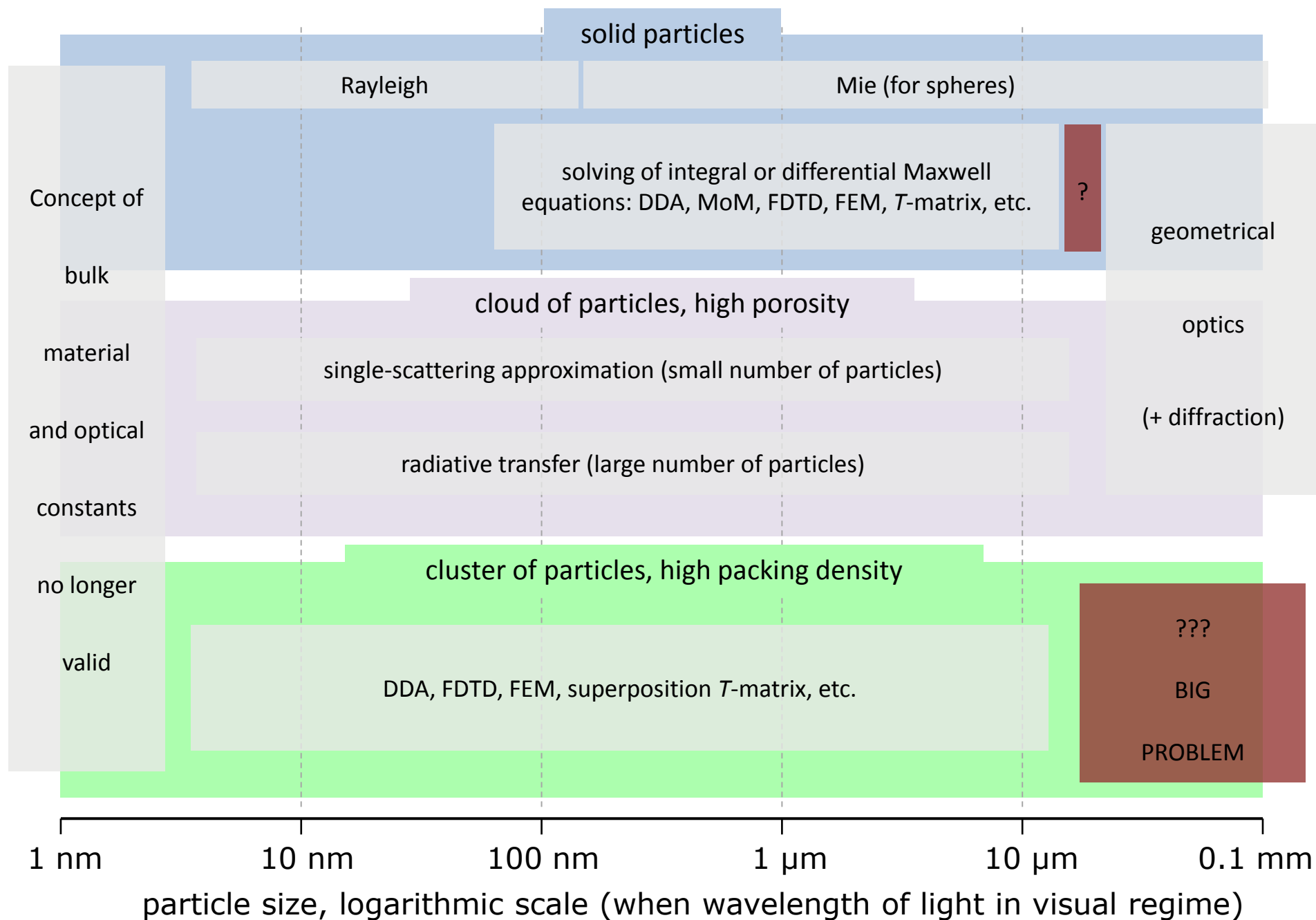


Schematic division of scattering problems



4.10.2011

The T-matrix method

Jani Tyynelä

History

- T -matrix method (TMM) is based on the extended boundary condition method (EBCM) by Waterman (1965-1979)
- Barber and Yeh (1975-1982) actually introduced the name EBCM and made the method more widely used
- the name ' T -matrix formalism' was introduced by Ström (1975)
- in acoustic applications, TMM is known as 'the null-field method'
- Iskander *et al.* (1982-1984) introduced an iterative version of TMM to improve the convergence
- Mishchenko (1990-1994) proposed to use of extended precision in order to use TMM for higher size parameters, and also developed an efficient way to use analytical averaging over orientations to speed up computations

Basics of TMM

- TMM can be considered to be an extension of Mie theory to particles without spherical symmetry
- in TMM incident, scattered and internal fields are expanded in vector spherical harmonic functions
- the T -matrix itself transforms the incident field expansion coefficients to the scattered field expansion coefficients
- the main advantage of TMM over volume-based methods like DDA is an efficient use of symmetries, better accuracy, and analytical averaging over orientations

Computing the T -matrix

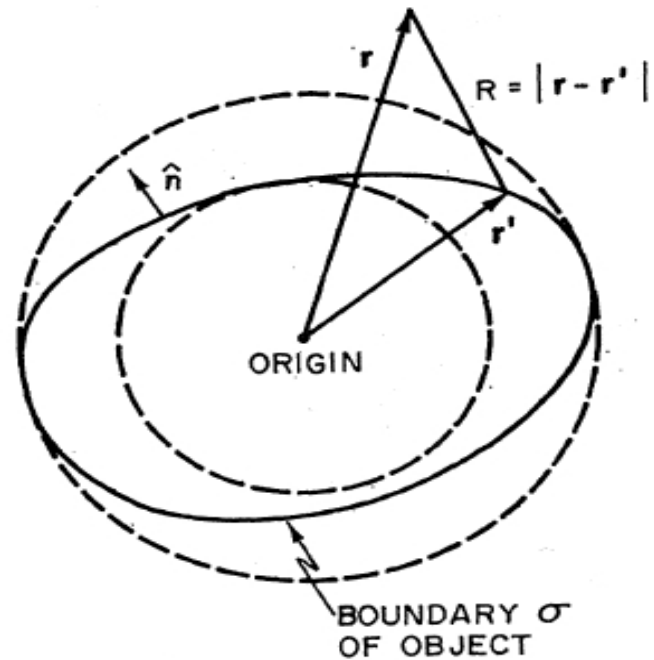


FIG. 1. Geometry of a scattering region bounded by the closed surface σ .

Computing the T -matrix

Huygens principle is used to establish a relationship between the total field and the incident field using the integral equation,

$$\begin{cases} \vec{E}_{tot}(\vec{r}) \\ 0 \end{cases} = \vec{E}_{inc}(\vec{r}) + \nabla \times \int_S (\vec{n} \times \vec{E}_{outside}) g(kR) dS - \frac{1}{i\omega\epsilon_0} \nabla \times \nabla \times \int_S (\vec{n} \times \vec{H}_{outside}) g(kR) dS, \vec{r} \begin{cases} \text{outside } \sigma \\ \text{inside } \sigma \end{cases}$$

where $g(kR) = \frac{e^{ikR}}{4\pi R}$ is the Green's function.

The surface integrals can be interpreted as surface currents that are the sources of the scattered field according to the equivalence theorem, but this also results in zero total field inside the scatterer.

The object is to solve the surface integrals using the incident field expansion and the physical characteristics of the scatterer.

Computing the T -matrix

Incident field:

1. Incident field is expanded in vector spherical harmonic functions

$$\vec{E}_{inc}(\vec{r}) = \sum_{n=1}^{N_{max}} \sum_{m=-n}^n [a_{mn} Rg \vec{M}_{mn}(k\vec{r}) + b_{mn} Rg \vec{N}_{mn}(k\vec{r})],$$

2. The surface integrals are also expanded and the surface currents $\vec{n} \times \vec{E}_{outside}$ and $\vec{n} \times \vec{H}_{outside}$ are solved using the incident field coefficients

$$\vec{E}_{inc} = - \int_S f(\vec{n} \times \vec{E}_{outside}, \vec{n} \times \vec{H}_{outside}) dS$$

Computing the T -matrix

Internal field:

3. The internal field is expanded

$$\vec{E}_{int}(\vec{r}) = \sum_{n=1}^{N_{max}} \sum_{m=-n}^n [c_{mn} \vec{M}_{mn}(mk\vec{r}) + d_{mn} \vec{N}_{mn}(mk\vec{r})]$$

4. The tangential components $\vec{n} \times \vec{E}_{inside}$ and $\vec{n} \times \vec{H}_{inside}$

are solved using the internal field coefficients

5. Using boundary conditions $\vec{n} \times \vec{E}_{outside} = \vec{n} \times \vec{E}_{inside}$

and $\vec{n} \times \vec{H}_{outside} = \vec{n} \times \vec{H}_{inside}$ a relation between the incident and internal field coefficients is obtained

in matrix form:

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix}$$

Computing the T -matrix

Scattered field:

6. The scattered field is expanded

$$\vec{E}_{sca}(\vec{r}) = \sum_{n=1}^{N_{max}} \sum_{m=-n}^n [p_{mn} \vec{M}_{mn}(k\vec{r}) + q_{mn} \vec{N}_{mn}(k\vec{r})], r > r_{sph}$$

7. Using the solved internal field coefficients, the tangential components

$$\vec{n} \times \vec{E}_{inside} \quad \text{and} \quad \vec{n} \times \vec{H}_{inside}$$

can be obtained, and the scattered field, when substituted into the integral equation

in matrix form:

$$\begin{bmatrix} p \\ q \end{bmatrix} = - \begin{bmatrix} Rg Q_{11} & Rg Q_{12} \\ Rg Q_{21} & Rg Q_{22} \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix}$$

