \mathbf{b}^{l0} \end{bmatrix} = \begin{bmatrix} \mathrm{Rg}\,\mathbf{A}(k\mathbf{R}_{0l}) & \mathrm{Rg}\,\mathbf{B}(k\mathbf{R}_{0l}) \\ \mathrm{Rg}\,\mathbf{B}(k\mathbf{R}_{0l}) & \mathrm{Rg}\,\mathbf{A}(k\mathbf{R}_{0l}) \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \qquad l = 1, \ldots, N, \tag{64}$$

$$\begin{bmatrix} \mathbf{p} \\ \mathbf{q} \end{bmatrix} = \sum_{j=1}^{N} \begin{bmatrix} \mathrm{Rg}\,\mathbf{A}(k\mathbf{R}_{j0}) & \mathrm{Rg}\,\mathbf{B}(k\mathbf{R}_{j0}) \\ \mathrm{Rg}\,\mathbf{B}(k\mathbf{R}_{j0}) & \mathrm{Rg}\,\mathbf{A}(k\mathbf{R}_{j0}) \end{bmatrix} \begin{bmatrix} \mathbf{p}^j \\ \mathbf{q}^j \end{bmatrix}. \tag{65}$$

Finally, using Eqs. (1), (2), (59), (64), and (65), we obtain Eq. (16), in which the cluster T matrix is given by

$$\mathbf{T} = \sum_{j,l=1}^{N} \begin{bmatrix} \mathrm{Rg}\,\mathbf{A}(k\mathbf{R}_{j0}) & \mathrm{Rg}\,\mathbf{B}(k\mathbf{R}_{j0}) \\ \mathrm{Rg}\,\mathbf{B}(k\mathbf{R}_{j0}) & \mathrm{Rg}\,\mathbf{A}(k\mathbf{R}_{j0}) \end{bmatrix} \mathbf{T}^{jl} \begin{bmatrix} \mathrm{Rg}\,\mathbf{A}(k\mathbf{R}_{0l}) & \mathrm{Rg}\,\mathbf{B}(k\mathbf{R}_{0l}) \\ \mathrm{Rg}\,\mathbf{B}(k\mathbf{R}_{0l}) & \mathrm{Rg}\,\mathbf{A}(k\mathbf{R}_{0l}) \end{bmatrix} \tag{66}$$

(Peterson and Ström, 1973; Mackowski, 1994). This cluster T matrix can be used in Eq. (18) to compute the amplitude matrix and in the analytical procedure for averaging over orientations described in Section III (Mishchenko and Mackowski, 1994; Mackowski and Mishchenko, 1996).

It is rather straightforward to derive a translation transformation law for the T matrix analogous to the rotation transformation law given by Eq. (24). Suppose that the T matrix of an arbitrary (single or clustered) nonspherical particle is known in coordinate system 1 and we seek the T matrix in a translated coordinate system 2 having the same spatial orientation. After simple manipulations, we obtain

$$\mathbf{T}(2) = \begin{bmatrix} \mathrm{Rg}\,\mathbf{A}(-k\mathbf{R}_{21}) & \mathrm{Rg}\,\mathbf{B}(-k\mathbf{R}_{21}) \\ \mathrm{Rg}\,\mathbf{B}(-k\mathbf{R}_{21}) & \mathrm{Rg}\,\mathbf{A}(-k\mathbf{R}_{21}) \end{bmatrix} \mathbf{T}(1) \begin{bmatrix} \mathrm{Rg}\,\mathbf{A}(k\mathbf{R}_{21}) & \mathrm{Rg}\,\mathbf{B}(k\mathbf{R}_{21}) \\ \mathrm{Rg}\,\mathbf{B}(k\mathbf{R}_{21}) & \mathrm{Rg}\,\mathbf{A}(k\mathbf{R}_{21}) \end{bmatrix}, \tag{67}$$

where the vector $\mathbf{R}_{21}$ originates at the origin of coordinate system 2 and connects it with the origin of coordinate system 1. Because the extinction and scattering cross sections averaged over a uniform orientation distribution must be independent of the choice of the coordinate system, Eqs. (32) and (33) lead to the following invariants with respect to translations of the coordinate system:

$$\sum_{nmk} T^{kk}_{mnmn}(2) = \sum_{nmk} T^{kk}_{mnmn}(1), \tag{68}$$

$$\sum_{nmn'm'kl} \left|T^{kl}_{mnm'n'}(2)\right|^2 = \sum_{nmn'm'kl} \left|T^{kl}_{mnm'n'}(1)\right|^2. \tag{69}$$

