Lorenz-Mie Scattering

Topics:
1. Lorenz-Mie theory
2. Scattering amplitudes/phase matrix
3. Mie scattering results: extinction, absorption, phase function vs. x
4. Anomalous Diffraction Theory
5. Index of refraction for water/ice/aerosols
6. Mie scattering results for size distributions

Reading: Liou 3.3.2& ; Thomas 9.3

Lorenz-Mie Theory

Mie scattering is a solution method for light scattering from spheres.
Applicable for any size parameter, but "Mie regime" $\sim\ 0.1 < x < 100$.

Overview of Mie scattering solution for spheres:
1) Express electric field inside and outside sphere in a vector spherical harmonic expansion, which satisfies Maxwell's equations.
2) Apply boundary conditions - match transverse fields at sphere surface to obtain outgoing spherical wave coefficients a_n and b_n.
3) Use series involving a_n and b_n to obtain extinction and scattering efficiencies (Q_{ext} and Q_{sca}).
4) Use series in Mie angular functions to obtain scattering amplitude functions $S_1(\Theta)$ and $S_2(\Theta)$, from which phase function is derived.

Scattering Amplitudes

Complex functions that describe pattern and polarization of scattered electric field in terms of the incident field.

The electric field in the *far field* ($R \gg kr^2, \;\; k = 2\pi/\lambda$) is

$$\begin{bmatrix} E_{\parallel} \\ E_{\perp} \end{bmatrix}_{sca} = \frac{\exp(-ikR + ikz)}{ikR} \begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix} \begin{bmatrix} E_{\parallel}^0 \\ E_{\perp}^0 \end{bmatrix}$$

The matrix $\begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix}$ is the amplitude scattering matrix (unitless).
For spheres $S_3 = S_4 = 0$.
The $\exp(ikz)$ is the incident plane wave. $\frac{\exp(-ikR)}{ikR}$ is the outgoing scattered wave.

Fundamental extinction formula (*optical theorem*):

$$\sigma_{ext} = C_{ext} = \frac{4\pi}{k^2}\mathrm{Re}[S_{1,2}(0°)]$$

Extinction cross section is related to scattering in forward direction.

Phase Matrix

The phase matrix is the phase function with polarization.
For randomly oriented particles it is

$$\begin{bmatrix} I_{sca} \\ Q_{sca} \\ U_{sca} \\ V_{sca} \end{bmatrix} = \frac{\sigma_{sca}}{4\pi R^2} \begin{bmatrix} P_{11} & P_{12} & 0 & 0 \\ P_{12} & P_{22} & 0 & 0 \\ 0 & 0 & P_{33} & P_{34} \\ 0 & 0 & -P_{34} & P_{44} \end{bmatrix} \begin{bmatrix} I_0 \\ Q_0 \\ U_0 \\ V_0 \end{bmatrix}$$

Each element depends on scattering angle ($1/R^2$ is from solid angle).
For spheres $P_{22} = P_{11}$ and $P_{44} = P_{33}$.
The off diagonal terms are usually small for Mie scattering, so polarization does not affect intensity (then need only P_{11} for I).
Intensity component of phase matrix

$$P_{11}(\Theta) = \frac{4\pi}{k^2\sigma_{sca}}\frac{|S_1|^2 + |S_2|^2}{2}$$

Mie Scattering Amplitudes

Mie theory scattering amplitudes

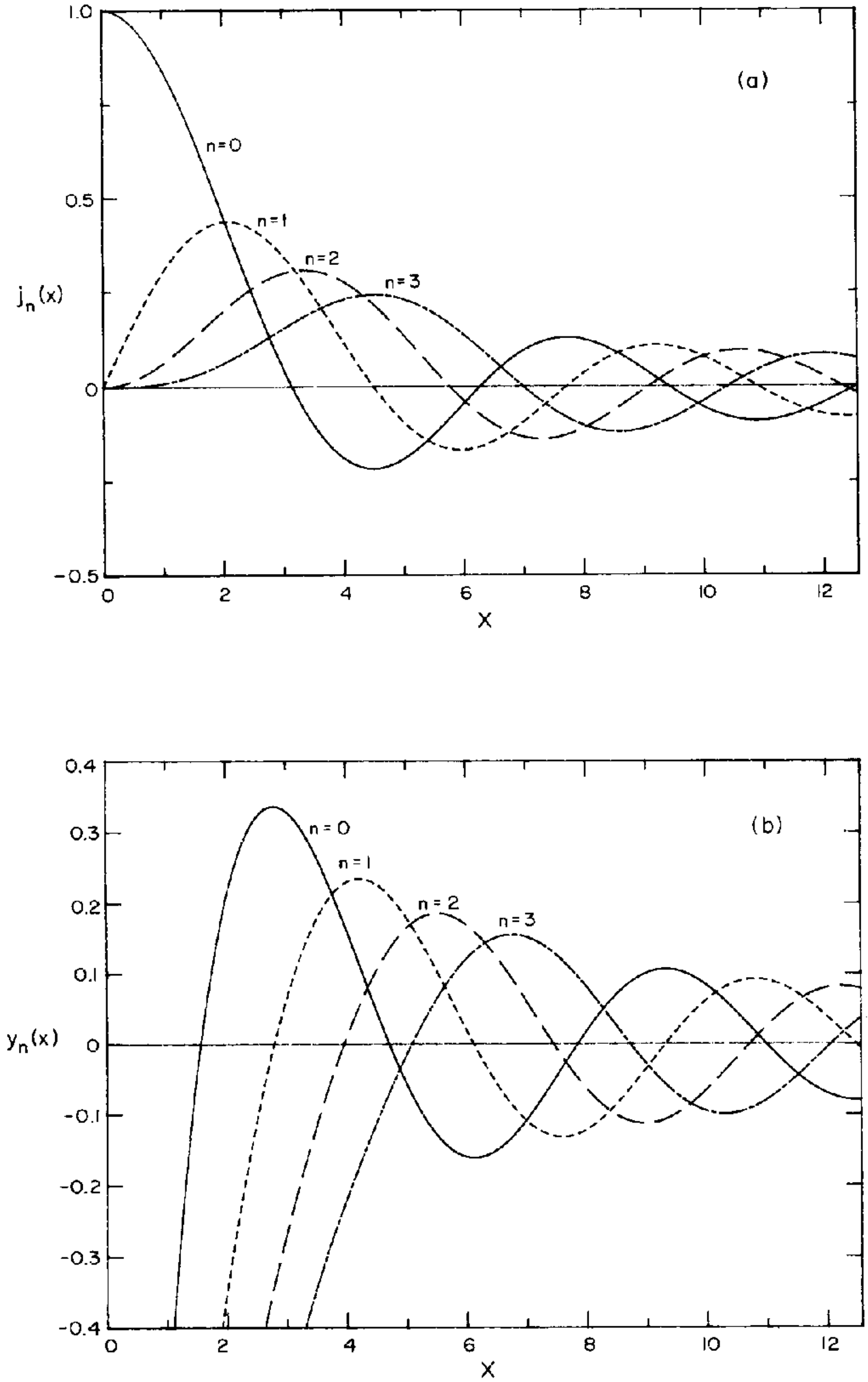
$$S_1(\Theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)}[a_n\pi_n(\cos\Theta) + b_n\tau_n(\cos\Theta)]$$

$$S_2(\Theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)}[b_n\pi_n(\cos\Theta) + a_n\tau_n(\cos\Theta)]$$