8. The T -matrix is:

$$T = -Rg Q Q^{-1}$$

Validity of TMM

- due to the singularity of Green's function, the expansion is only valid for the regions outside the circumscribing sphere ($r > r_{\text{sph}}$)
- according to Rayleigh hypothesis the expansion is valid anywhere outside the boundary, but this has never been proved/disproved
- some investigations (Doicu, 1999) imply that it may not be valid in certain cases
- convex shape is not required in the TMM formulation (proved by Waterman, 1979)

Practical matters

- in practical applications, particle symmetries are used to enhance the computational speed, and codes are used only on certain simple shapes like spheroids, finite circular cylinders etc.
- if the particle has a rotational symmetry with respect to the Z-axis, all surface integrals reduce to single integrals over the polar angle (θ), and the T -matrix becomes symmetric with respect to the azimuth angle (ϕ)
- the integrals can be easily evaluated with Gauss quadrature or the trapezium rule
- it is also possible to factor out the shape dependence $R(\theta, \phi)$ in the expansions, this allows efficient computation for general star-like shapes, such as Gaussian random spheres

Advantages of TMM

- computationally fast for rotationally symmetric particles, $O(N^6)$ for computing Q and RgQ matrices, DDA is a magnitude slower $O(N^7)$ (N is number of coefficients)
- exact solution for many nonspherical particles, largest simulated cylinder about $x=160$
- for particles with spherical symmetry, it is the same as Mie theory
- when the T -matrix of a particle in any orientation is known, it can be computed in any other orientation a lot faster than doing the T -matrix computations again
- T -matrix itself is a function of particle shape, size, refractive index, and orientation, but is independent on incident polarization and direction as well as the scattered direction
- orientation averaging can be done analytically using Euler angle rotations, and it can be about a factor of several tens faster than doing the numerical integration

Maximum size for T -matrix computations $X = 160$

What it means in physical units for a sphere diameter in different wavelengths:

- Near UV 0.1 μm , 5 μm
- Visible 0.6 μm , 30 μm
- W-band radar 2.7 mm, 138 mm
- C-band radar 4 cm, 204 cm

Limitations of TMM

- for particles with no symmetry, TMM is generally not faster than DDA
- no available TMM codes for general starlike particles
- applicable only for homogeneous particles, but can be extended to a layered structure
- small errors in the Q-matrix can become large errors in Q^{-1} , these errors increase as size or aspect ratio is increased

More limitations for T -matrix method

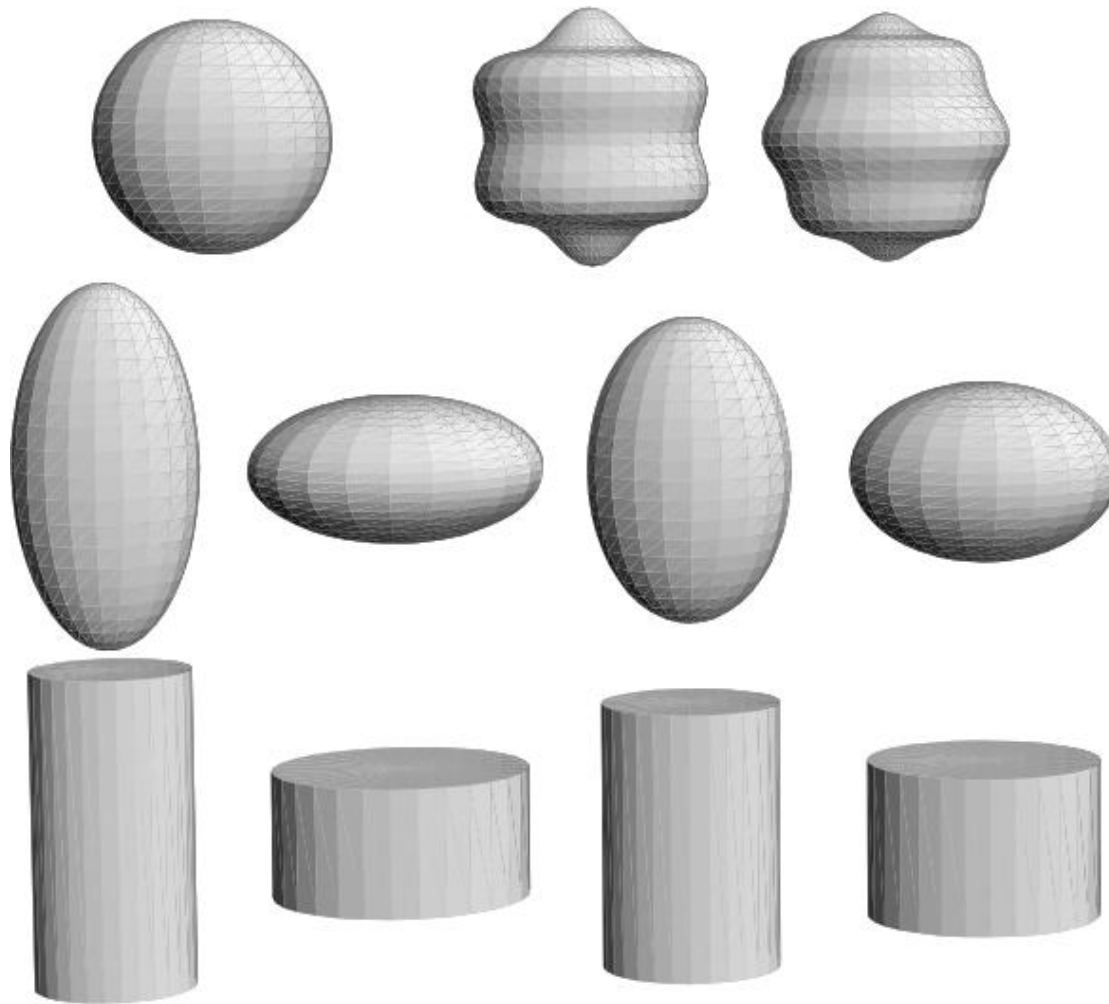
- When approaching very large size parameters, the additional memory space needed for the analytical orientation may become significant. In those cases the fixed orientation version with numerical averaging might be beneficial.
- Recent studies [1] suggest that there are sources of severe numerical instabilities in the way the surface integrals are computed numerically in the extended boundary condition method. These are independent of the possible errors in the Q -matrix inversion.
- With difficult cases, the convergence is sometimes reached, sometimes not, but the convergence limit seems arbitrary.
- The T -matrix method is very precise to a certain level when it converges. However, it can be difficult to improve the accuracy by introducing more terms to the series, due to numerical problems. In DDA the accuracy will improve when the size of a single dipole is decreased.

[1] Somerville, Auguie, LeRu (2012). Severe loss of precision in calculations of T -matrix integrals. *JQSRT* **113**.

TMM applications

- shapes that can be modeled with the available TMM codes:
 - spheroids
 - finite circular cylinders
 - Chebyshev-polynome shapes
 - finite polyhedral cylinders
 - cluster of spheres (uses the T -matrix formalism)
- in the near future, general star-like geometries will (hopefully) be publicly available

Axisymmetric geometries for T -matrix



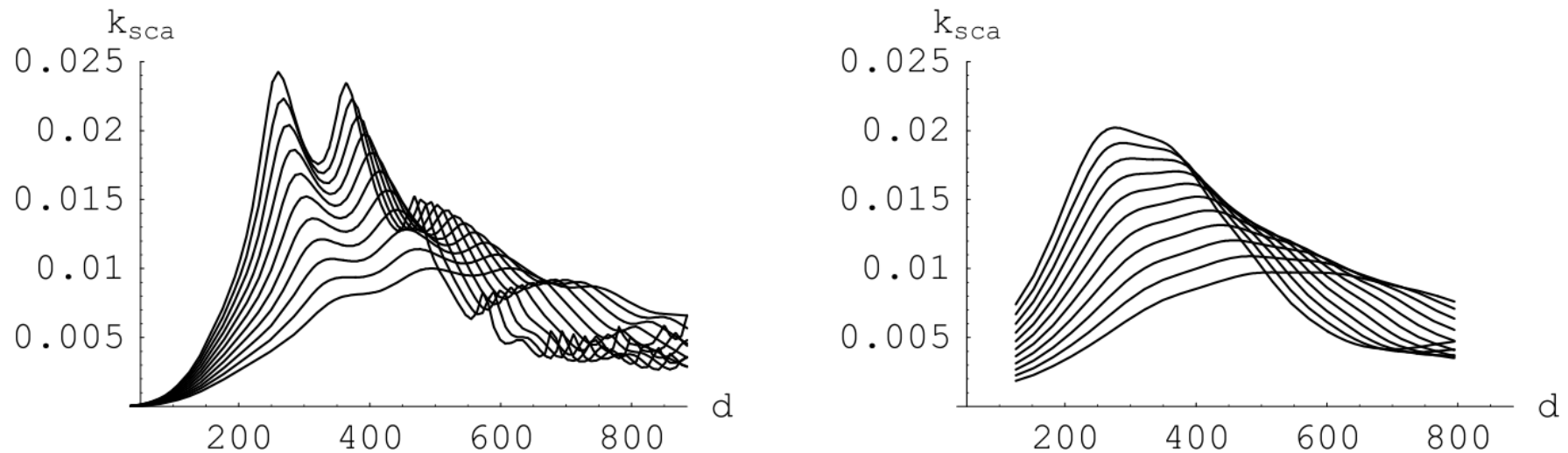
Sphere, Chebyshev particles, spheroids, circular cylinders

Computer implementation of the T -matrix method

- Several exists, but probably the most popular are the fixed- and analytical orientation codes by Mishchenko
- Written in Fortran 77, publically available.
 - + Well tested, efficient, several shapes
 - No dynamical memory allocation, problem with difficult cases
 - Problematic if difficulties in convergence
 - Input coded inside program, requires compiling for each set of input parameters
- Includes possibility to average over size distribution, several possibilities for a size distribution.
- Produces: Extinction and scattering cross-sections, asymmetry parameter, expansion coefficients and scattering matrix elements as a function of scattering angle.

Why size distribution is important?