Different versions of the superposition T-matrix approach were derived by Chew *et al.* (1994), Tseng and Fung (1994), and Şahin and Miller (1998). An important modification of the T-matrix superposition method was developed by Ström and Zheng (1988), Zheng (1988), and Zheng and Ström (1989, 1991). Several alternative expressions for the T matrix of a composite object were derived, which enabled the authors to avoid the geometrical constraints inherent in the standard approach. As a result, this technique can be applied to composite particles with concavo-convex components and can also be used in computations for particles with extreme geometries, for example, highly elongated or flattened spheroids. In this regard, the technique can be considered a supplement to the methods for suppressing the numerical instability of the regular T-matrix approach described in the previous section.

VI. PUBLIC-DOMAIN *T*-MATRIX CODES

Several Fortran T-matrix codes for computing electromagnetic scattering by rotationally symmetric particles in fixed and random orientations are available on the World Wide Web at http://www.giss.nasa.gov/~crmim. The codes incorporate all the latest developments, including the analytical orientation averaging procedure for randomly oriented scatterers (Mishchenko, 1991a) and an automatic convergence procedure (Mishchenko, 1993), are extensively documented, have been thoroughly tested, and provide a reliable and efficient practical instrument. The codes compute the complete set of scattering characteristics, that is, the amplitude matrix for particles in a fixed orientation (Section IV of Chapter 1) and the optical cross sections, expansion coefficients, and scattering matrix for randomly oriented particles (Section XI of Chapter 1).

The code for two-sphere clusters with touching and separated components is based on the superposition T-matrix technique (Mackowski, 1994; Mishchenko and Mackowski, 1994, 1996). The codes for homogeneous nonspherical particles are based on EBCM and are provided in two versions. One version utilizes only double-precision floating-point variables, whereas the other one computes the T-matrix elements using extended-precision variables. The extended-precision code is slower than the double-precision code, especially on supercomputers, but allows computations for significantly larger particles. The EBCM codes have an option for inverting the **Q** matrix using either standard Gaussian elimination with partial pivoting or a special form of the LU factorization (Wielaard *et al.*, 1997). The latter approach is especially beneficial for nonabsorbing or weakly absorbing scatterers. In the present setting, the EBCM codes are directly applicable to spheroids, finite circular cylinders, and even-order Chebyshev particles (Fig. 2). Note that Chebyshev particles are rotationally symmetric bodies obtained by continuously deforming a sphere by means of a Chebyshev polynomial of degree n (Wiscombe and Mugnai, 1986). Their shape in the particle coordinate system with the z axis along the axis of symmetry is given by

$$r(\vartheta, \varphi) = r_0\left[1 + \xi T_n(\cos\vartheta)\right], \qquad |\xi| < 1, \tag{70}$$

where r_0 is the radius of the unperturbed sphere, ξ is the deformation parameter, and $T_n(\cos\vartheta) = \cos n\vartheta$ is the Chebyshev polynomial of degree n. The codes can be easily modified to accommodate any rotationally symmetric particle having a plane of symmetry perpendicular to the axis of rotation. Mishchenko and Travis (1998) provide a detailed user guide to the EBCM codes.

