Week 9: October 22-26

Nonspherical Particle Scattering
Scattering Radiative Transfer

Topics:
1. Discrete Dipole Approximation for scattering
2. Ray tracing scattering method
3. Radiative transfer equation with scattering
4. First order scattering solution
5. Legendre series and Henyey-Greenstein phase functions

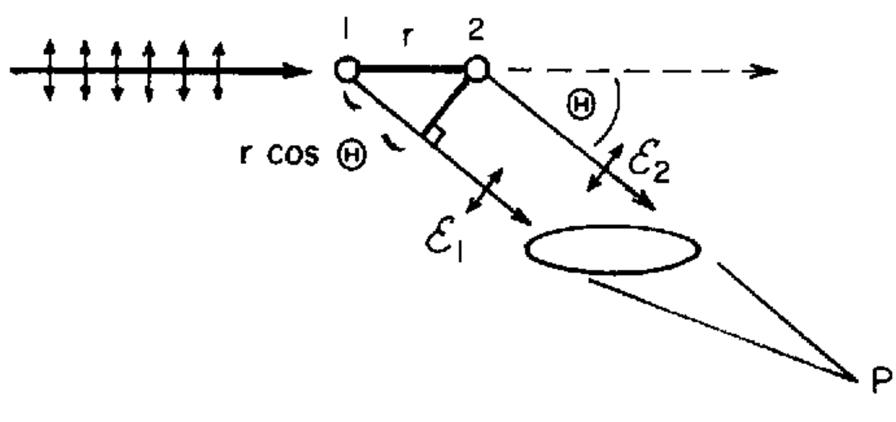
Reading: Liou ; Thomas 6.2,6.3,6.7,7.2

Rayleigh-Gans limit

Rayleigh-Gans limit is $x(m-1) \ll 1$ ($x \ll 1$ is not required). In Rayleigh-Gans limit, the field inside the particle is the same as the incident. The field is not reflected by the particle and there is no phase difference across particle.

Conceptual model: A particle may be divided into "dipoles" of size $2\pi d/\lambda < 1$.

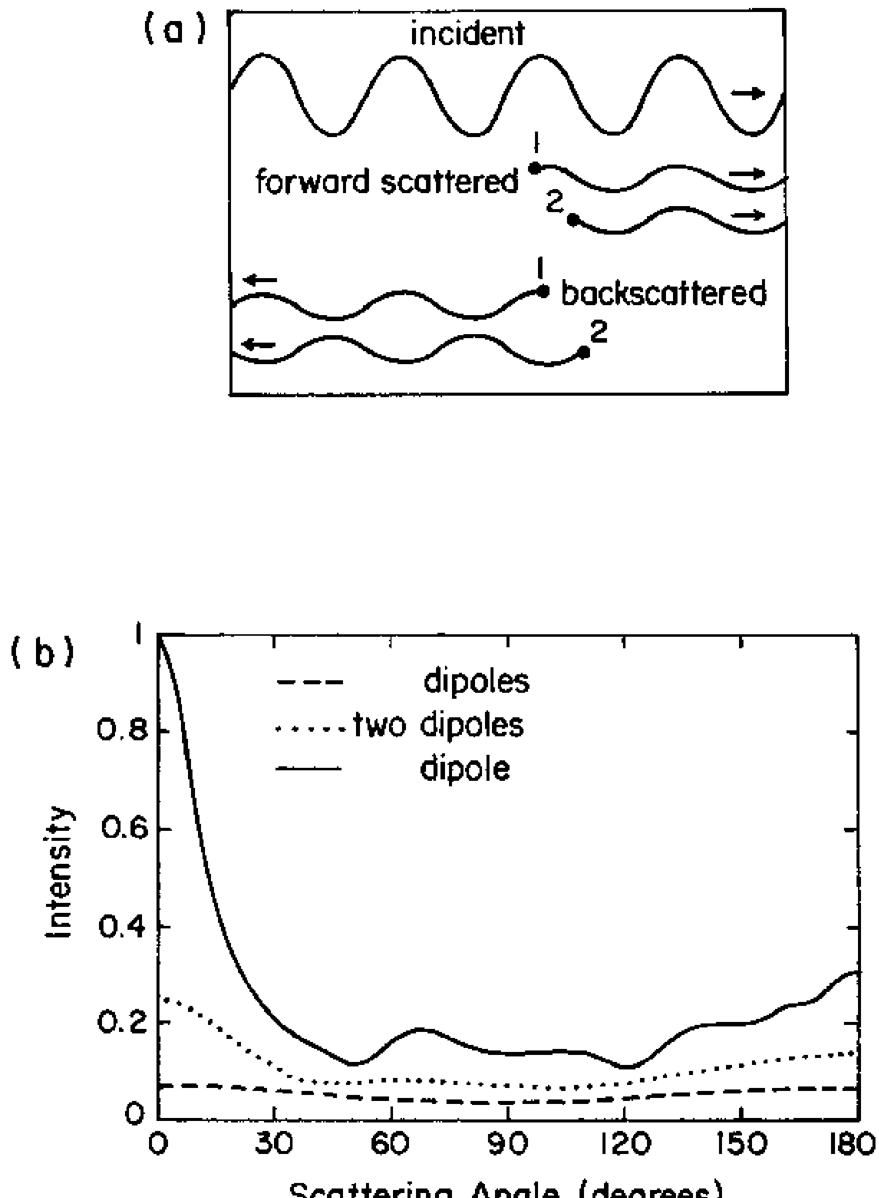
Example: two dipoles along incident field direction - distance r apart
 Outgoing scattered wave phase difference $\Delta\phi = kr(1 - \cos\Theta)$
 Far from particle superpose fields: $E_{1+2} = E_1 e^{i\phi} + E_2 e^{i(\phi+\Delta\phi)}$
 Intensity: $I_{sca} \propto E_1^2 + E_2^2 + 2E_1E_2 \cos\Delta\phi$