Perfect shapes (spheres, spheroids etc.) do not exist in nature. Naturally-occurring particles have always size distribution. Especially sphere, which is perfectly symmetric, has strong fluctuations in its scattering behavior, which is rarely seen in practice.



k_{sca} (scattering coefficient, scattering cross section C_{sca} divided by the volume) as a function of sphere diameter with n_{re} running from 1.5 (starting at lowest) to 2 (starting at highest) and n_{im} as 0.001. The figure on the left is for the exact-sized particles, and on the right is the result after convolution with the size distribution.

TMM applications: spheroids

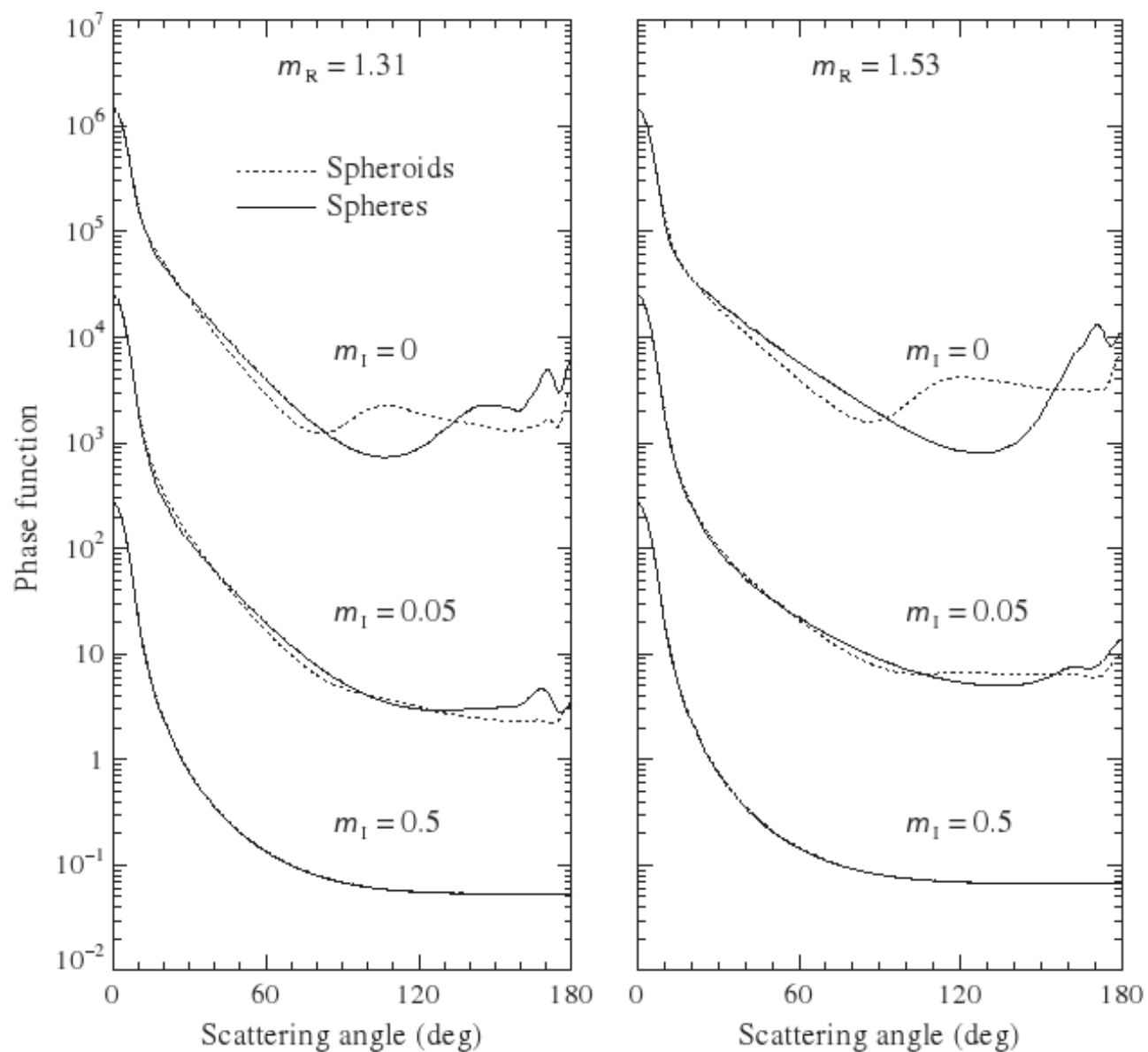


Figure 10.15. Phase function α_1 versus scattering angle Θ for polydisperse, randomly oriented oblate spheroids with an axis ratio 1.7 and for surface-equivalent spheres. The results are shown for two values of the real part of the relative refractive index ($m_R = 1.31$ and 1.53) and three values of the imaginary part ($m_I = 0, 0.05$, and 0.5). The size distribution is given by Eq. (5.246) with $\alpha = -3$ and $\nu_{\text{eff}} = 0.1$. The effective size parameter is $x_{\text{eff}} = 15$. The vertical axis scale applies to the curves with $m_I = 0.5$, the other curves being successively displaced upward by a factor of 100.

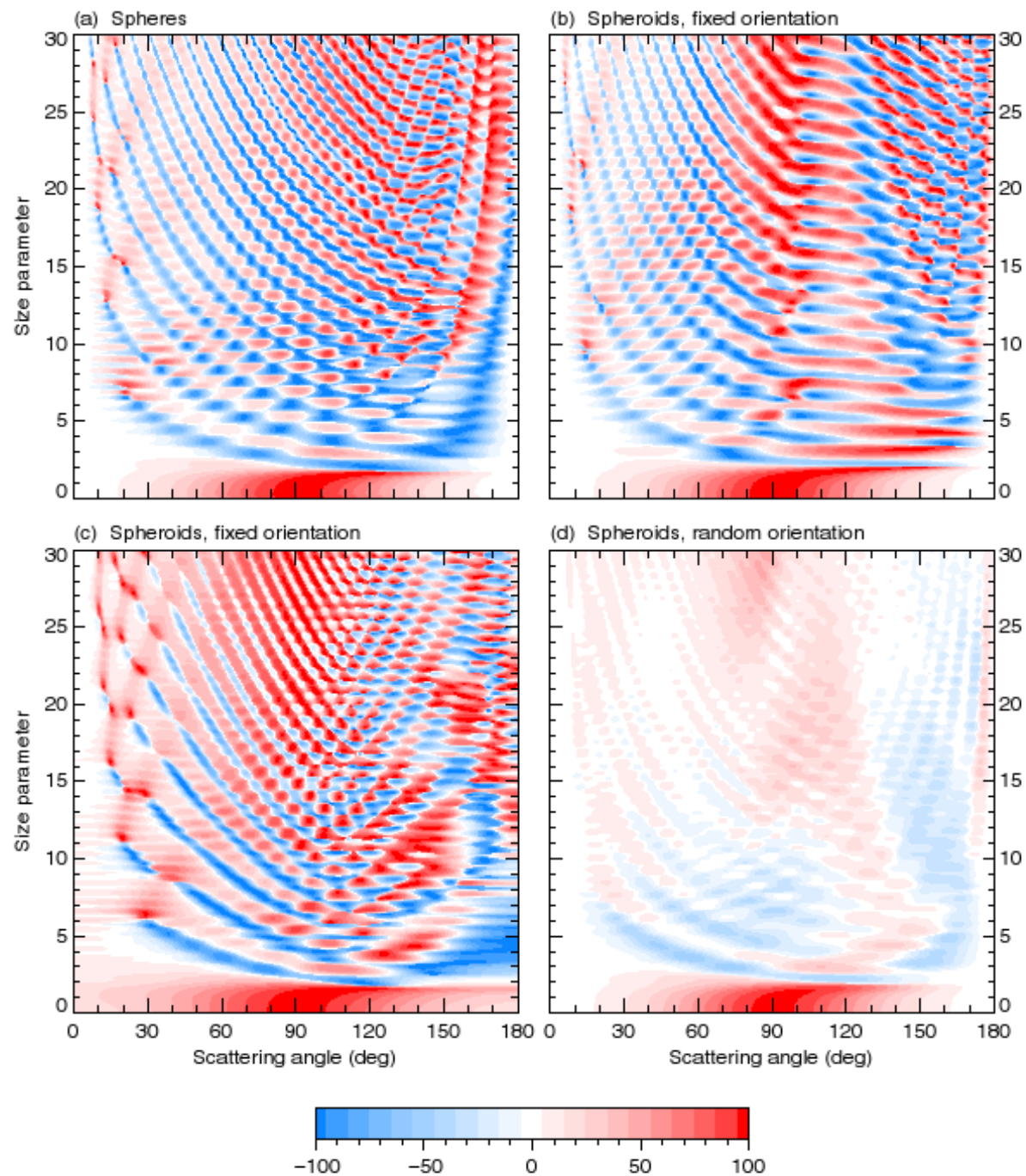


Plate 10.1. The ratio $-Z_{21}(\vartheta^{sca}, \varphi^{sca} = 0; \vartheta^{inc} = 0, \varphi^{inc} = 0) / Z_{11}(\vartheta^{sca}, \varphi^{sca} = 0; \vartheta^{inc} = 0, \varphi^{inc} = 0)$ in % versus ϑ^{sca} and size parameter for monodisperse spheres and surface-equivalent oblate spheroids in fixed 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 $a/b = 1.7$.