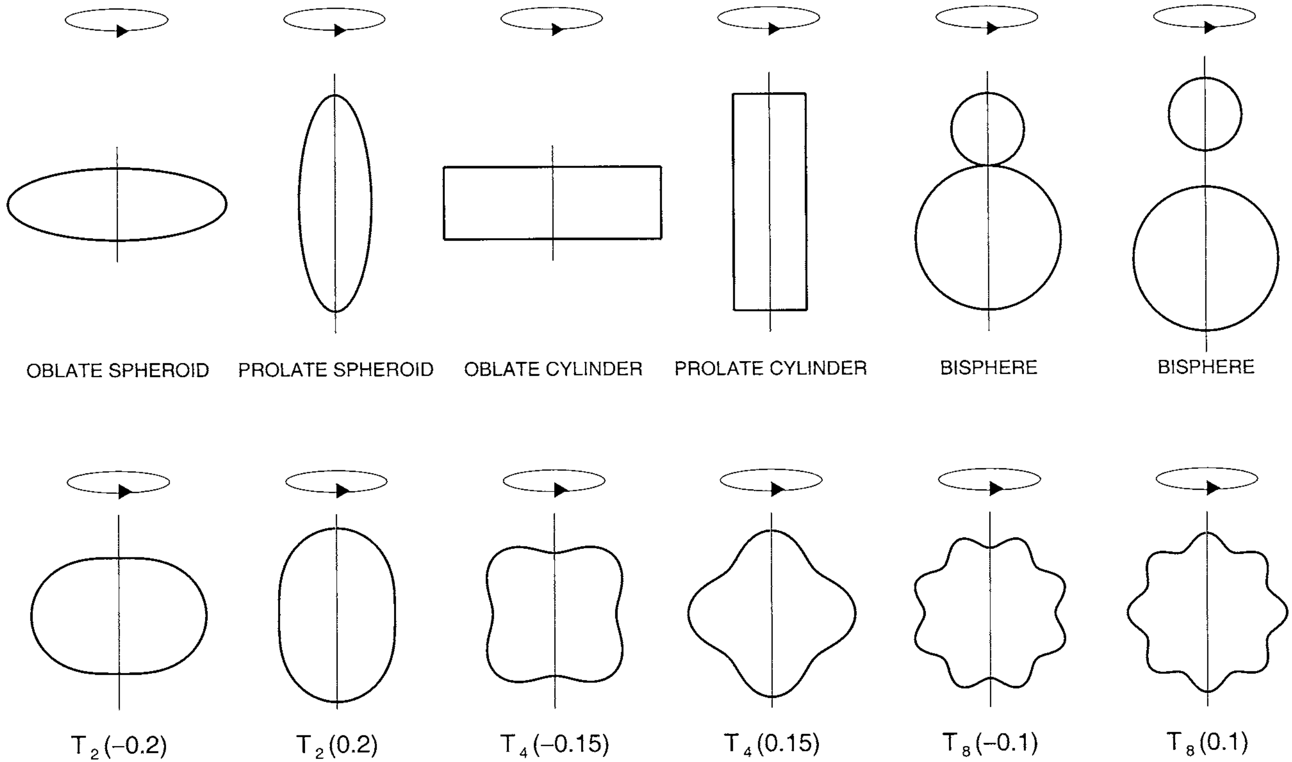

Figure 2 Types of rotationally symmetric particles that can be accommodated by publicly available T-matrix codes. $T_n(\xi)$ denotes the nth-degree Chebyshev particle with deformation parameter ξ.