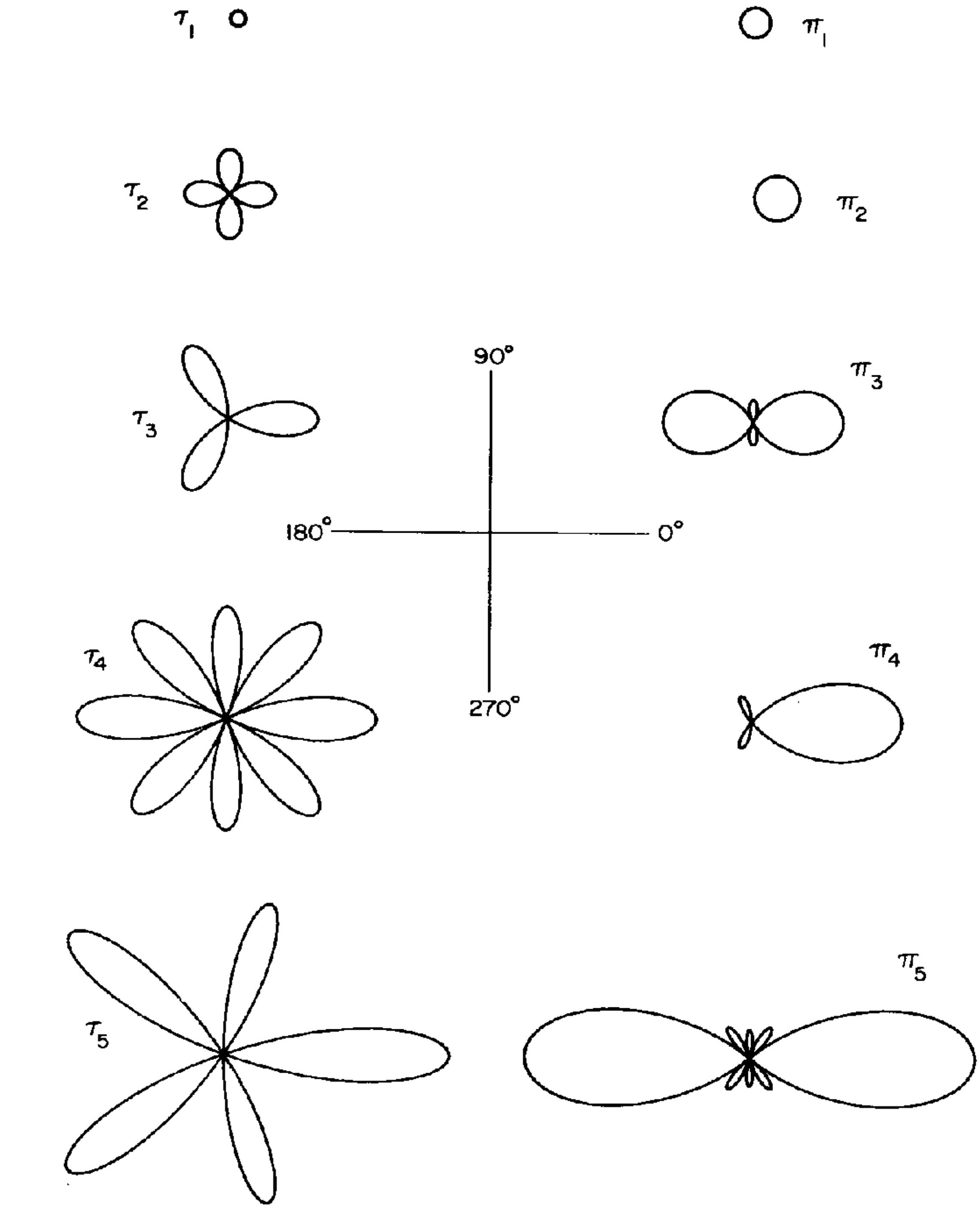
The complex Mie coefficients a_n and b_n are obtained from matching the boundary conditions at the surface of the sphere. They are expressed in terms of spherical Bessel functions evaluated at x and mx.
The Mie angular functions are

$$\pi_n(\cos\Theta) = \frac{1}{\sin\Theta}P_n^1(\cos\Theta) \qquad \tau_n(\cos\Theta) = \frac{d}{d\Theta}P_n^1(\cos\Theta)$$

P_n^1 are associate Legendre functions.
The number of terms needed and amount of angular structure is proportional to size parameter x.



Spherical Bessel functiuons of the first (a) and second (b) kind. [Bohren and Huffman, 1993; Fig. 4.2]



Polar plots of the first five Mie angular functions π_n and τ_n. Both functions are plotted to the same scale. [Bohren and Huffman, 1993; Fig. 4.3]

Mie Efficiency Factors

The Mie efficiency factors are derived from the scattering amplitudes.
Extinction efficiency:

$$Q_{ext} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) \mathrm{Re}(a_n + b_n)$$

Scattering efficiency:

$$Q_{sca} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1)(|a_n|^2 + |b_n|^2)$$

Asymmetry parameter:

$$Q_{sca} g = \frac{4}{x^2} \left[\sum_n \frac{n(n+2)}{n+1} \mathrm{Re}(a_n a_{n+1}^* + b_n b_{n+1}^*) \; + \; \frac{2n+1}{n(n+1)} \mathrm{Re}(a_n b_n^*) \right]$$

Mie Code Algorithm

How a Mie code works:

1. Compute a_n and b_n for $n = 1 \ldots N$ from size parameter x and index of refraction m (uses recursion relations for the spherical Bessel functions). $N \approx x + 4x^{1/3} + 2$.
2. Compute Q_{ext}, Q_{sca}, and g from a_n and b_n.
3. (optional) Compute $S_1(\Theta)$ and $S_2(\Theta)$ at desired scattering angles from a_n and b_n and $\pi_n(\Theta)$ and $\tau_n(\Theta)$ (π_n and τ_n from recursion). Compute phase matrix elements $P_{11}, P_{12}, P_{33}, P_{34}$ from S_1, S_2.
4. Integrate numerically over a size distribution $n(r)$ to get volume extinction β, single scattering albedo ω, and phase function $P(\Theta)$.

Mie Scattering Results

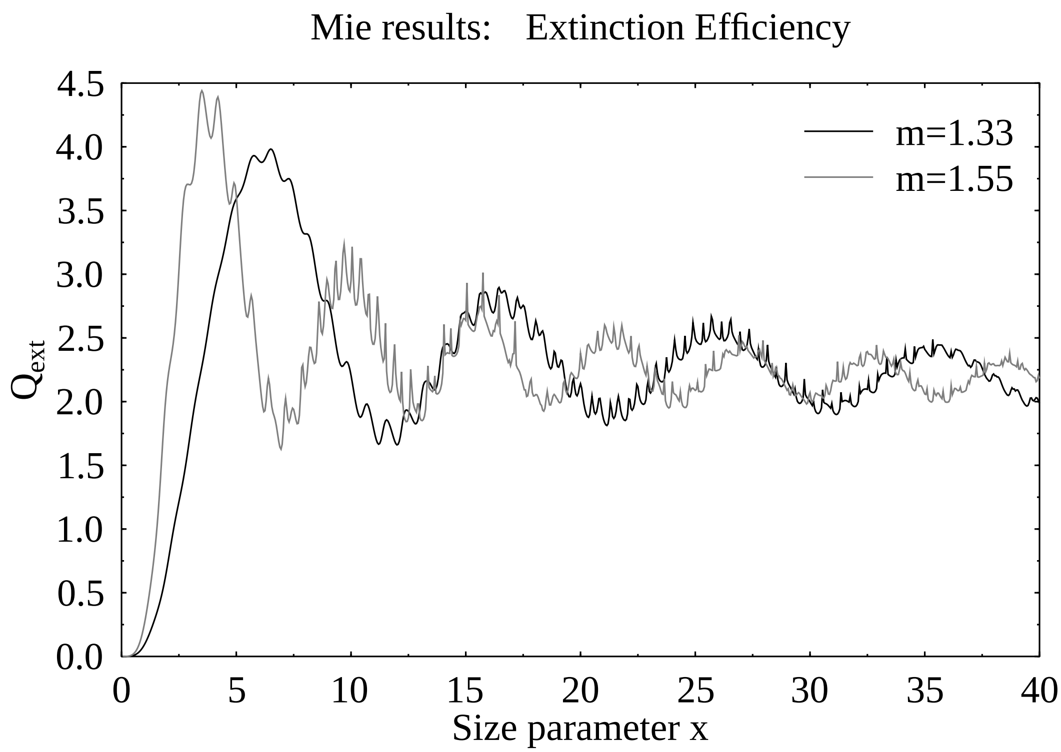
Lorenz-Mie theory applies to spheres of all size parameters x.