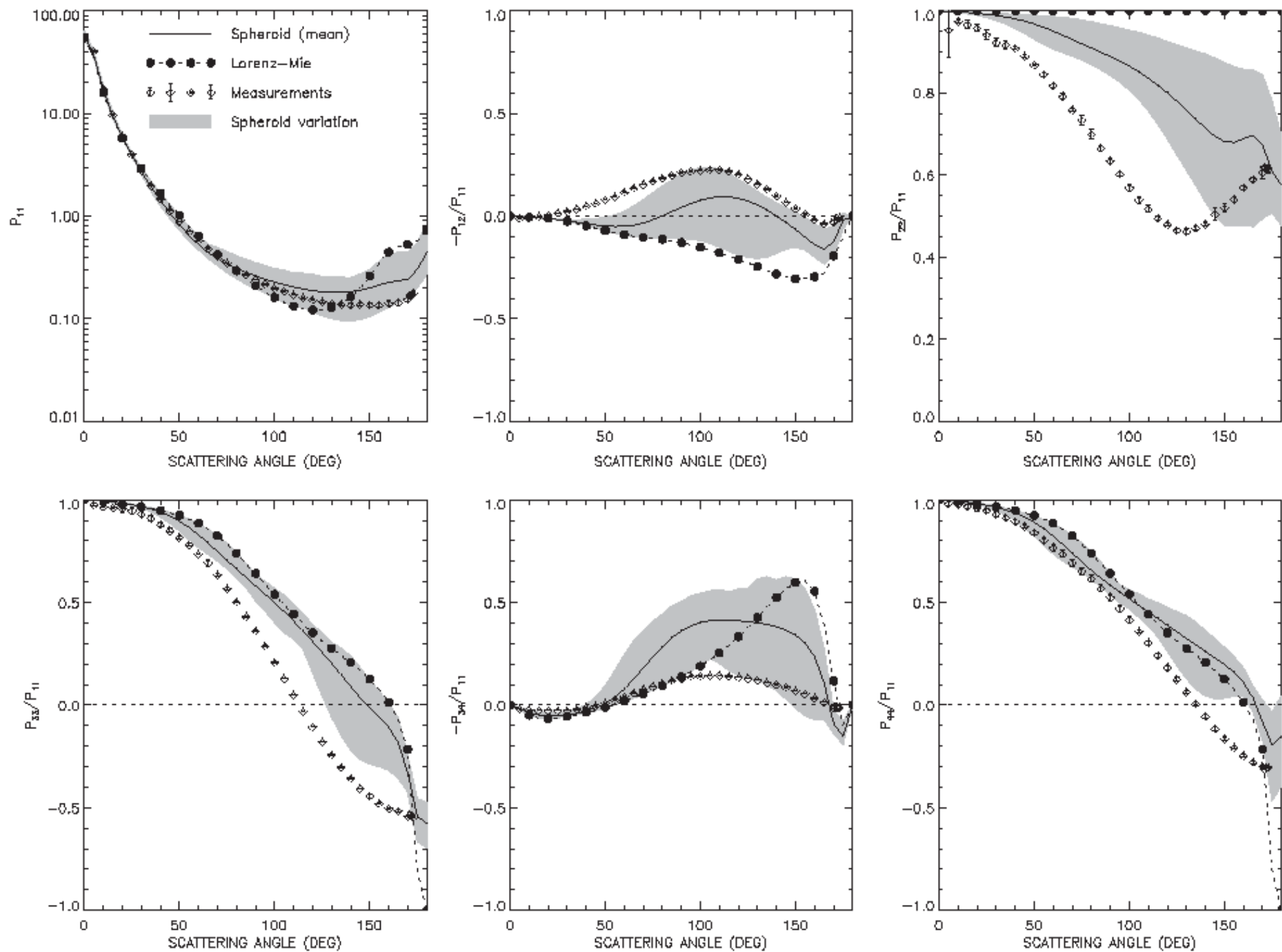


Fig. 3. Same as Fig. 2, except for equi-probable distribution of oblate spheroids.

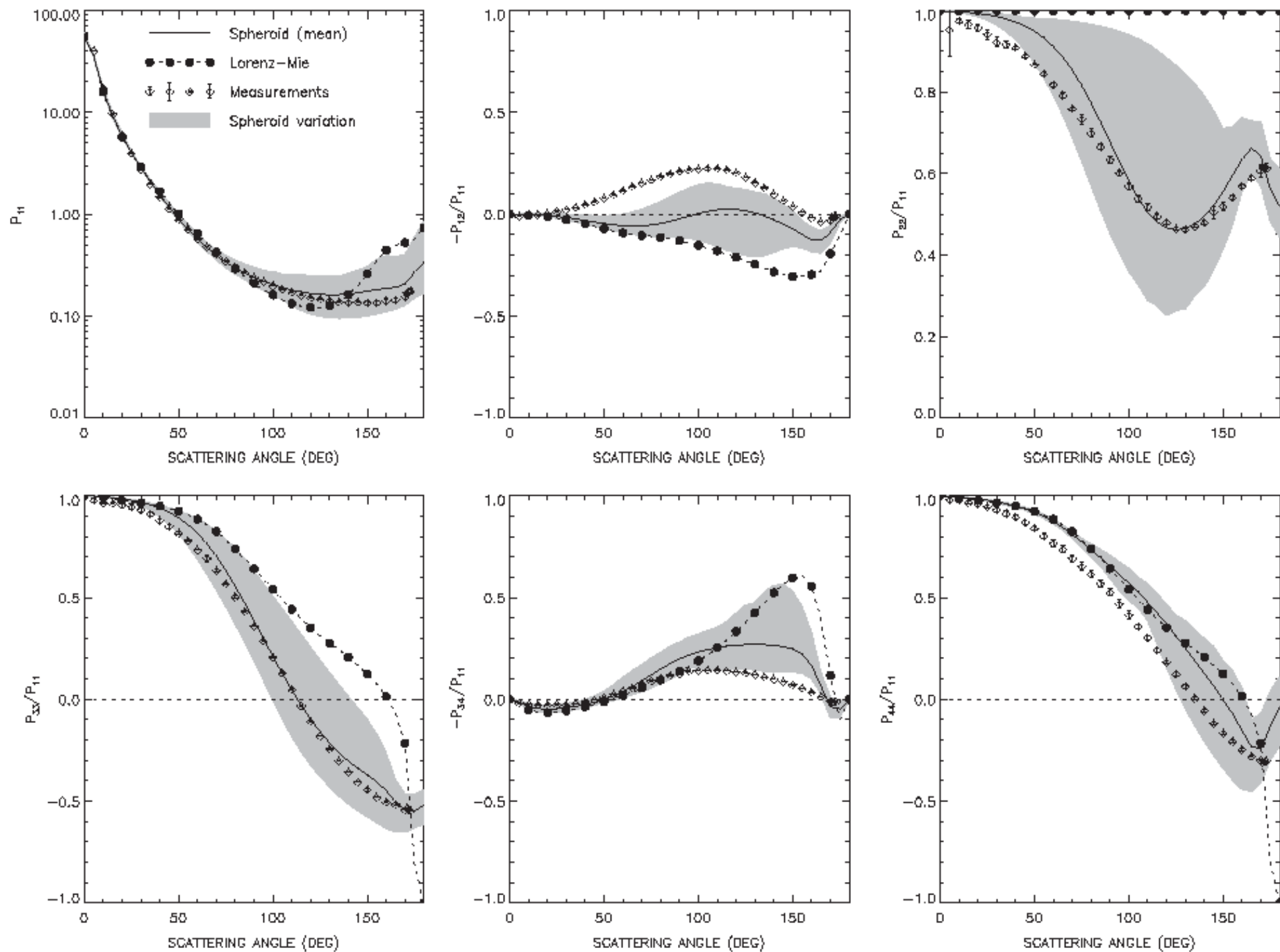


Fig. 4. Same as Fig. 2, except for equi-probable distribution of prolate spheroids.

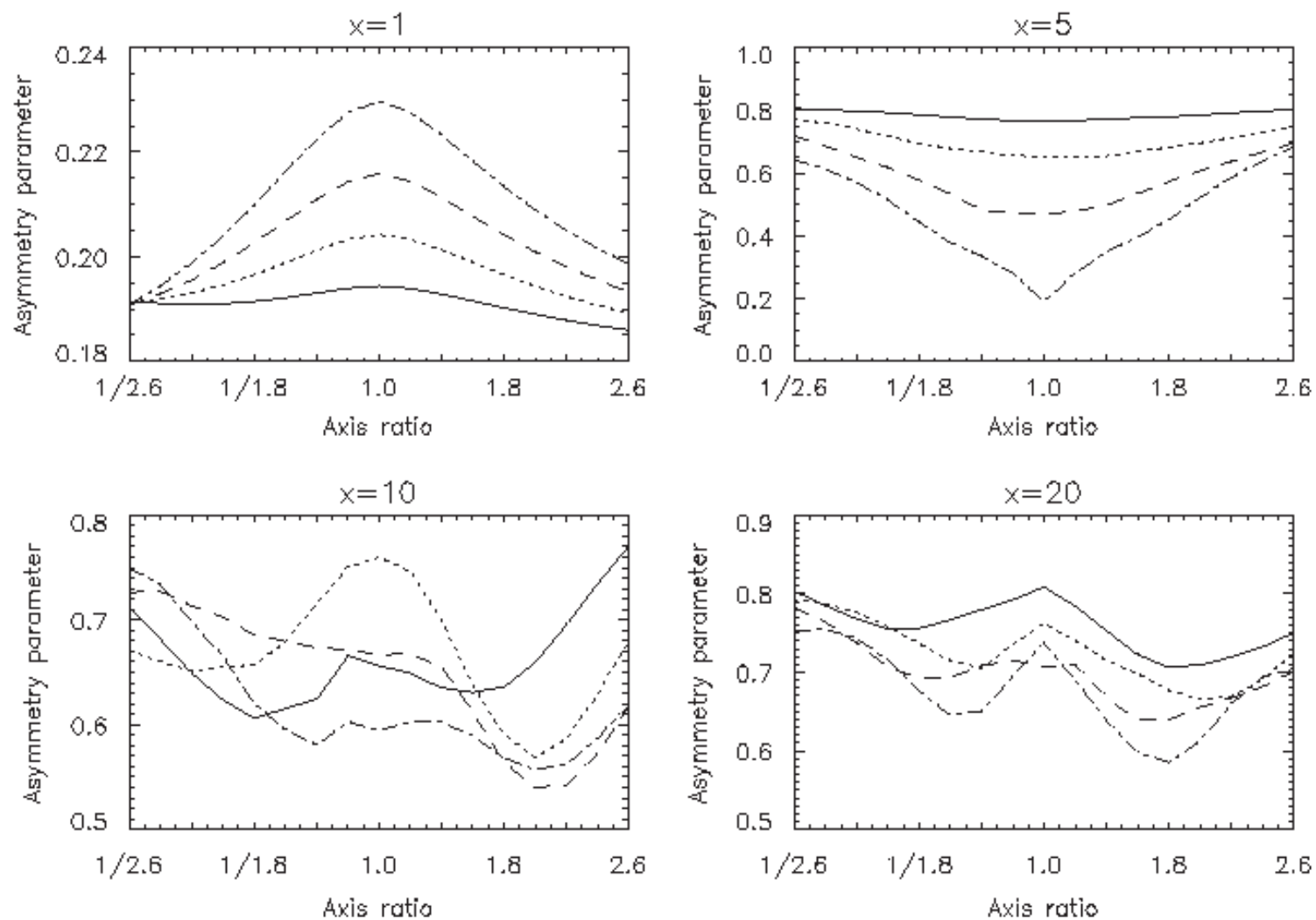


Fig. 2. As Fig. 1 but for $\text{Re}(m)$ values of 1.45 (solid line), 1.55 (dotted line), 1.65 (dashed line), and 1.75 (dash-dotted line). $\text{Im}(m)$ has been fixed to 0.001.