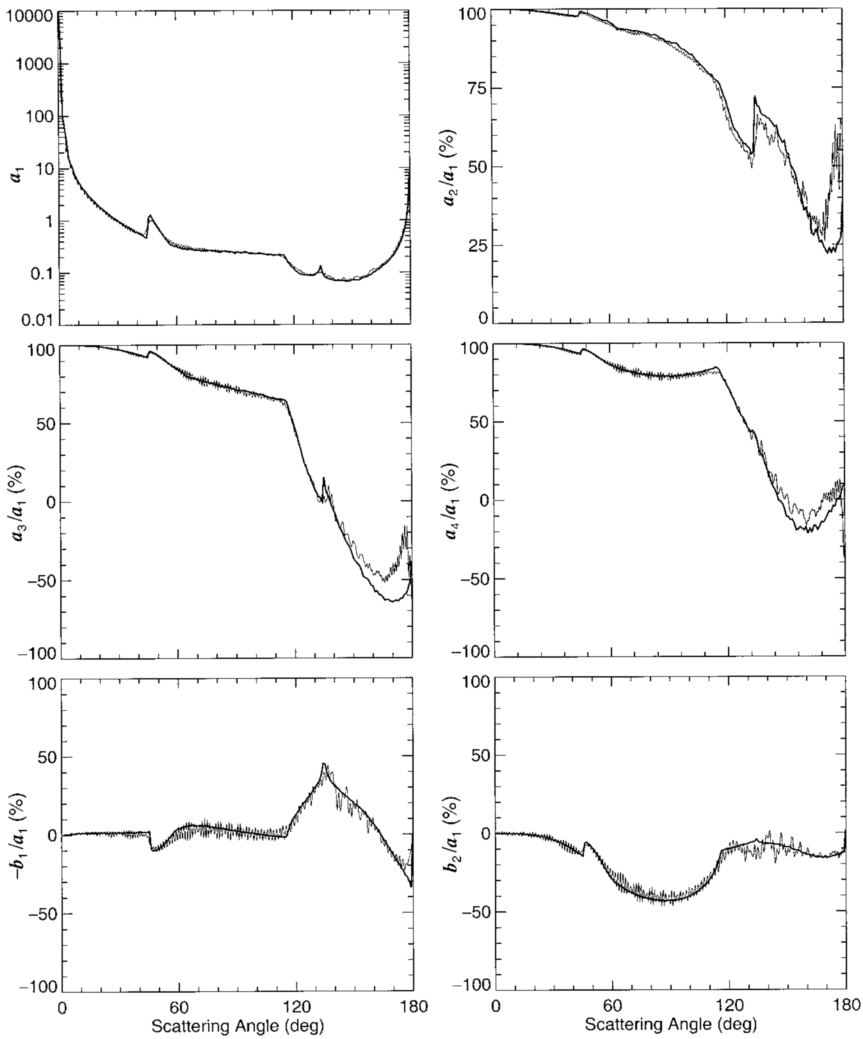

Figure 3 Scattering matrix elements for randomly oriented circular cylinders with diameter-to-length ratio 1, surface-equivalent sphere size parameter 180, and refractive index 1.311. Thin curves show T-matrix computations; thick curves represent ray-tracing results.

As for all exact numerical techniques for computing electromagnetic scattering by nonspherical particles, the performance of the T-matrix codes in terms of convergence and memory and CPU time requirements strongly depends on the options used and such particle characteristics as shape, size parameter (defined