Two isolated dipoles emit waves in all directions. At some point P far from the "particle", these waves superimpose to create the scattered wave along the directions Θ. These waves either constructively or destructively interfere depending on their relative phase phase difference $\Delta\phi$. [Stephens, 1994; Fig. 5.7]

Scattered waves from dipoles are in phase for forward direction $\Theta = 0$, giving constructive interference $\rightarrow$ forward peak in phase function.

Destructive and constructive interference alternates as Θ increases $\rightarrow$ oscillations in phase function. More oscillations for larger particle.



(a) Excited by an incident wave, two dipoles scatter in all directions. In the forwarrd direction, the two waves are exactly in phase regardless of the separation of the dipoles. (b) The greater the number of dipoles (larger the particle), the more they collectively scatter towards the forward direction. [Stephens, 1994; Fig. 5.8]

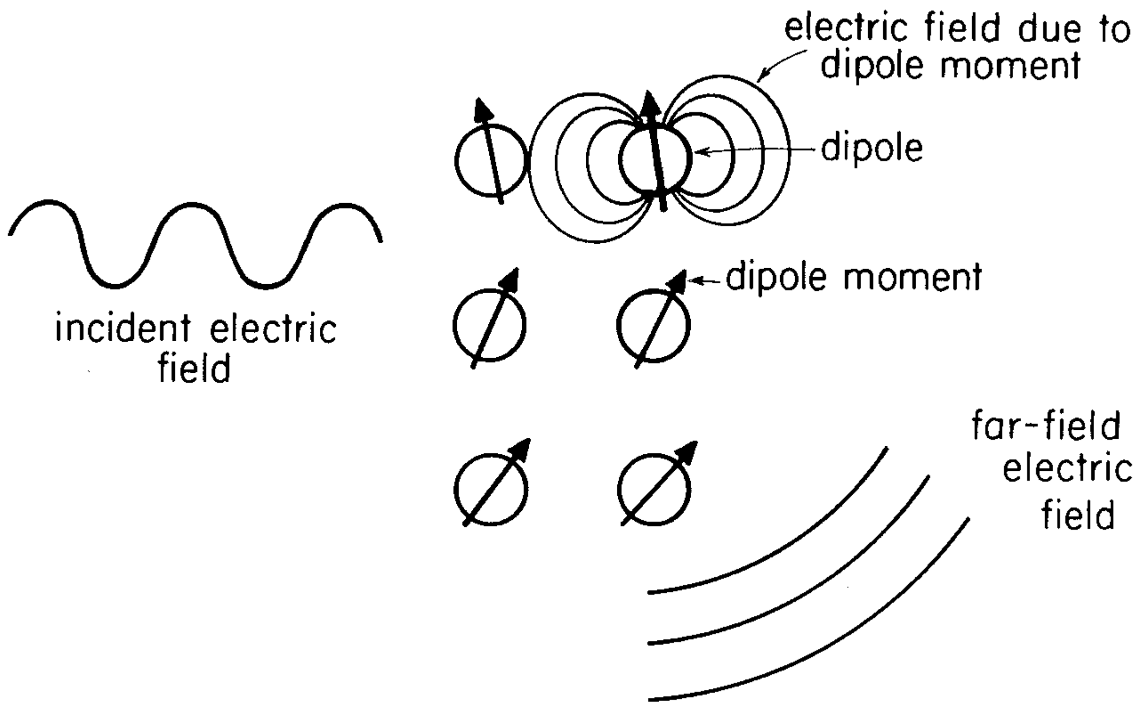
Discrete Dipole Approximation (DDA)