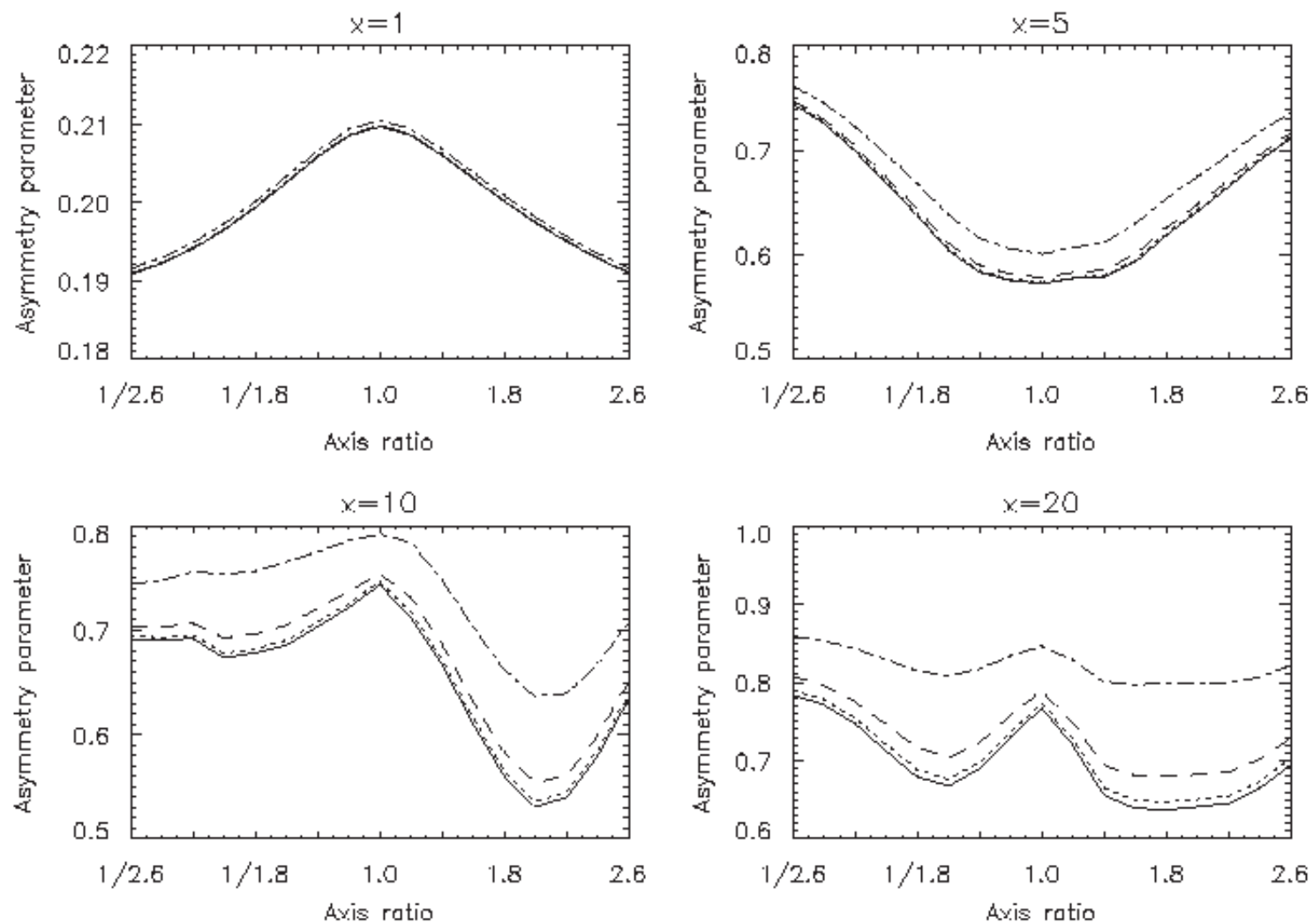


Fig. 1. The dependence of the asymmetry parameter g on the spheroid axis ratio. The panels show the results for size parameters 1, 5, 10, and 20. The different lines stand for $\text{Im}(m)$ values of 0.0001 (solid line), 0.0005 (dotted line), 0.002 (dashed line), and 0.01 (dash-dotted line). $\text{Re}(m)$ has been fixed to 1.6.

TMM applications: cylinders

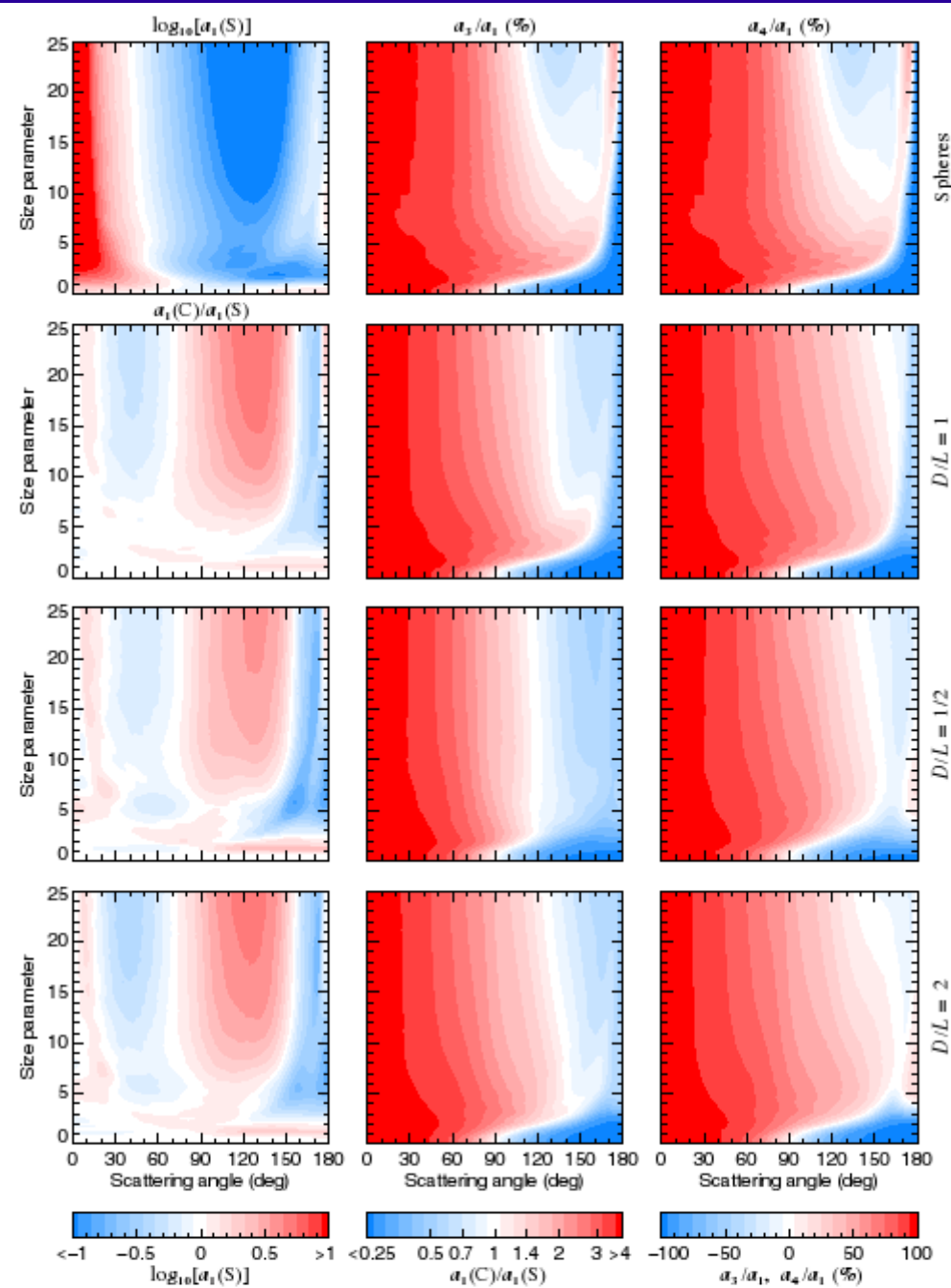


Plate 10.5. The top left panel shows the logarithm of the phase function versus scattering angle and effective size parameter for polydisperse spheres. The three lower diagrams in the left-hand column show the ratio of the phase function $a_1(C)$ for polydisperse randomly oriented cylinders with $D/L = 1, 1/2$, and 2 and the phase function $a_1(S)$ for surface-equivalent spheres. The middle and right-hand columns show a_3/a_1 and a_4/a_1 for spheres (top panels) and for surface-equivalent cylinders (lower three pairs of panels). Each diagram is quantified by the corresponding color bar at the bottom of the plate. All particles have the same relative refractive index, $1.53 + i0.008$. The distribution of surface-equivalent-sphere radii is given by Eq. (5.246) with $\alpha = -3$ and $v_{\text{eff}} = 0.1$.