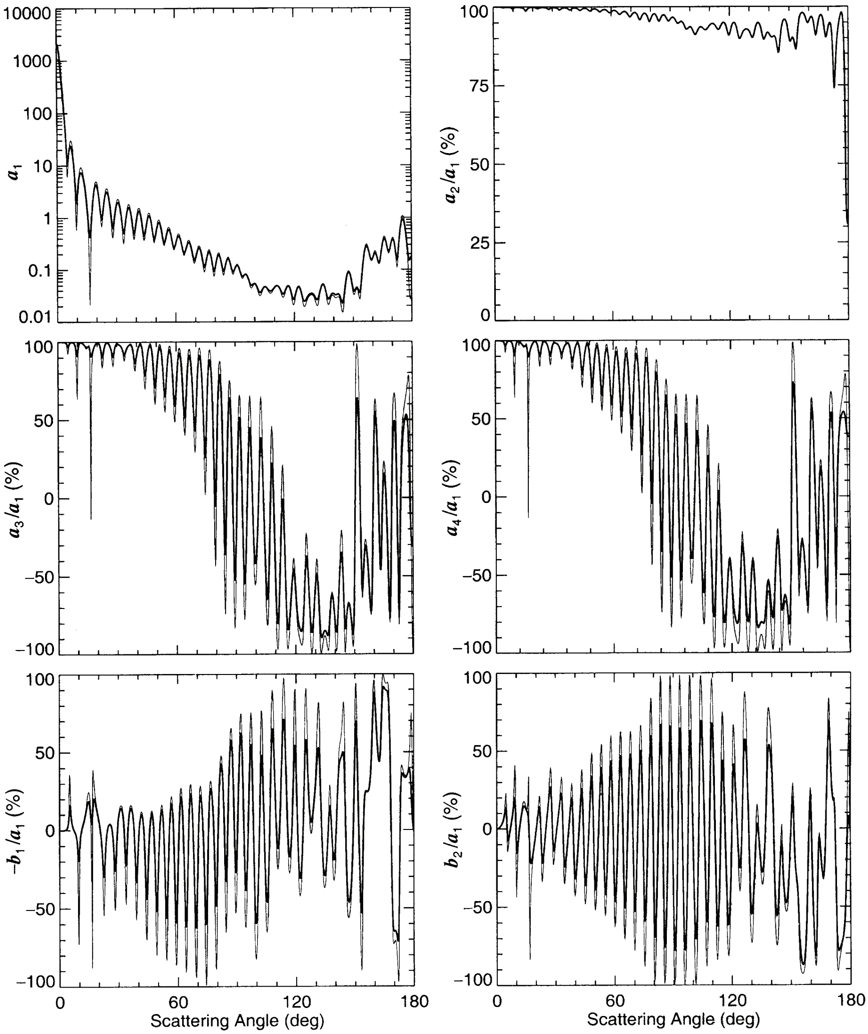

Figure 4 Scattering matrix elements for a two-sphere cluster in random orientation (thick curves) and a single sphere (thin curves). The component spheres and the single sphere have the same size parameter 40 and the same refractive index $1.5 + 0.005i$.

here as the wavenumber times the surface-equivalent sphere radius), and refractive index. For example, the maximal convergent size parameter increases from 12 for oblate spheroids with an aspect ratio of 20 and a refractive index of 1.311 to more than 160 for composition-equivalent oblate spheroids with an aspect ratio of 1.5. The sensitivity to refractive index is weaker but is also significant. The use of extended-precision variables more than doubles the maximal convergent size parameter, but makes computations slower. The use of the special LU-factorization scheme in place of standard Gaussian elimination to compute the $\mathbf{Q}^{-1}$ matrix can more than triple the maximal convergent size parameter for nonabsorbing or weakly absorbing particles. All these factors should be carefully taken into account, especially in planning massive computer calculations for large particle ensembles (Mishchenko and Travis, 1998).

Figures 3 and 4 exemplify the capabilities of the T-matrix codes. Figure 3 compares T-matrix and geometric optics computations for randomly oriented circular cylinders with diameter-to-length ratio 1, surface-equivalent sphere size parameter 180, and refractive index 1.311. The small-amplitude oscillations in the T-matrix curves are a manifestation of the interference structure typical of monodisperse particles (Section V.A of Chapter 2). For this large size parameter, the T-matrix computations closely reproduce the asymptotic geometric optics behavior, in particular, such pronounced phase function features as the 46° halo caused by minimum deviation at 90° prisms and the strong backscattering peak caused by double internal reflections from mutually perpendicular facets (Macke and Mishchenko, 1996). Figure 4 compares scattering matrix elements for a randomly oriented two-sphere cluster with identical touching components and a single sphere with size parameter equal to that of the cluster component spheres. It is obvious that the dominant feature in the cluster scattering is the single scattering from the component spheres, although this feature is somewhat reduced by cooperative scattering effects and orientation averaging (Mishchenko *et al.*, 1995). The only distinct manifestations of the cluster nonsphericity are the departure of the ratio a_2/a_1 from unity and the inequality of the ratios a_3/a_1 and a_4/a_1 (cf. Section V.B of Chapter 2).

An older collection of EBCM codes developed by Barber and Hill (1990) is also available on the World Wide Web (Flatau, 1998). The codes use single-precision floating-point variables and do not incorporate the most recent developments.

VII. APPLICATIONS

Because of its high numerical accuracy, the T-matrix method is ideally suited for producing benchmark results. Benchmark numbers for particles in fixed and random orientations were reported by Mishchenko (1991a), Kuik *et al.* (1992), Mishchenko *et al.* (1996a), Mishchenko and Mackowski (1996), Hovenier *et al.* (1996), and Wielaard *et al.* (1997). They cover a range of equivalent-sphere size parameters from a few units to 60 and are given with up to nine correct decimals.

The great computational efficiency of the T-matrix approach has been employed by many authors to study electromagnetic scattering by representative ensembles of nonspherical particles with various shapes and sizes. Systematic computations for homogeneous and layered spheroids, finite circular cylinders, Chebyshev particles, and two-sphere clusters in random orientation were reported and analyzed by Mugnai and Wiscombe (1980, 1986, 1989), Wiscombe and Mugnai (1986, 1988), Kuik *et al.* (1994), Mishchenko and Travis (1994b, c), Mishchenko and Hovenier (1995), Mishchenko *et al.* (1995, 1996a, b), and Quirantes (1999).