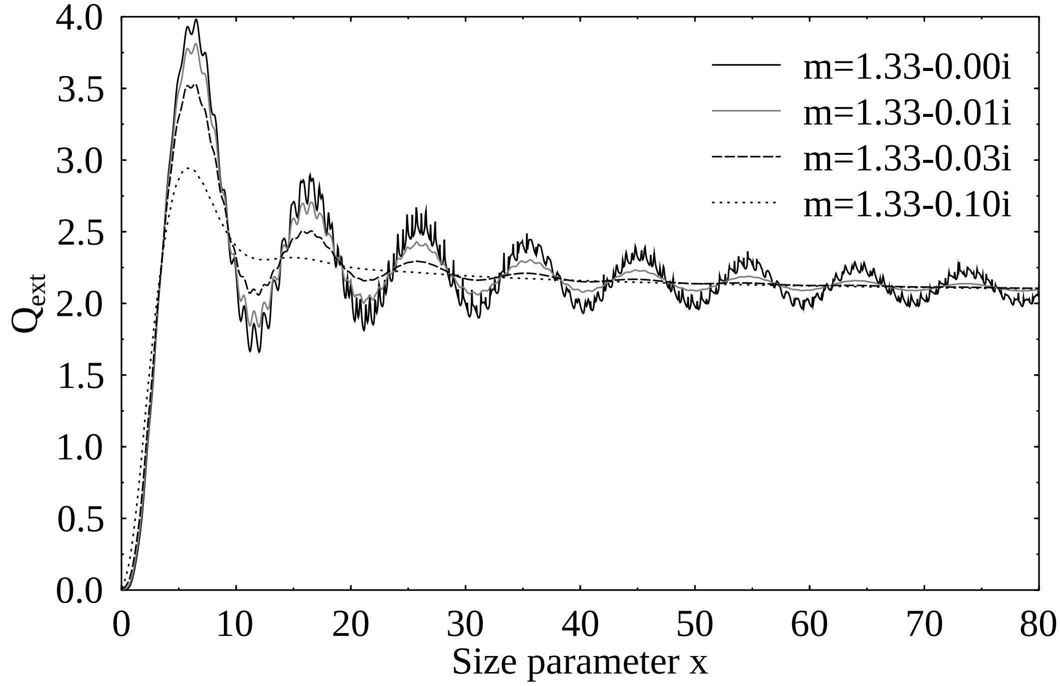
Extinction efficiency vs size parameter (no absorption):
1) Small in Rayleigh limit $Q_{ext} \propto x^4$
2) Largest Q_{ext} when particle and wavelength have similar size.
3) $Q_{ext} \to 2$ in geometric limit ($x \to \infty$).
4) Oscillations from interference of transmitted and diffracted waves.
5) Ripple structure from surface waves - resonance effects

Period in x of interference oscillation depends on m.
Absorption reduces interference oscillations and kills resonance ripples.

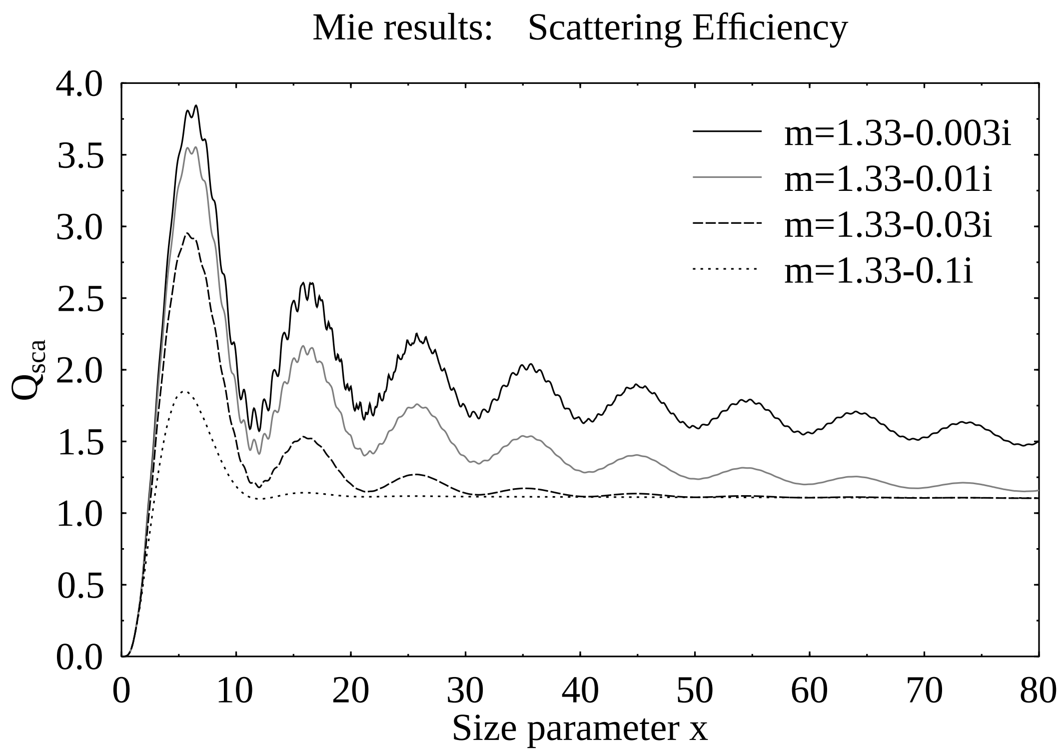
Scattering and absorption efficiency vs size parameter with absorbing m:
as $x \to \infty$, $Q_{sca} \to 1$, $Q_{abs} \to 1$; entering rays are absorbed inside particle.
Smaller imaginary part of m requires larger particle to fully absorb internal rays.

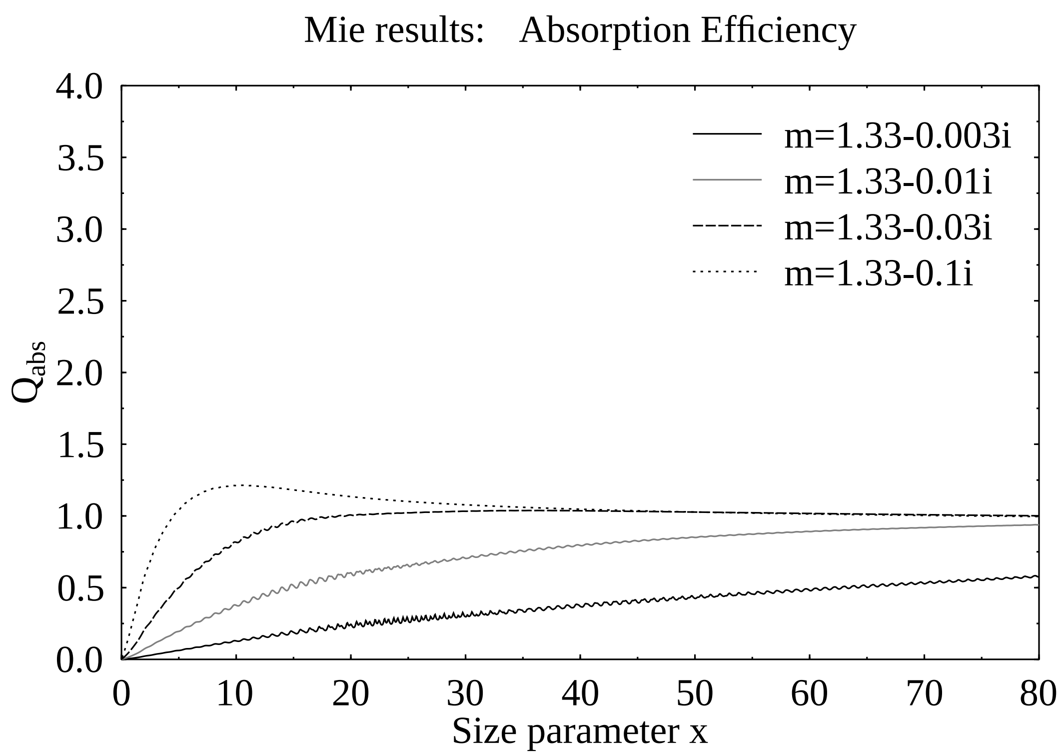
Phase functions: Forward peak height increases dramatically with x.
For single particles - number of oscillations in $P(\Theta)$ increases with x.