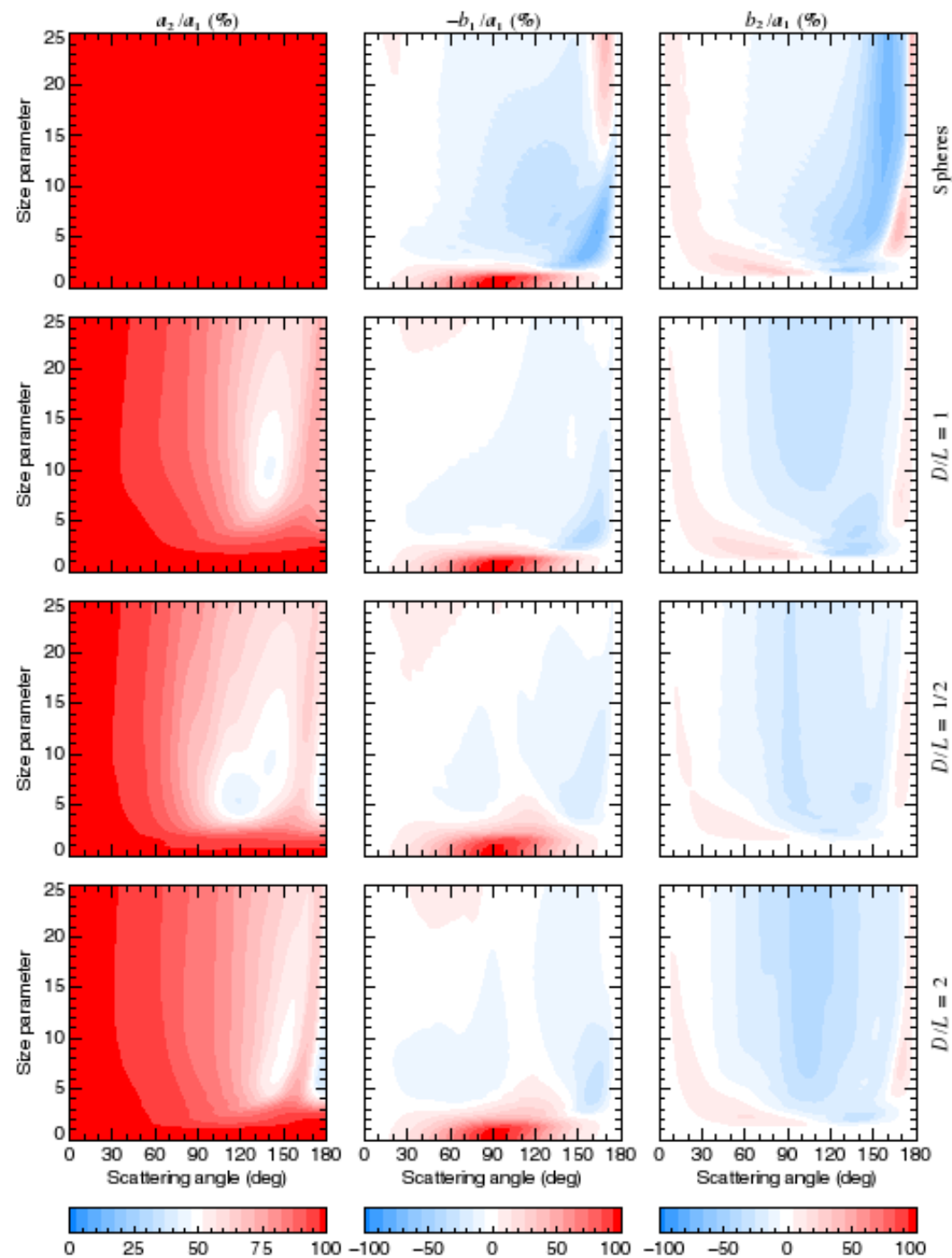


Plate 10.6. The ratios a_2/a_1 , $-b_1/a_1$, and b_2/a_1 for polydisperse spheres and for surface-equivalent randomly oriented cylinders with $D/L = 1, 1/2$, and 2. The diagrams in each column are quantified using the color bar below the column. All particles have the same relative refractive index, $1.53 + i0.008$. The distribution of surface-equivalent-sphere radii is given by Eq. (5.246) with $\alpha = -3$ and $v_{eff} = 0.1$.

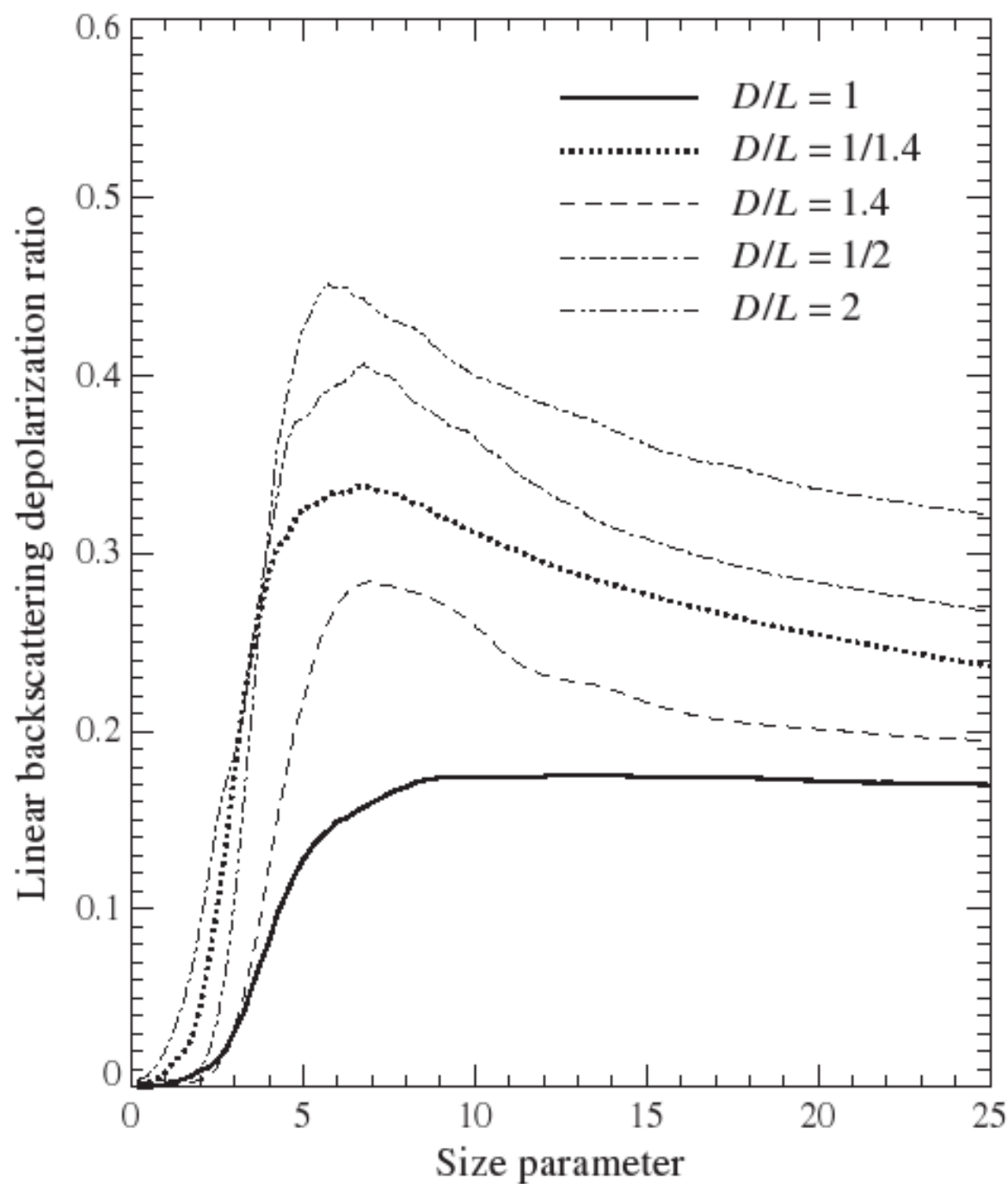


Figure 10.26. Linear backscattering depolarization ratio versus effective size parameter for randomly oriented polydisperse cylinders.