The T-matrix approach has been used in many practical applications. Warner and Hizal (1976), Bringi and Seliga (1977b), Yeh *et al.* (1982), Aydin and Seliga (1984), Kummerow and Weinman (1988), Vivekanandan *et al.* (1991), Sturniolo *et al.* (1995), Haferman *et al.* (1997), Bringi *et al.* (1998), Aydin *et al.* (1998), Seow *et al.* (1998), Czekala (1998), Czekala and Simmer (1998), Prodi *et al.* (1998), and Roberti and Kummerow (1999) used T-matrix computations in remote-sensing studies of precipitation, whereas Toon *et al.* (1990), Flesia *et al.* (1994), Mannoni *et al.* (1996), and Mishchenko and Sassen (1998) analyzed depolarization measurements of stratospheric aerosols and contrail particles. Bantges *et al.* (1998) computed cirrus cloud radiance spectra in the thermal infrared wavelength region. Mishchenko *et al.* (1997b) and Mishchenko and Macke (1998) studied zenith-enhanced lidar backscatter and δ-function transmission by ice plates. Hill *et al.* (1984), Iskander *et al.* (1986), Lacis and Mishchenko (1995), Khlebtsov and Mel'nikov (1995), Mishchenko *et al.* (1997a), Kahn *et al.* (1997), Liang and Mishchenko (1997), Krotkov *et al.* (1997, 1999), Pilinis and Li (1998), and von Hoyningen-Huene (1998) modeled scattering properties of soil particles and mineral and soot aerosols using size/shape mixtures of randomly oriented spheroids. Carslaw *et al.* (1998), Tsias *et al.* (1998), and Trautman *et al.* (1998) applied the T-matrix technique to remote sensing of polar stratospheric clouds. Kouzoubov *et al.* (1998) computed the scattering matrix for nonspherical ocean water particulates. Kolokolova *et al.* (1997) used T-matrix computations to model the photometric and polarization properties of nonspherical cometary dust grains. Khlebtsov *et al.* (1996) calculated the extinction properties of colloidal gold sols. Quirantes and Delgado (1995, 1998) and Jalava *et al.* (1998) applied the T-matrix method to particle size/shape determination. Nilsson *et al.* (1998) analyzed near and far fields originating from light interaction with a spheroidal red blood cell. Latimer and Barber (1978), Barber and Wang (1978), Wang *et al.* (1979), Goedecke and O'Brien (1988), Iskander *et al.* (1989a), Evans and Fournier (1994), Streekstra *et al.* (1994), Macke *et al.* (1995), Peltoniemi (1996), Wielaard *et al.* (1997), Mishchenko *et al.* (1997b), Baran *et al.* (1998), Mishchenko and Macke (1998), and Liu *et al.* (1998) used numerically exact T-matrix computations to check the accuracy of various approximate and numerical approaches. Lai *et al.* (1991), Mazumder *et al.* (1992), Ngo and Pinnick (1994), and Borghese *et al.* (1998) analyzed the effect of nonsphericity and inhomogeneity on morphology-dependent resonances in small particles.

Mishchenko (1996) studied coherent effects in two-sphere clusters. Pitter *et al.* (1998) analyzed second-order fluctuations of the polarization state of light scattered by ensembles of randomly positioned spheroidal particles. Ruppin (1998) studied polariton modes of spheroidal microcrystals of dispersive materials over a wide range of spheroid sizes and eccentricities. Ho and Allen (1994) and Liu *et al.* (1999) analyzed the effect of nonsphericity on numerical solutions of inverse problems. Other applications of the T-matrix method were reported by Geller *et al.* (1985), Hofer and Glatter (1989), Ruppin (1990), Ryde and Matijević (1994), Xing and Greenberg (1994), Lumme and Rahola (1998), Balzer *et al.* (1998), Mishchenko and Macke (1999), Evans *et al.* (1999), and Petrova (1999).