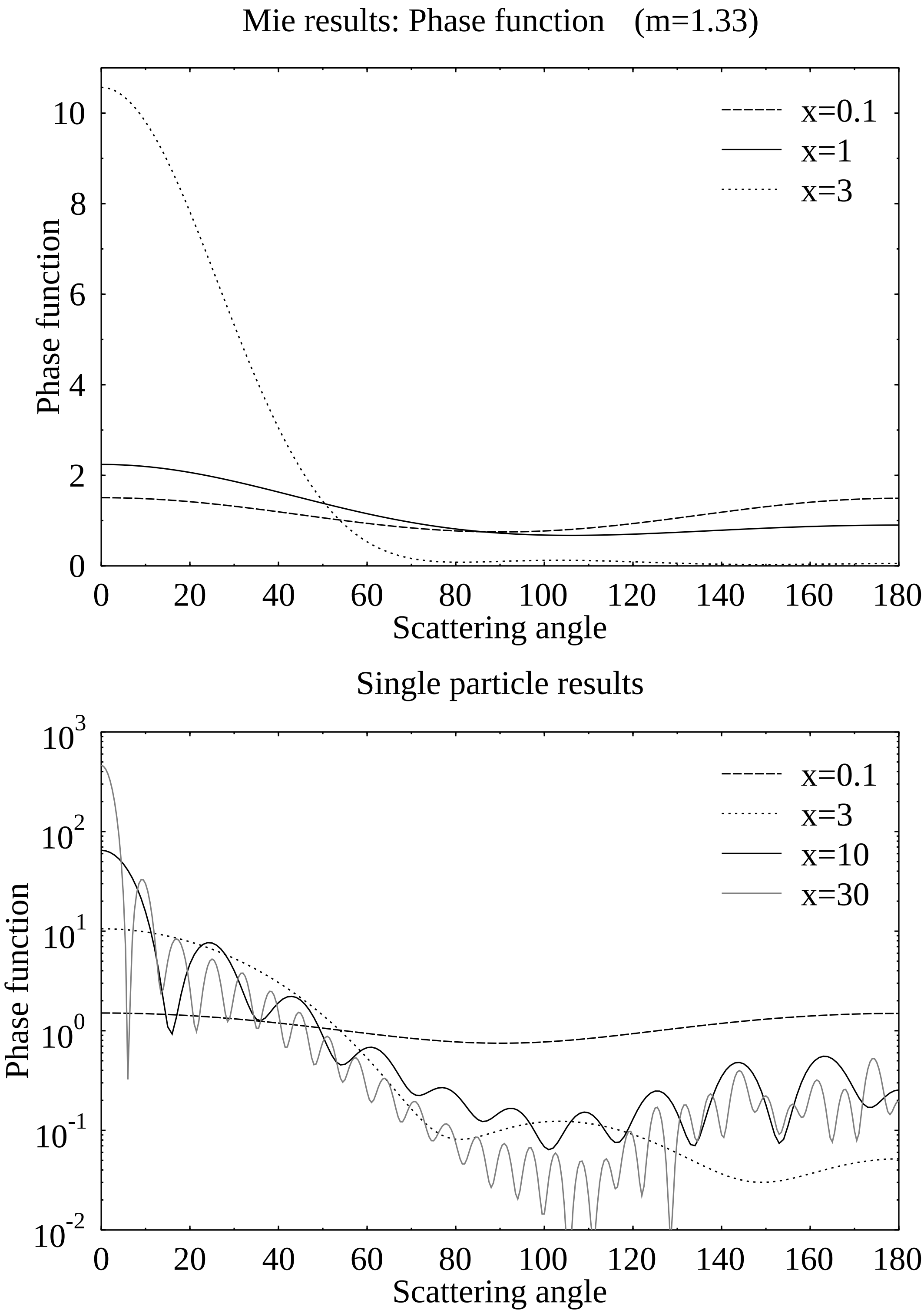


Extinction efficiency vs. size parameter. Top panel shows effect of real part of index of refraction, while bottom panel shows effect of imaginary part.





Scattering and absorption efficiencies vs. size parameter for varying amounts of absorption.



Phase functions for single nonabsorbing spheres of increasing size parameter x: linear scale (top), log scale (bottom).

Extinction Paradox and Geometric Optics Limit

Geometric optics limit is $x \to \infty$.

As $x \to \infty$ extinction efficiency is $Q_{ext} = 2$.
Extinction cross section is *twice* particle area!
One πr^2 from blockage by particle, second πr^2 from diffraction.
Light diffracted by particle edge is scattered by small angles.
Solution to paradox: need to be in far field ($xr \gg 1$) to see diffraction.

If optical path in particle $4\pi\kappa r/\lambda \gg 1$, all light entering is absorbed:
$C_{abs} = \pi r^2 \quad C_{sca} = \pi r^2 \quad \omega = 0.5$
If $4\pi\kappa r/\lambda \ll 1$, all light entering particle is transmitted:
$C_{abs} = 0 \quad C_{sca} = 2\pi r^2 \quad \omega = 1$

Optical depth is proportional to second moment of size distribution:

$$\tau = \int \int_0^\infty 2\pi r^2 n(r) dr\, dz \;\; = \frac{3}{2}\frac{\mathrm{LWP}}{\rho_l r_e} \qquad \text{for } x \to \infty$$

where LWP is liquid water path and r_e is effective radius.

Anomalous Diffraction Theory (ADT)

Simple scattering theory - explains main Mie $Q_{ext}(x)$ oscillations.
ADT applies to limits:
$x \gg 1$ so treat waves as rays,
$m - 1 \ll 1$ so no refraction or reflection.
But phase lag in particle is significant $\rho = 2x(m-1)$.

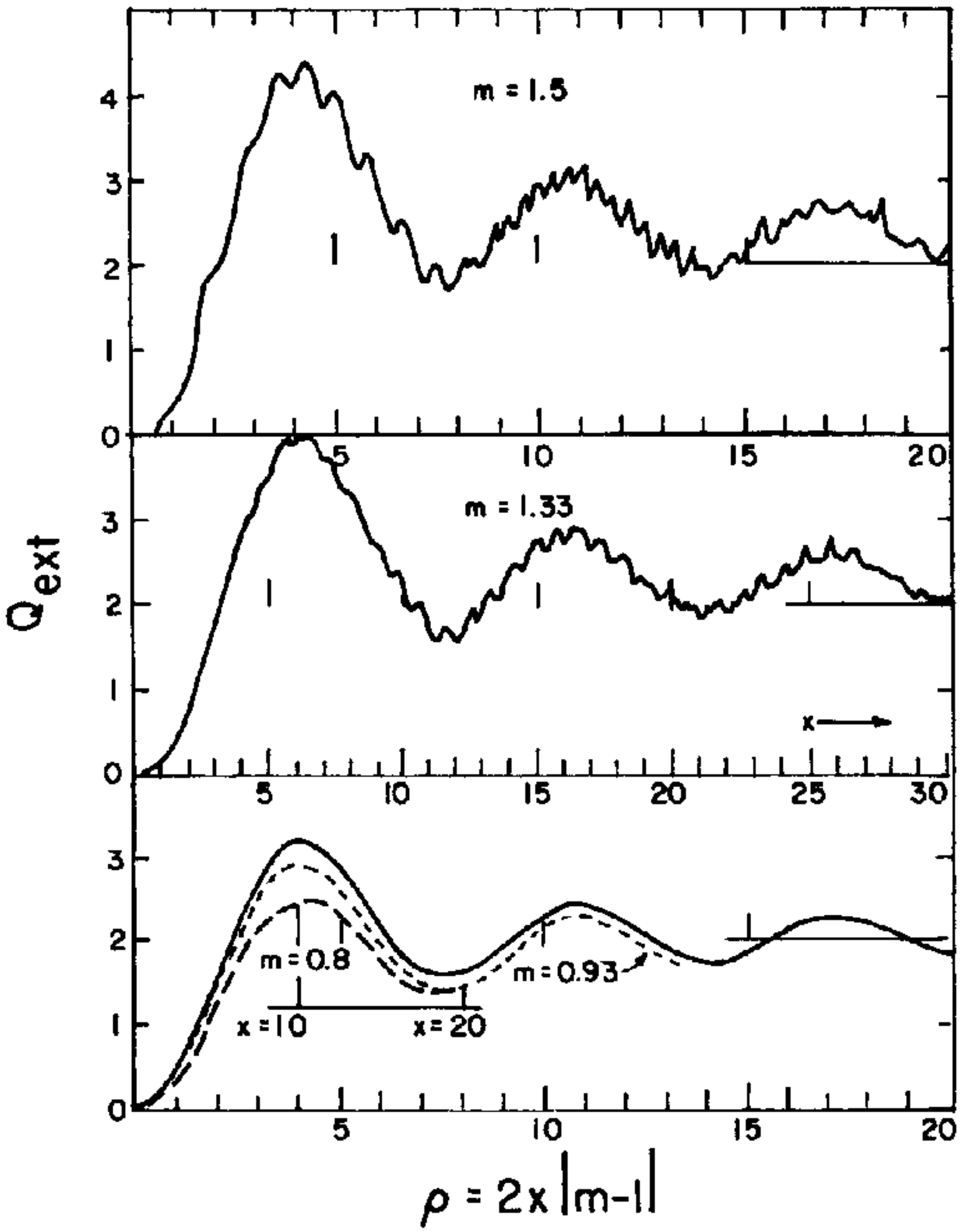
ADT integrates sum of incident and transmitted E field (in $\Theta = 0$ direction) for all rays through particle. Then uses optical theorem ($C_{ext} = (4\pi/k^2)\mathrm{Re}[S(0)]$) to obtain extinction cross section, and bulk absorption coefficient ($4\pi \mathrm{Im}[m]/\lambda$) to obtain absorption cross section.