TMM applications: Chebyshev shapes

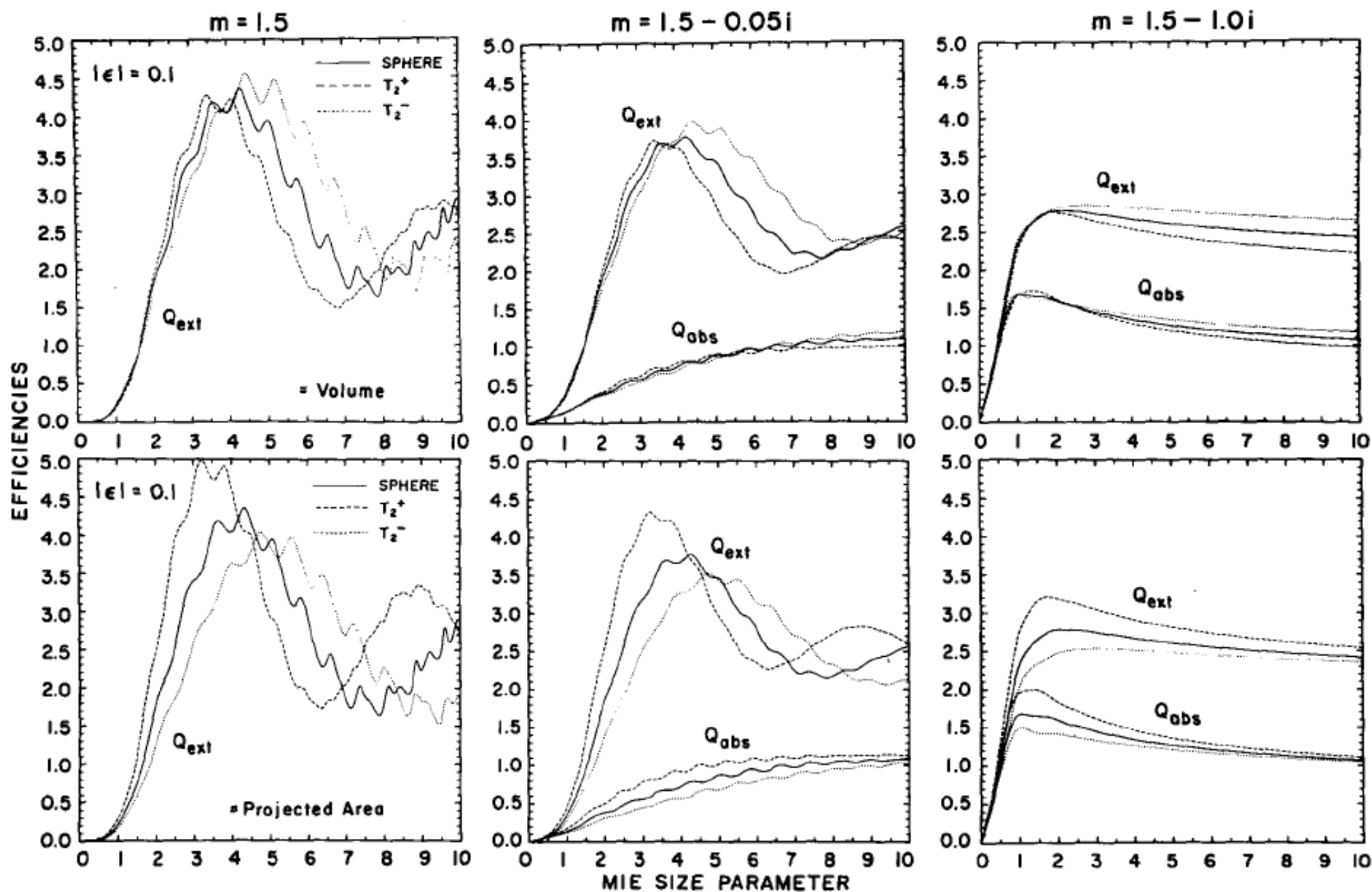


FIG. 3. Q_{ext} and Q_{obs} versus x_{ev} (top row) and versus x_{epa} (bottom row) for T_2^\pm particles with $|\epsilon| = 0.1$ at nose-on incidence. Corresponding results for a sphere are also shown. Refractive indices of 1.5, $1.5 - 0.05i$, and $1.5 - i$ in the three columns, respectively.

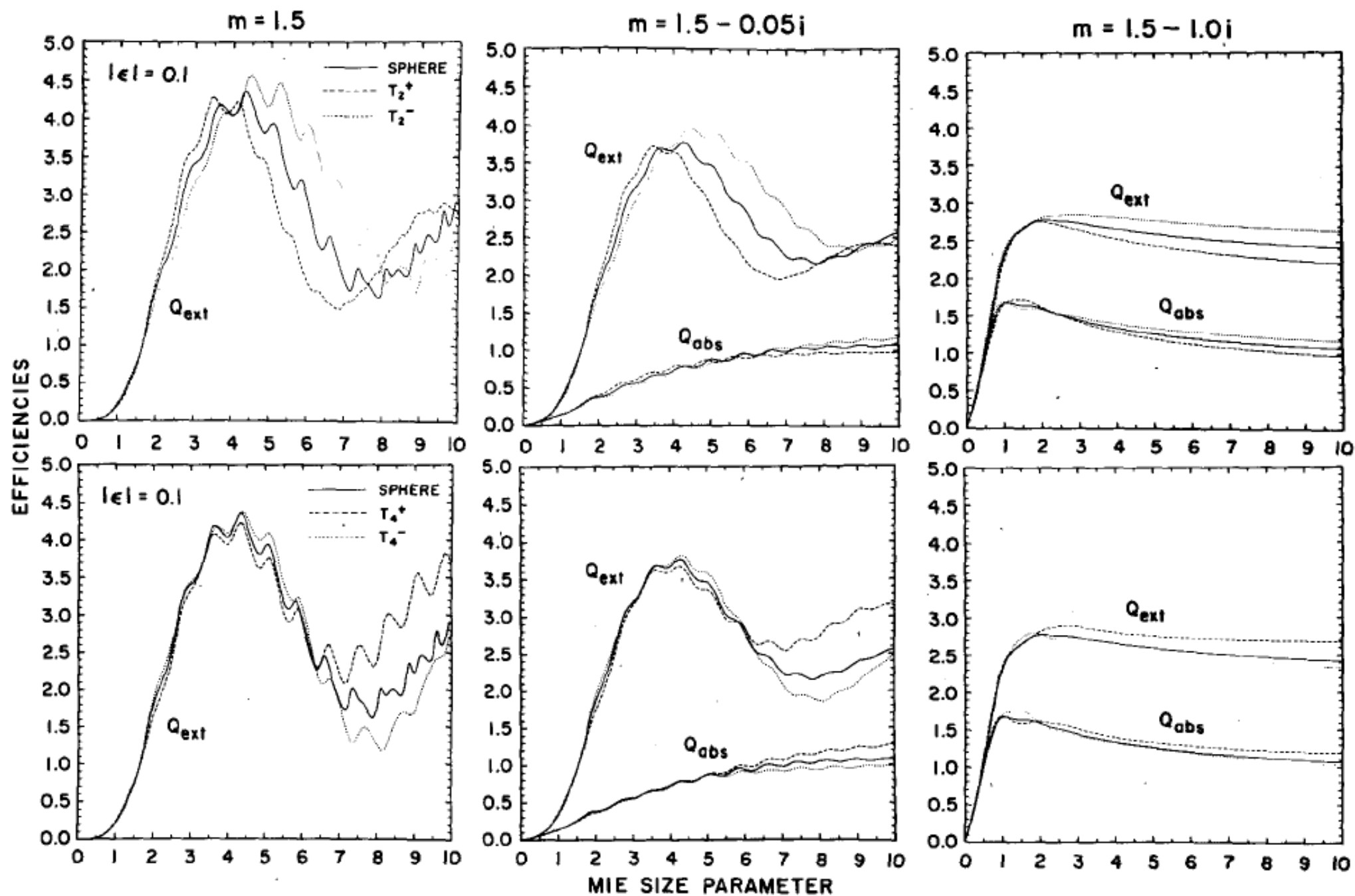


FIG. 4. Q_{ext} and Q_{abs} versus x_{ev} for T_2^\pm (top row) and T_4^\pm (bottom row) particles with $|\epsilon| = 0.1$ at nose-on incidence. Also corresponding spherical results.

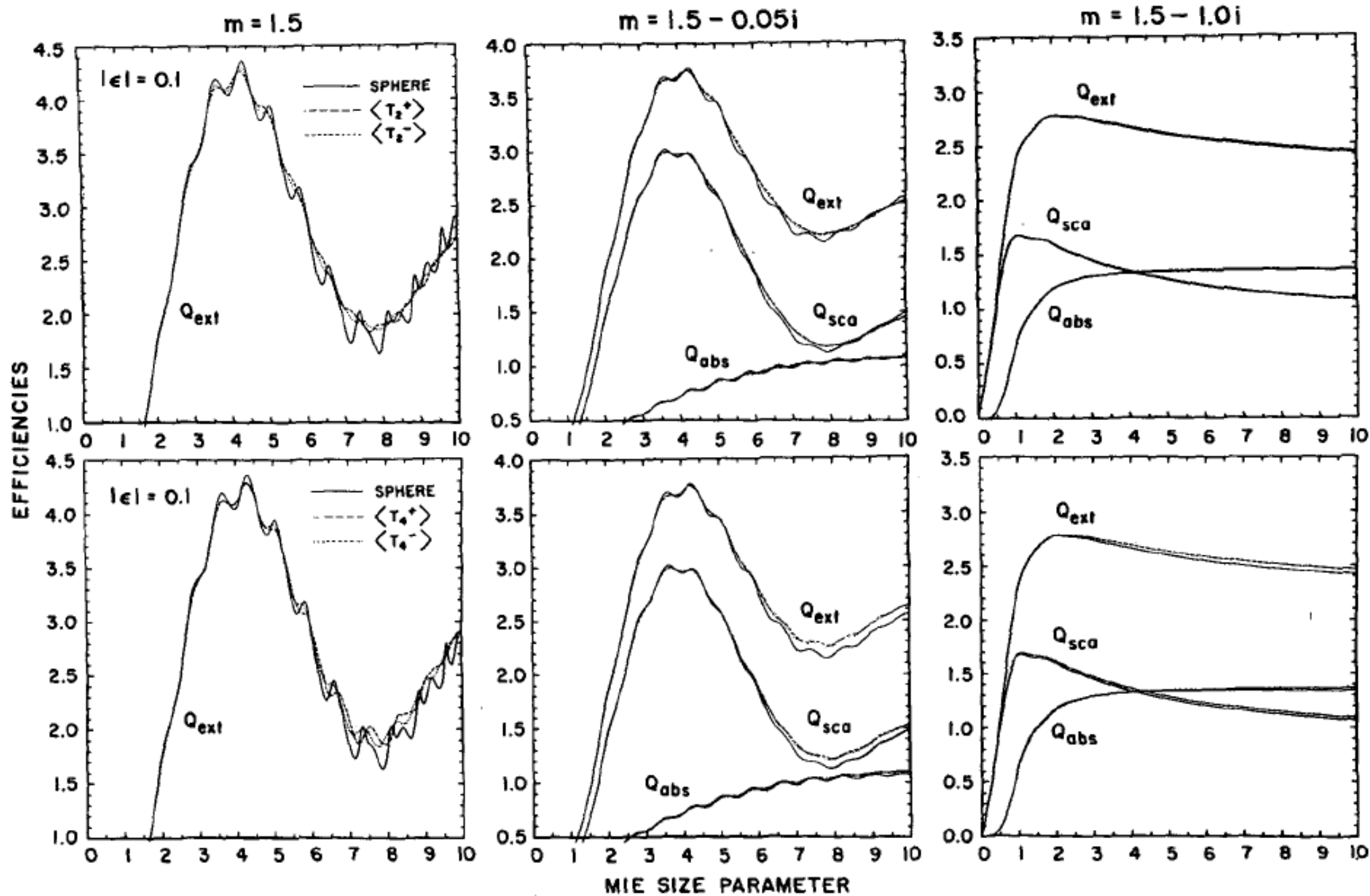


FIG. 5. Q_{ext} and Q_{abs} versus x_{ev} for randomly oriented T_2^\pm (top row) and T_4^\pm (bottom row) particles with $|\epsilon| = 0.1$. Also corresponding spherical results.