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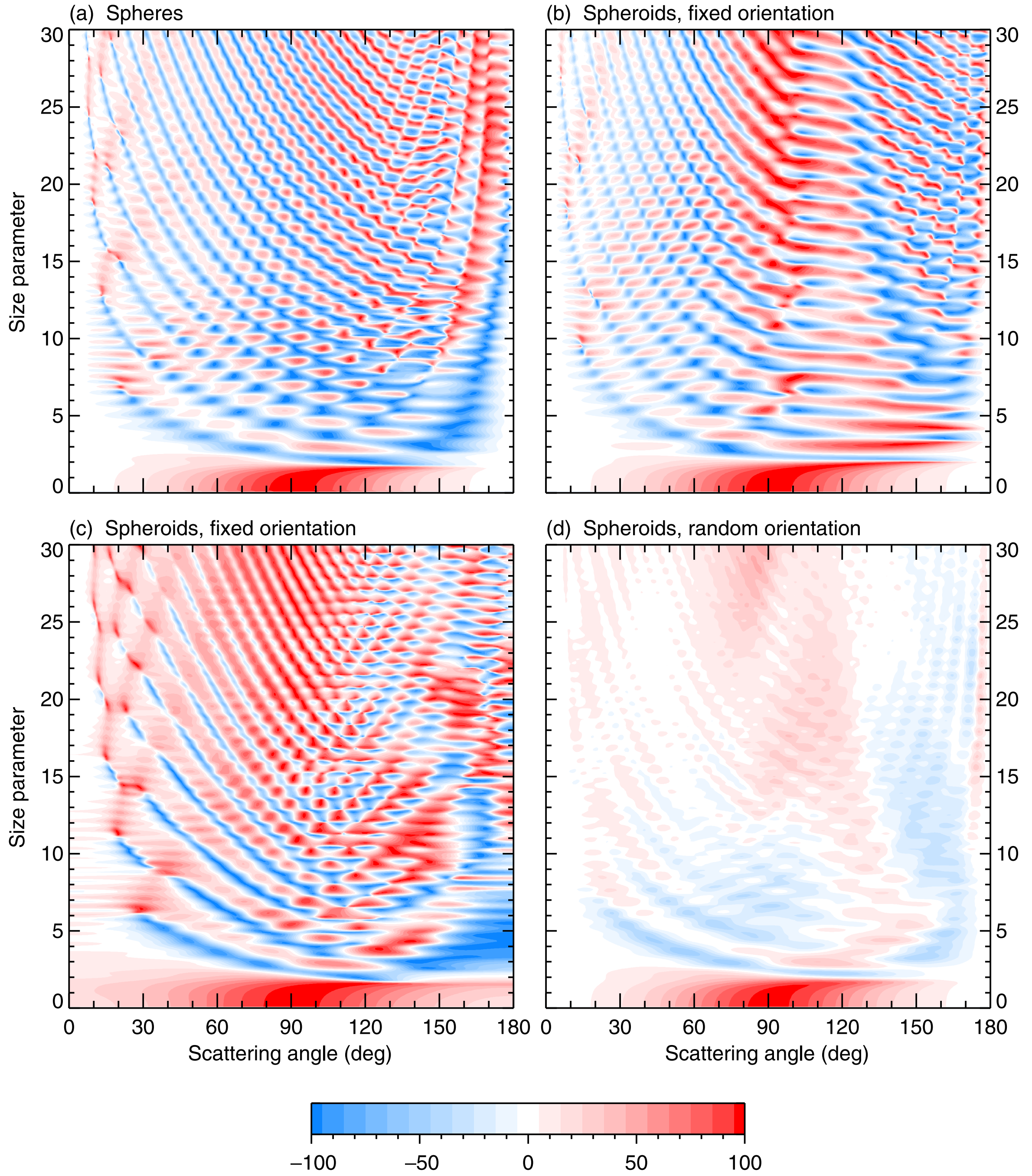

Plate 10.1. The ratio $-Z_{21}(\vartheta^{\text{sca}}, \varphi^{\text{sca}} = 0; \vartheta^{\text{inc}} = 0, \varphi^{\text{inc}} = 0)/Z_{11}(\vartheta^{\text{sca}}, \varphi^{\text{sca}} = 0; \vartheta^{\text{inc}} = 0, \varphi^{\text{inc}} = 0)$ in % versus ϑ^{sca} and size parameter for monodisperse spheres and surface-equivalent oblate spheroids in fixed and random orientations. In panels (b) and (c), the rotation axis of the spheroids is oriented respectively along the *z*-axis and along the *x*-axis of the laboratory reference frame. The relative refractive index is 1.53 + i0.008 and the spheroid axis ratio $a/b = 1.7$.