A numerical method for scattering from any shape particle that is not too large ($x < 5$). See review paper by Draine and Flatau, J. Opt. Soc. Am. A, **11,** 1491.

1) Particle is divided into dipoles of size d small compared to wavelength.
2) Given all the dipole moments, the field due to all other dipoles can be found at one dipole j: $\mathbf{E}_j = \mathbf{E}_{inc,j} - \sum_{k \neq j} A_{jk}\mathbf{p_k}$
3) For a particular incident E field, the linear system may be solved for the dipole moments $\mathbf{p_k}$.
4) The far field scattering properties are calculated from the $\mathbf{p_k}$.

Finite-Difference Time Domain (FDTD) is a competing method that is also used for small nonspherical particles.

In both DDA and FDTD the number of dipoles or elements is proportional to the particle volume $\rightarrow$ quickly becomes computationally prohibitive.

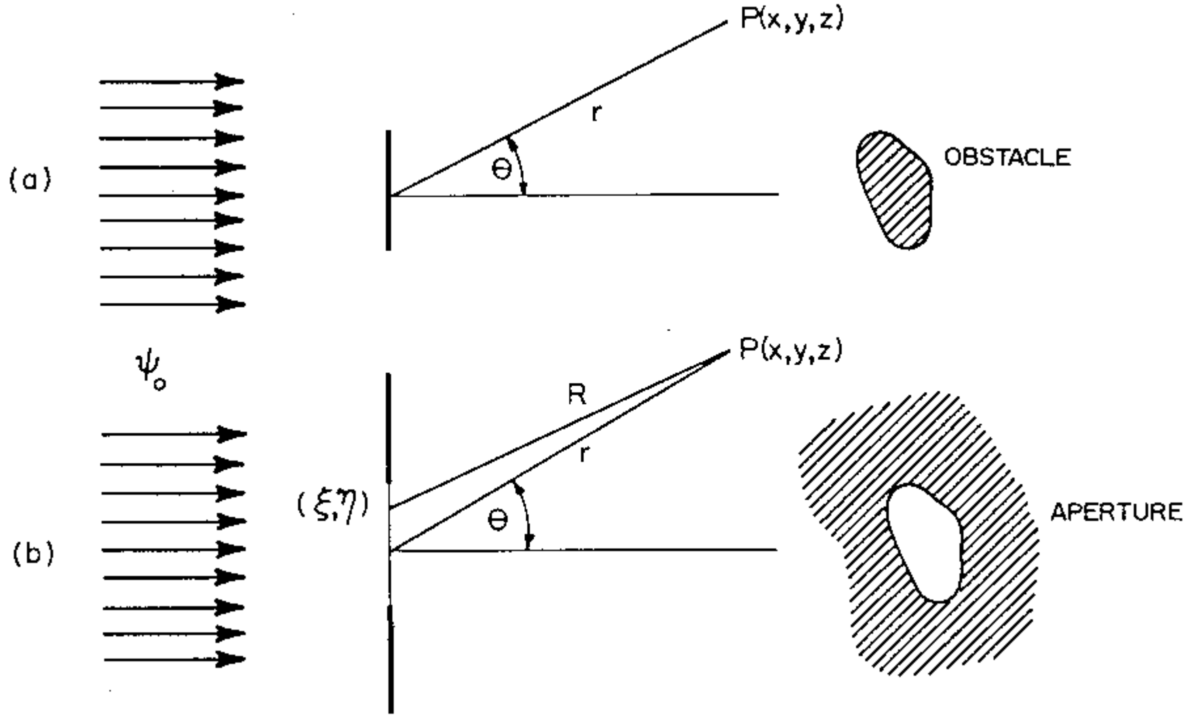


The Discrete Dipole Approximation divides a particle up into many dipoles which are small compared to the wavelength. The oscillating electric field produced by each dipole depends on the dipole moment. The dipole moment depends on the applied electric field from the incident field and other dipoles and the dielectric properties of the dipole. The far-field electric field is a sum of the dipole fields from all the dipoles.