Oscillations in Q_{ext} due to constructive and destructive interference of diffracted and transmitted waves.
For non-absorbing spheres ADT gives

$$Q_{ext} = 2 - \frac{4}{\rho}\sin\rho + \frac{4}{\rho^2}(1 - \cos\rho)$$

First maximum at $\rho \approx 4.1$. Asymptotically, maxes at $\rho = 2\pi(n + 3/4)$.

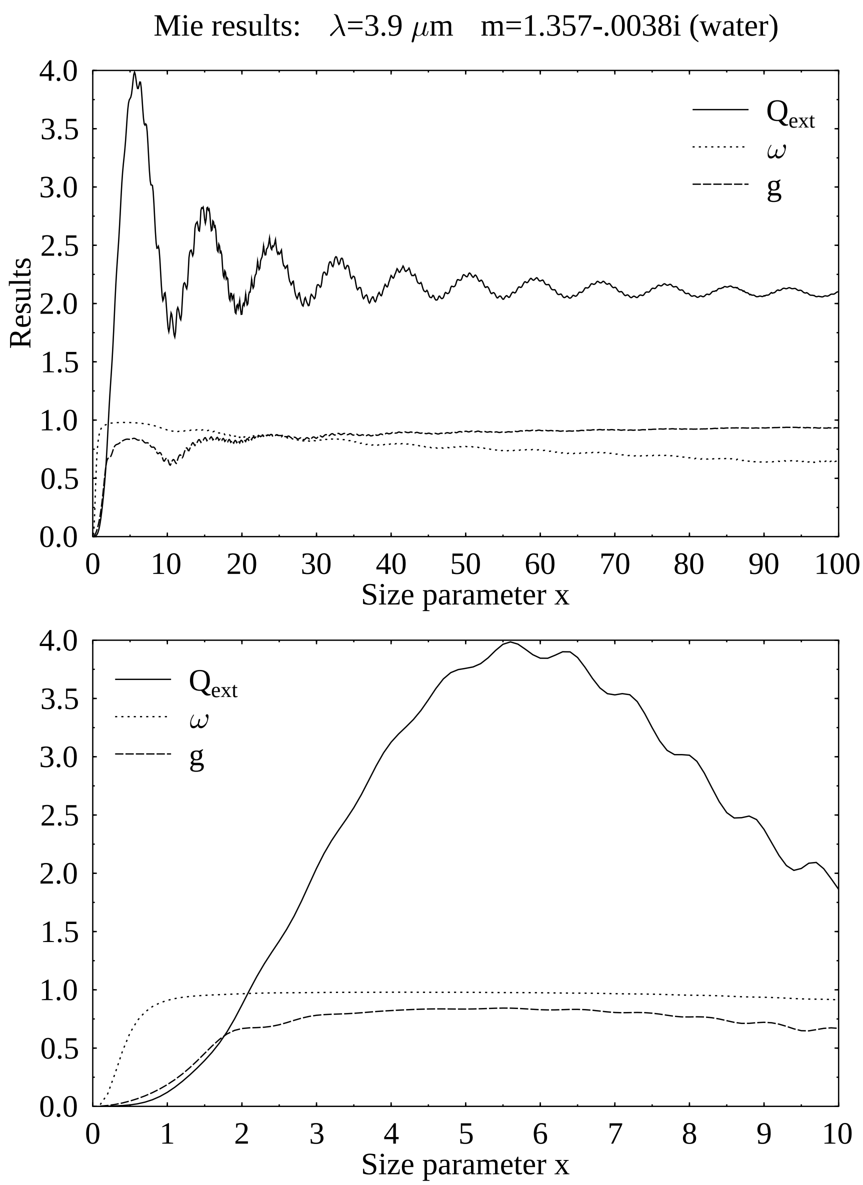
ADT provides extinction and absorption, but not phase function.
ADT can be used on any convex shaped particle. But not that accurate for realistic index of refraction.



Extinction curves computed from Lorenz-Mie theory for m=1.5,1.33,0.93,0.8. The abscissa is $\rho = 2x(m-1)$ and is common to the upper two Lorenz-Mie curves as well as to the bottom anomalous diffraction theory (ADT) curves [van del Hulst, 1957; Stephens, 1994]

Single Particle Mie Scattering Summary

	$x \to 0$	$0.2 < x < 50$	$x \to \infty$
C_{ext}	$\propto r^3$ or $\propto r^6$	Q_{ext} oscillations	$\to 2\pi r^2$
ω ($\kappa > 0$)	0	reaches maximum	$\to 1/2$
g	$\to 0$	increases	constant ($\sim$.7–1)



Extinction efficiency (Q_{ext}), single scattering albedo (ω), and asymmetry parameter (g) as a function of size parameter for a slightly absorbing index of refraction.

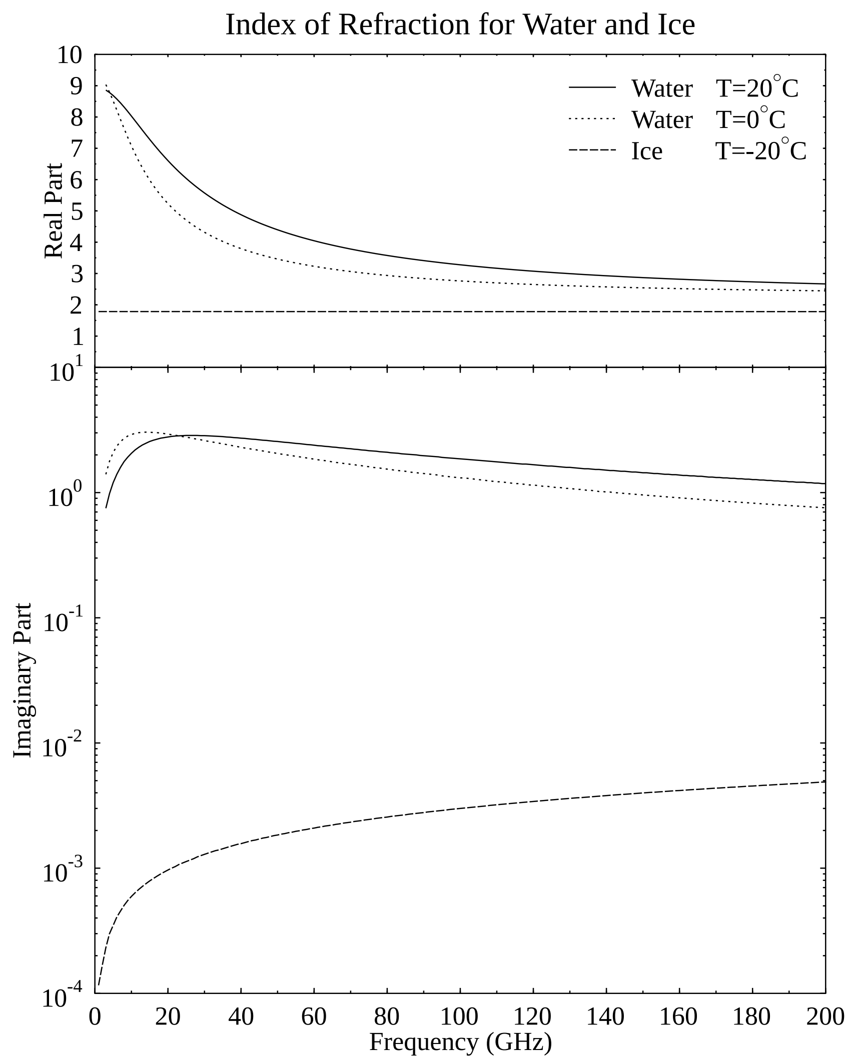
Index of Refraction of Water and Ice

See graphs for complex index of refraction $m = n - i\kappa$
Debye and Lorentz models used to understand index (see Stephens).