TMM applications: Prisms

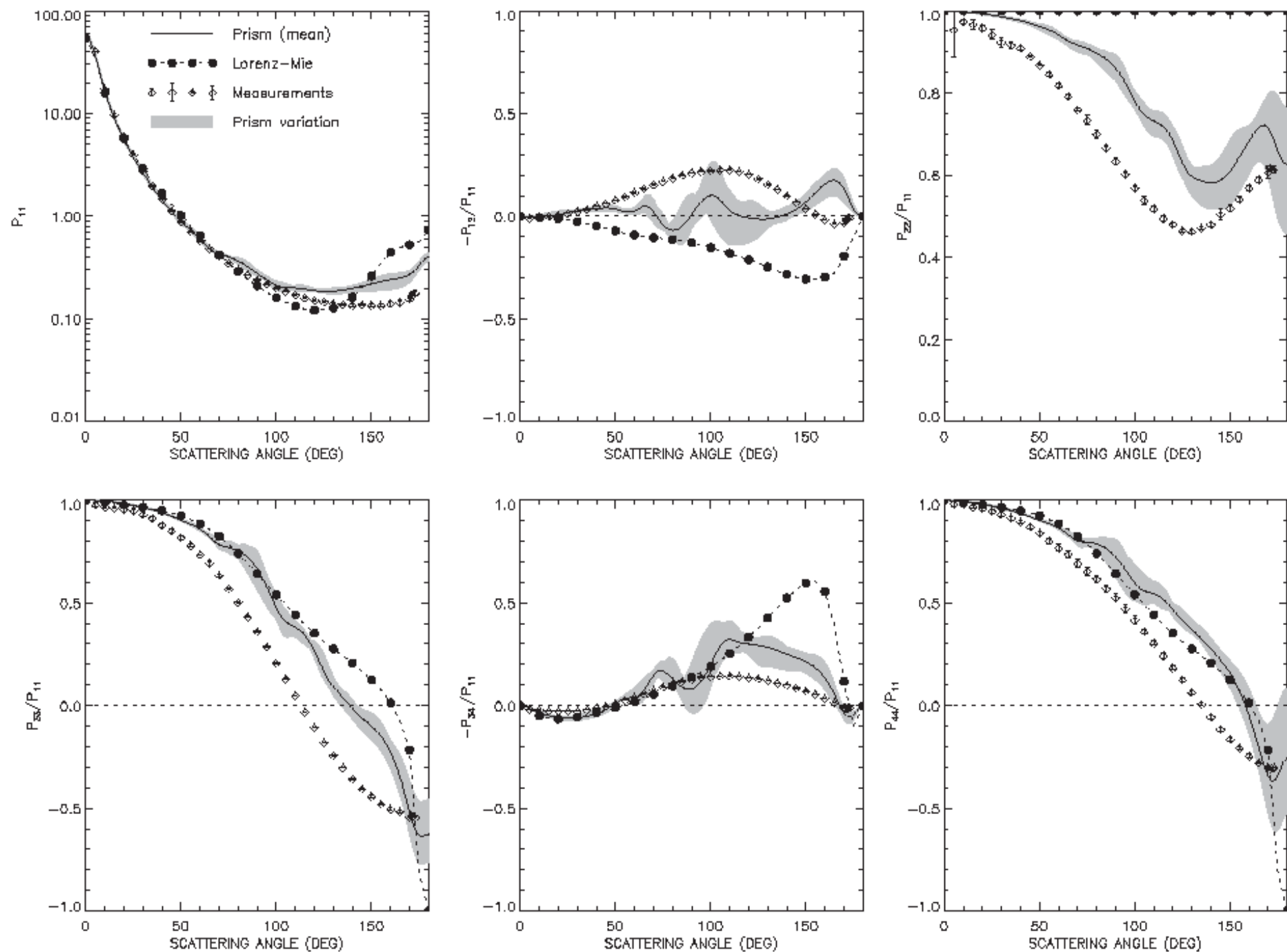


Fig. 2. Comparison of the laboratory measurement with light scattering simulations based on an equi-probable distribution of all 12 different model polyhedral prisms. A Lorenz-Mie solution for perfect spheres is shown for comparison.

TMM applications: Bi-spheres

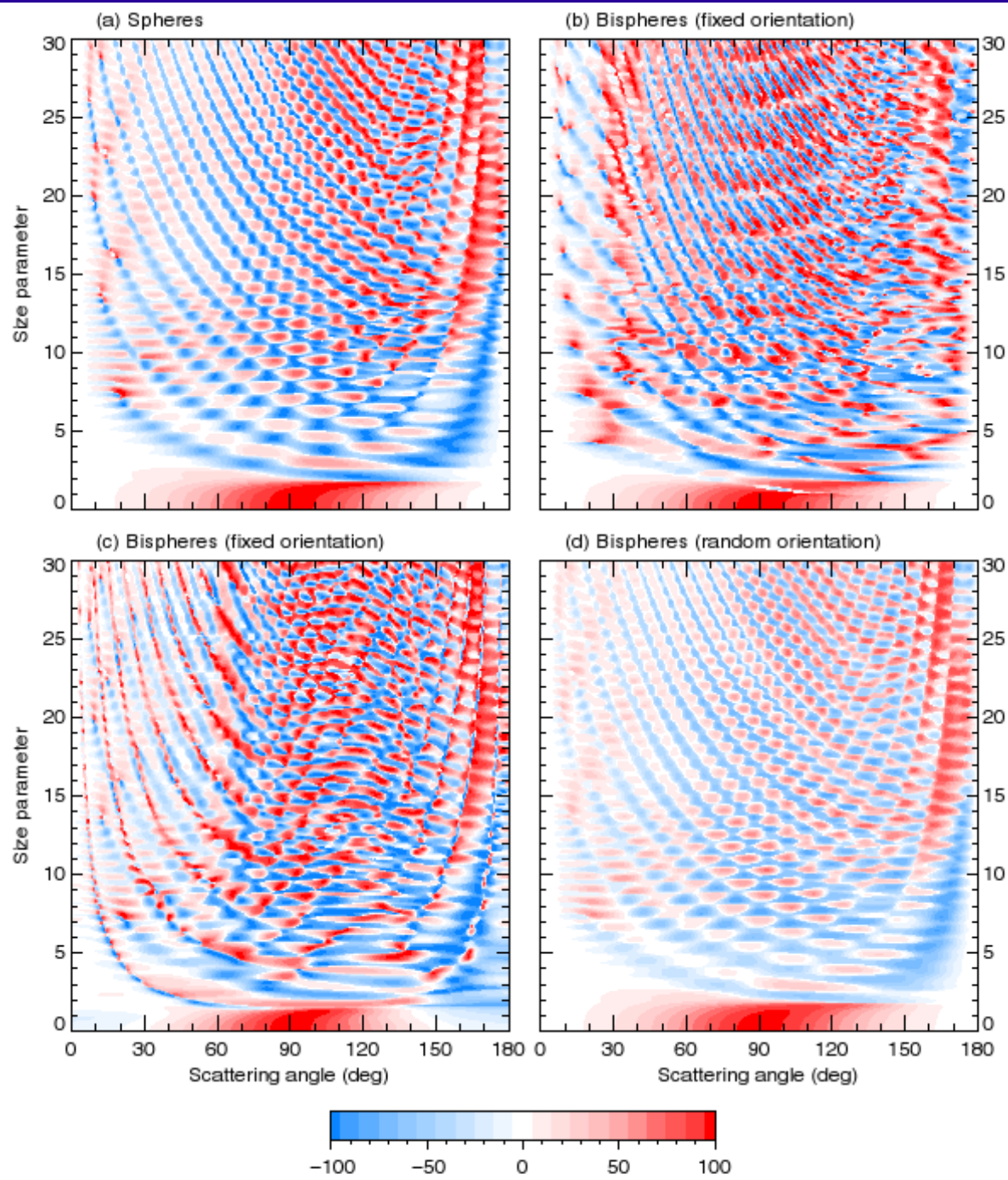


Plate 10.8. Panel (a): the ratio $-Z_{21}(\vartheta^{ca}, \varphi^{ca}=0; \vartheta^{inc}=0, \varphi^{inc}=0) / Z_{11}(\vartheta^{ca}, \varphi^{ca}=0; \vartheta^{inc}=0, \varphi^{inc}=0)$ in % versus ϑ^{ca} and size parameter for monodisperse single spheres. Panels (b)–(d): the same ratio versus ϑ^{ca} and constituent-sphere size parameter for monodisperse bispheres with equal touching components in fixed and random orientations. In panels (b) and (c) the bisphere axis is oriented respectively along the z -axis and along the x -axis of the laboratory reference frame. The relative refractive index is $1.5 + i0.005$.

Available TMM codes

- Thomas Wriedt: www.t-matrix.de
- Michael Mishchenko:
http://www.giss.nasa.gov/staff/mmishchenko/t_matrix.html
- Daniel Mackowski:
<http://www.eng.auburn.edu/users/dmckwski/scatcodes/>
- Yu-lin Xu: <http://www.scattport.org/files/xu/codes.htm>