Diffraction

In geometric optics limit ($x \gg 1$) light may be treated as rays, except for Fraunhofer diffraction around a particle.

Babinet's principle - diffraction pattern is the same from an aperture as for opaque particle of same size.



(a) Diffraction by an opaque planar obstacle. (b) Diffraction by an aperture with the same shape as the obstacle. [Liou, 1980; Fig. 4.7]

Integrate the far field contribution of incident wave over the aperture.

$$E = -\frac{iE_0}{R\lambda}\int_A e^{-ikR} dA$$

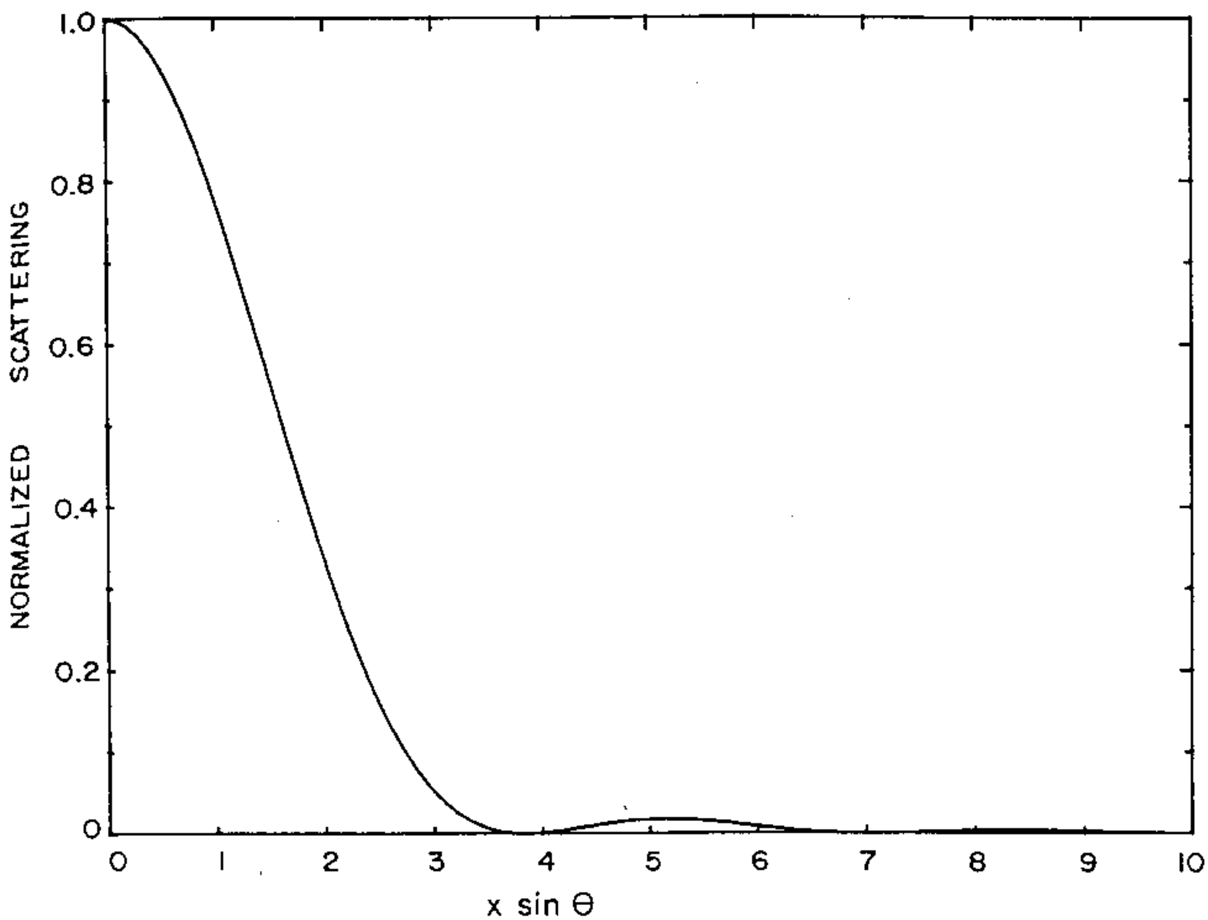
Huygens principle - each point is a source of circular wave fronts.