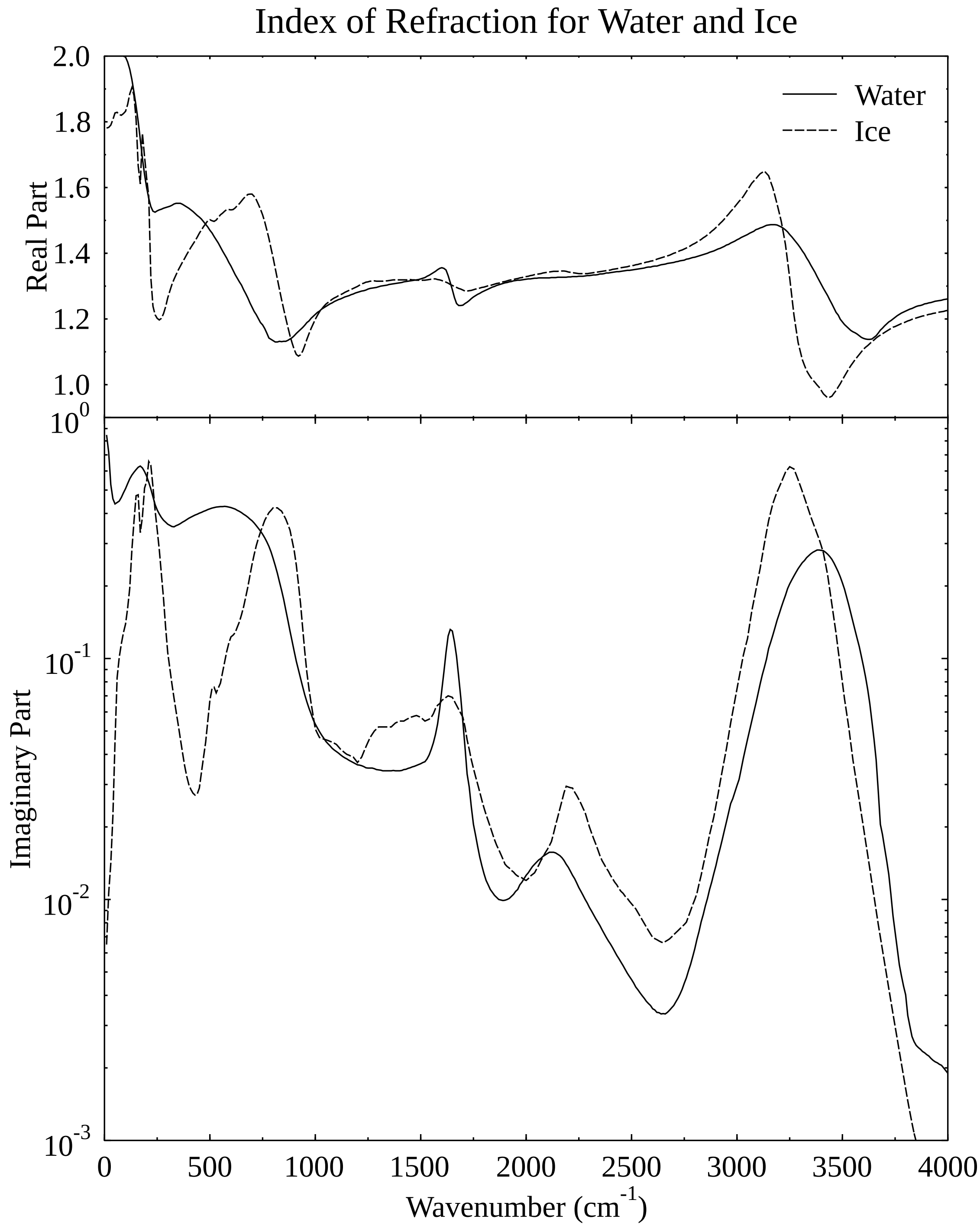
Microwave: water - very high n and κ,   ice - $n = 1.78$, low κ
Index is temperature dependent for water but not much for ice.

Thermal IR: high κ (highest at 3 μm); wiggle in n with each peak in κ.

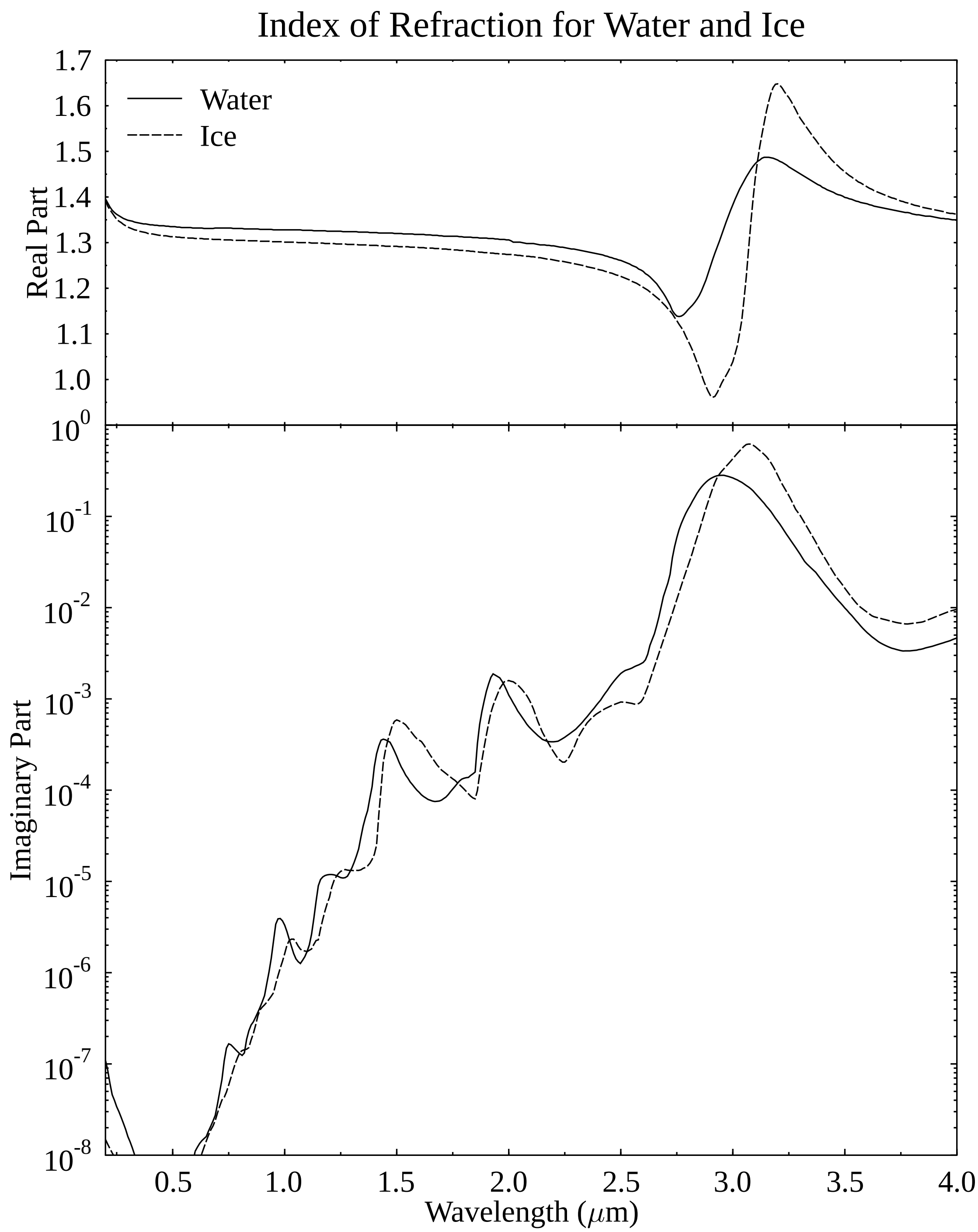
Visible/near IR: mostly constant n,
$\kappa = 0$ in visible and increases with wavelength in near IR.