For sphere (circular aperture) the diffraction pattern is

$$I(\Theta) = \frac{I_0}{k^2R^2}\,\frac{x^4}{4}\left[\frac{2J_1(x\sin\Theta)}{x\sin\Theta}\right]^2$$

where x is the size parameter, $k = 2\pi/\lambda$, and J_1 is a Bessel function.

Diffraction peak in phase function: width $\Theta \sim 1/x$, height $P(0) \propto x^2$.
First zero at $x \sin \Theta = 3.83$, max at $x \sin \Theta = 5.14$.



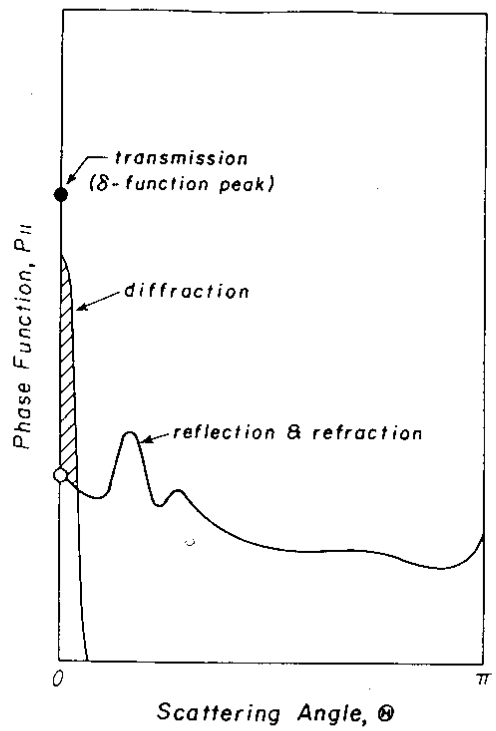
Scattering diagram for diffraction by a circular disk. [Liou, 1980; Fig. 4.8]

Ray Tracing

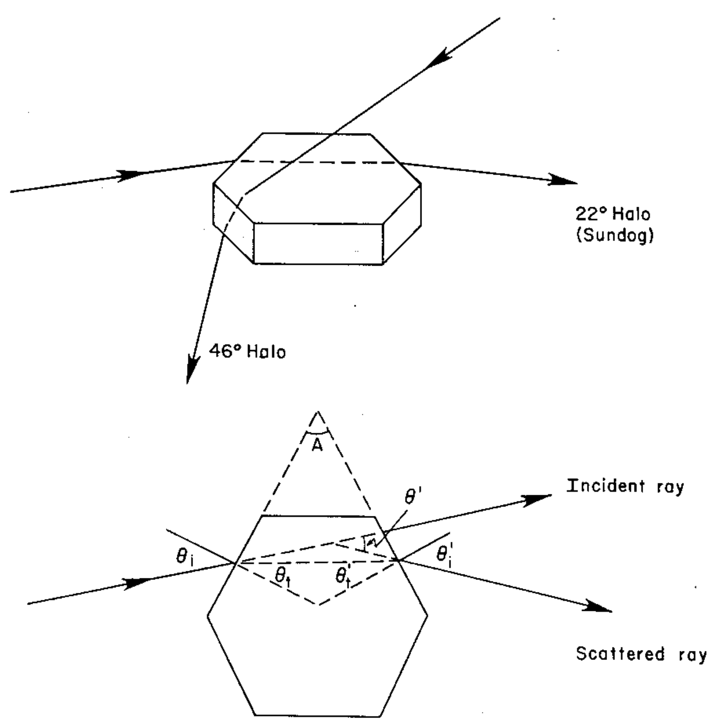
In the geometric optics limit (say $x > 100$) ray optics provide an accurate scattering method for nonspherical particles.

Ray optics consists of two parts:

1) Diffraction theory for the forward scattering peak,
2) Ray tracing using Fresnel reflection and transmission formulas.
   Many rays incident on particle are followed to determine
   what fraction scatter in each direction or are absorbed.



A schematic representation of the components of the phase function P_{11} for randomly oriented hexagonal ice crystals. [Liou, 1992; Fig. 5.5]



Geometrical reflection and refraction by hexagonal crystals. [Liou, 1980; Fig. 5.10]

Fresnel Reflection and Transmission

Plane wave incident on planar dielectric surface. Solve for reflection and transmission using boundary conditions from Maxwell's equations (tangential components of fields are continuous).

Snell's Law gives refraction angle θ_t: $\sin\theta_i = m\sin\theta_t$

Fresnel formula for polarized reflection *amplitude* coefficients:

$$r_\parallel = \frac{\sqrt{m^2-\sin^2\theta_i} - m^2\cos\theta_i}{\sqrt{m^2-\sin^2\theta_i} + m^2\cos\theta_i} \qquad r_\perp = \frac{\cos\theta_i - \sqrt{m^2-\sin^2\theta_i}}{\cos\theta_i + \sqrt{m^2-\sin^2\theta_i}}$$

m is relative index of refraction: $m = m_2/m_1$

Reflection and transmission coefficients for intensity:

$$\mathcal{R}_\parallel = |r_\parallel|^2 \quad \mathcal{R}_\perp = |r_\perp|^2 \quad \mathcal{T}_\parallel = 1 - \mathcal{R}_\parallel \quad \mathcal{T}_\perp = 1 - \mathcal{R}_\perp$$

Reflection for $\theta = 0$ is $R = \left|\frac{m-1}{m+1}\right|^2$. Reflectivity increases with index of refraction.