Real and imaginary part of the index of refraction of water and ice in the microwave.

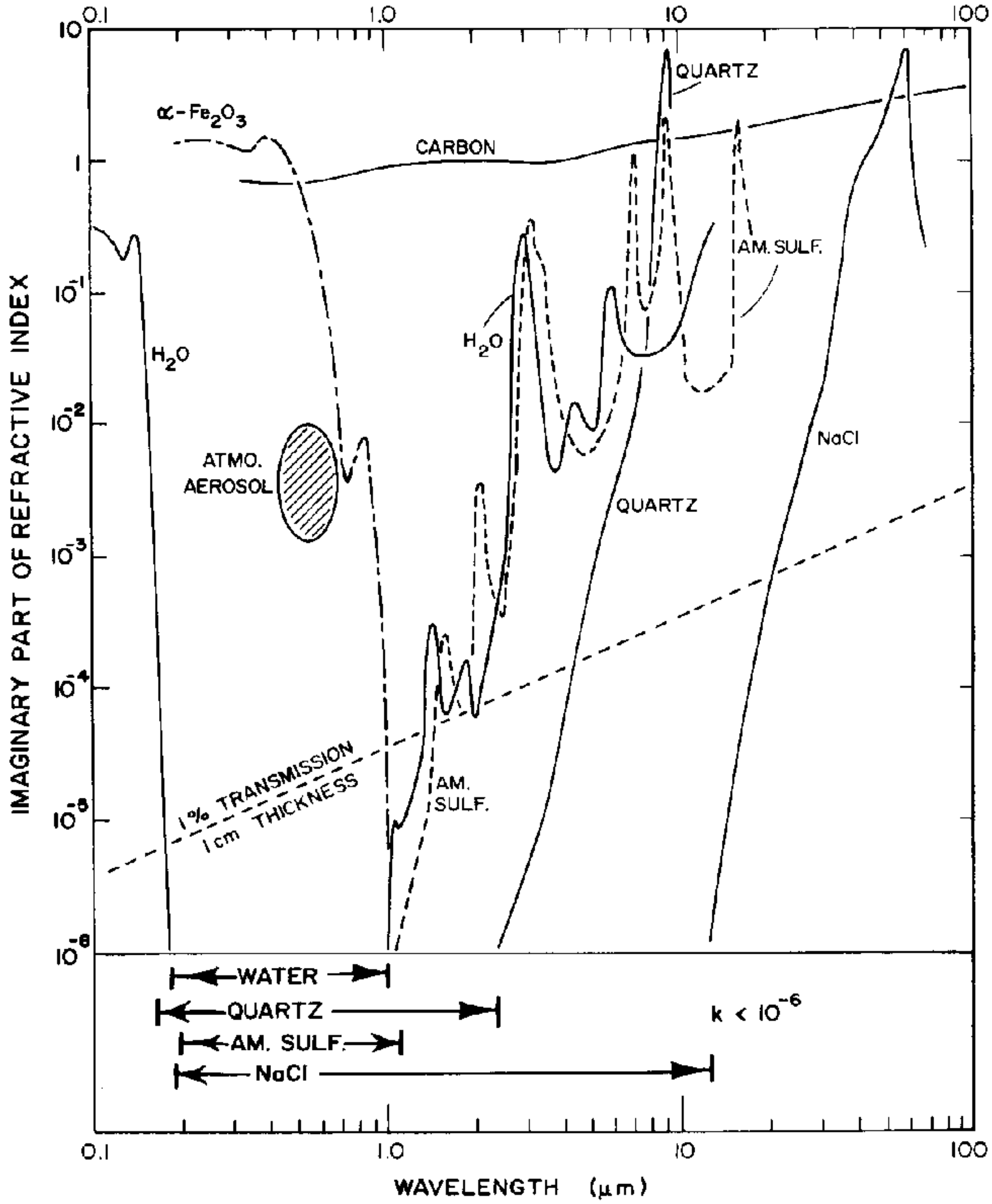


Real and imaginary part of the index of refraction of water and ice in the infrared.



Real and imaginary part of the index of refraction of water and ice in the visible and near infrared.

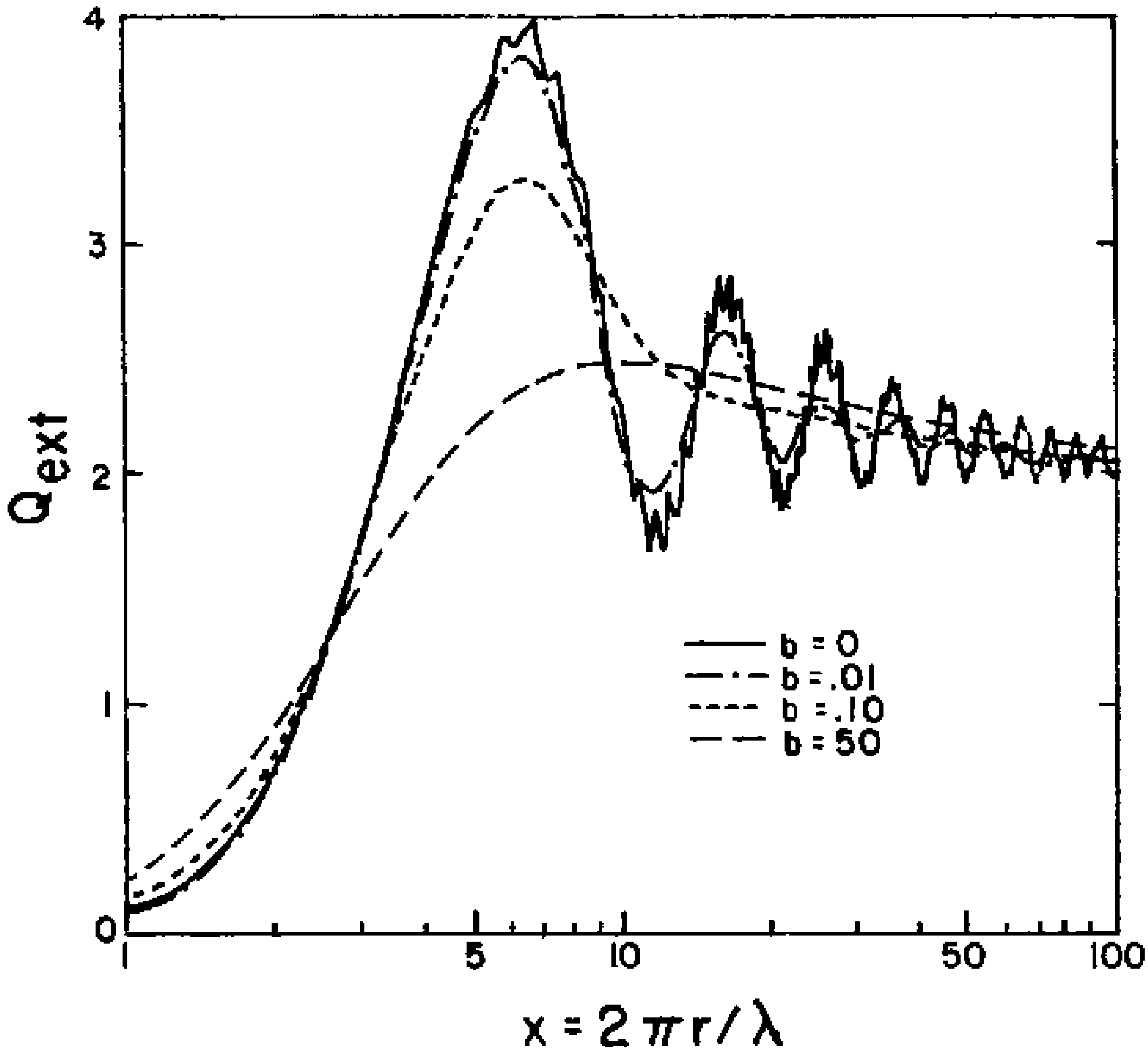
Index of refraction of aerosol materials: mostly nonabsorbing in shortwave, except for soot (carbon) and dust (e.g. hematite) aerosols. Sulfates and quartz absorb in 8-12 μm region.