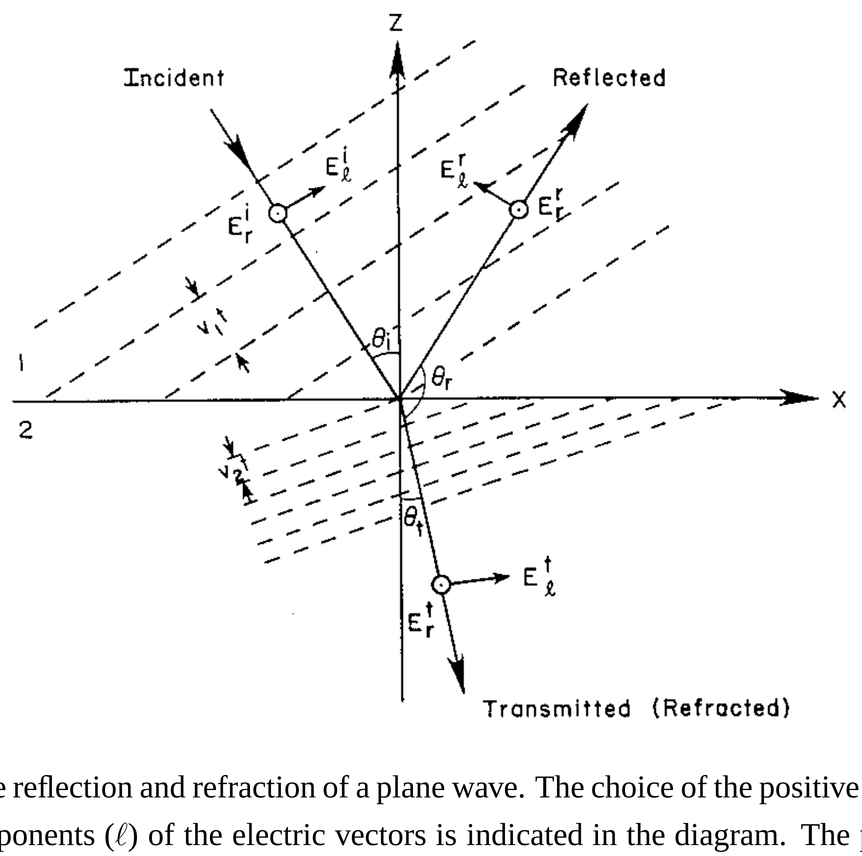
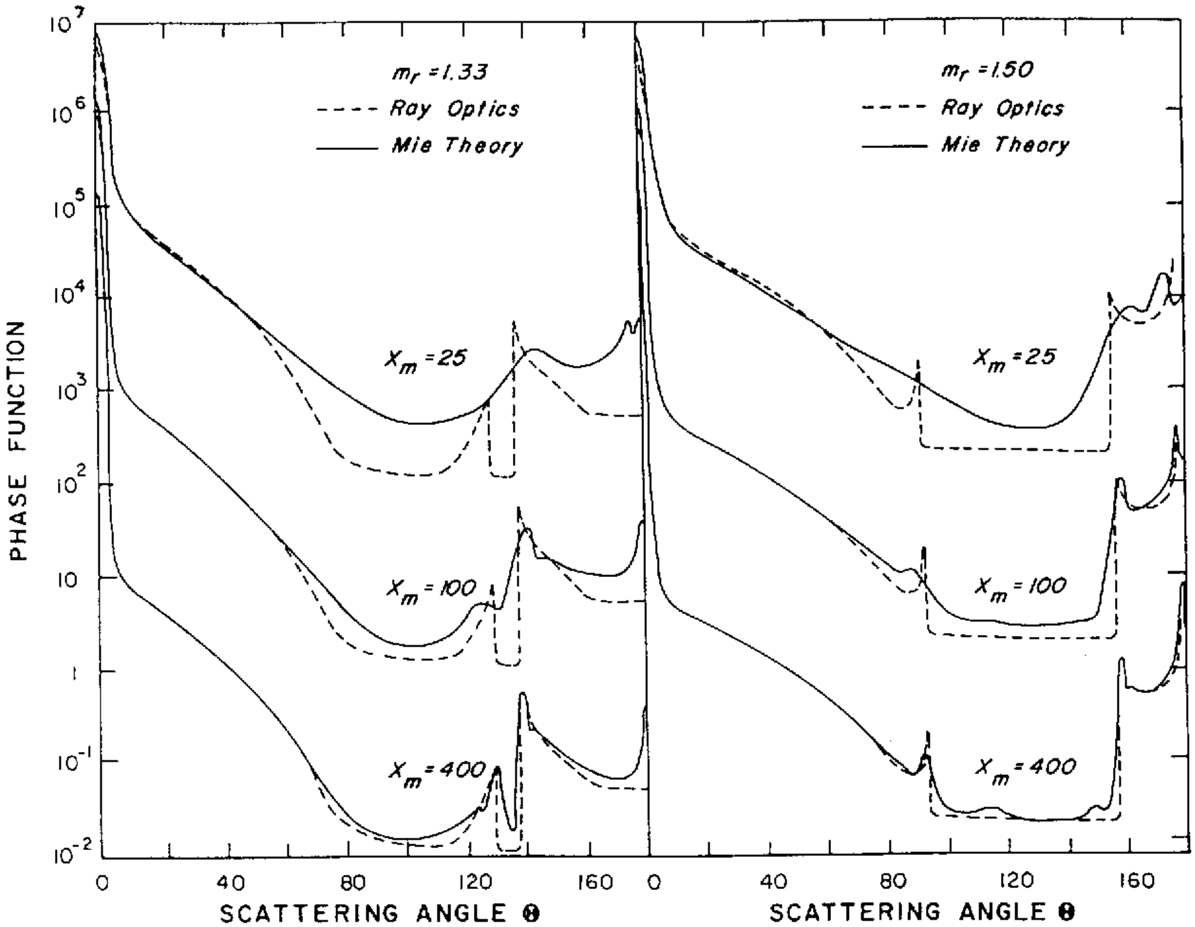


Illustration of the reflection and refraction of a plane wave. The choice of the positive directions for the parallel components (ℓ) of the electric vectors is indicated in the diagram. The perpendicular components are at right angles into the plane of reference. [Liou, 1994; Fig. 5.8]

Ray Tracing Results

Ray tracing compares well with Mie theory for large size parameters:
For water drops in the visible ($m = 1.33$) the primary rainbow is at $\Theta = 137°$ from one internal reflection.
Rainbow angle depends on index of refraction through Snell's Law.
Ray tracing cannot explain glory (at $\Theta = 180°$) for cloud droplets.