Imaginary part of index of refraction as a function of wavelength for some common aerosol materials. [Bohren and Huffman; Fig. 5.16]

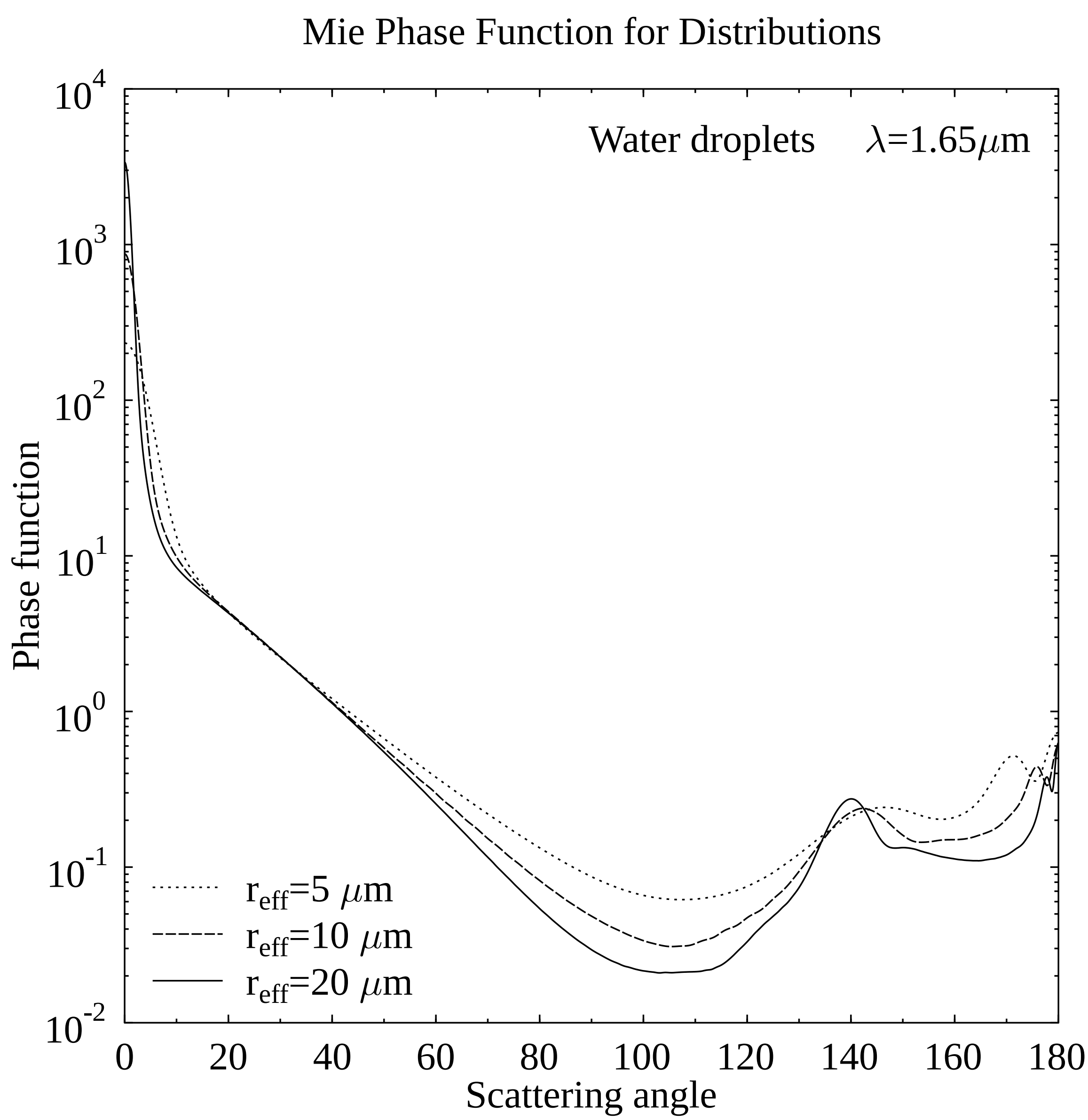
Mie Scattering Results for Distributions

Real distributions of particles smooth out oscillations in extinction efficiency $Q_{ext}(x)$ and phase function $P(\Theta)$.



The extinction efficiency as a function of the effective size parameter $x_e = 2\pi r_e/\lambda$ for gamma size distributions of various effective variances b. Mie theory with index $m = 1.33$ was used. [after Hansen and Travis, 1974; Stephens, Fig. 5.16]

For cloud droplets at solar wavelengths: still have forward diffraction peak (width $\Delta\Theta \sim 1/x$), rainbow near $\Theta = 140°$, and glory at $\Theta = 180°$.



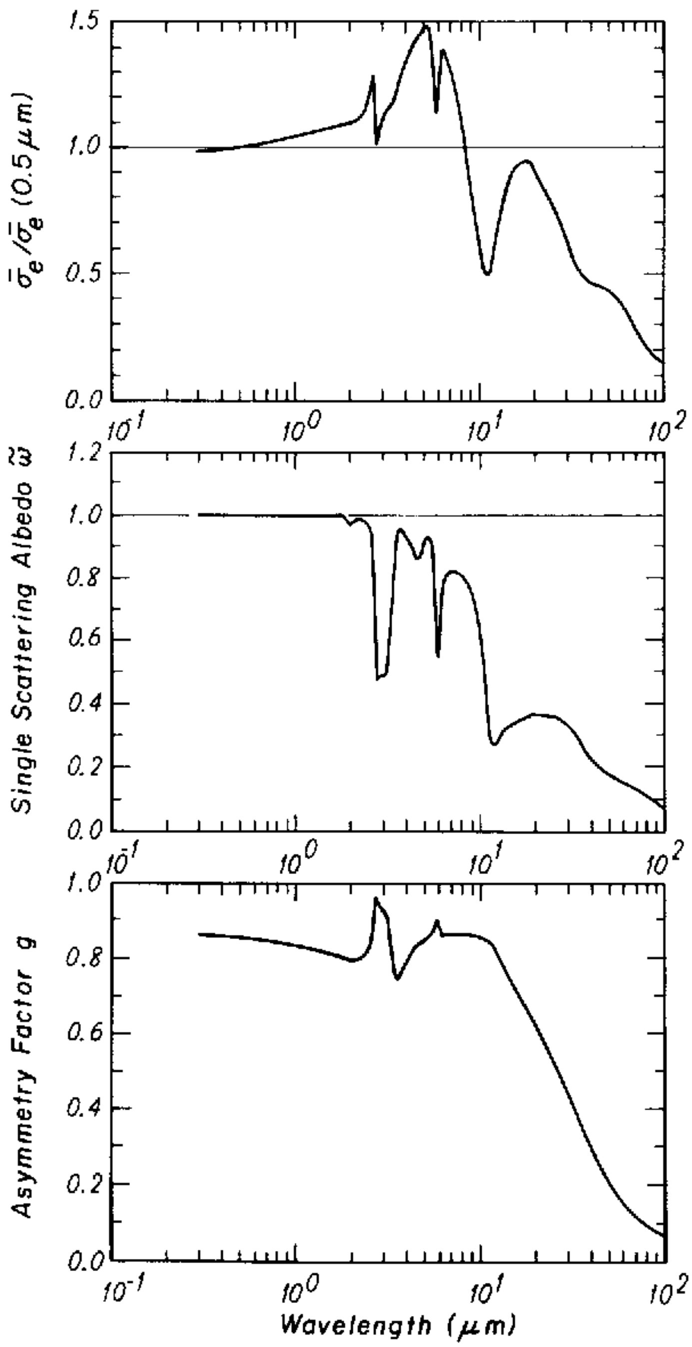
The phase function for gamma distributions ($\alpha = 7$) of water droplets for three different effective radii.

Mie scattering results vs. wavelength for cloud droplets:

Extinction: constant in visible and near IR; decreases in far IR.

Single scattering albedo: 1 for $\lambda < 1.6$ μm; low in mid IR.

Asymmetry parameter: 0.8 to 0.9 from visible to mid IR.



Normalized extinction coefficient, single scattering albedo, and asymmetry parameter for a cloud droplet size distribution with $r_{eff} = 6$ μm. [Liou, 1992; Fig. 5.3]