Comparison of ray tracing and Mie phase functions for spheres. Two refractive indices are shown along with three size distributions; the vertical scale is shifted by 10^2 and 10^4 for the $X_m = 100$ and $X_m = 25$ curves. [Liou, 1980; Fig. 5.11]

Visible light ray tracing in randomly oriented hexagonal ice crystals explains $22°$ and $46°$ halos.

Modeled and measured nonspherical phase functions for ice crystals show that Mie theory gives too little side scattering.

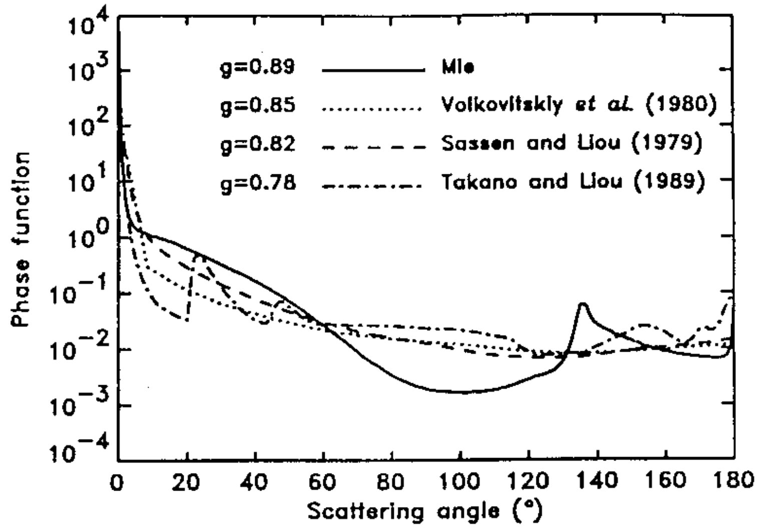


FIG. 7. Phase functions used in this study, including the corresponding values of the asymmetry parameter g.

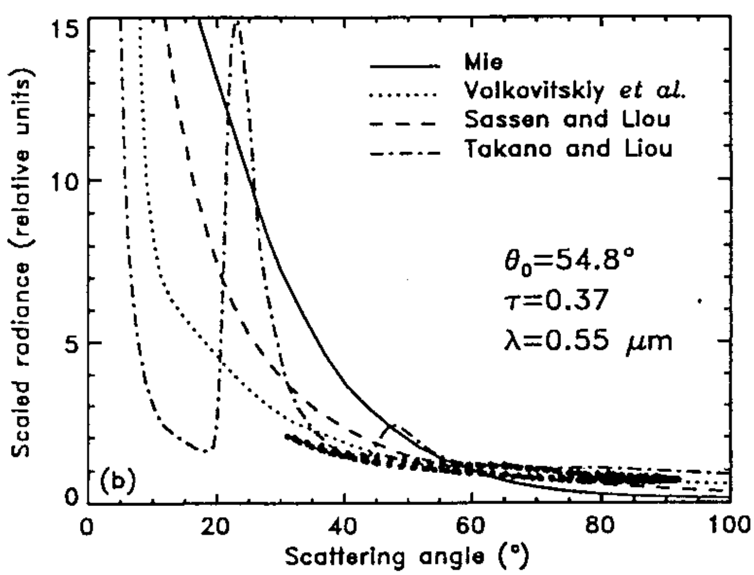


FIG. 8. (a) Comparisons between measured radiances (●) and Monte Carlo simulations for A189 orbit 1 (30°) at a wavelength of 0.55 μm. (b) As in (a) but for A189 orbit 2 (45°).

Mie and modeled or lab measured phase functions for cirrus cloud ice crystals. (from Francis, 1995: Some Aircraft Observations of the Scattering Properties of Ice Crystals. J. Atmos. Sci., 52, 1142.)

Radiative Transfer with Scattering

Scattering represents a loss of radiation from a beam, but also a source, as light is scattered into the beam from other directions.

The source of radiation scattered from a small volume depends on the
  radiation intensity in the incident direction, $I(\Omega')$
  fraction of radiation that interacts, βds
  fraction of that which is scattered, ω
  fraction scattered into the new direction, $P(\Theta) d\Omega/4\pi$
Integrate over all incident directions, to give the scattering source function:

$$J(\Omega) = \frac{\omega}{4\pi} \int_{4\pi} P(\Omega, \Omega')\, I(\Omega')\, d\Omega'$$

Scattered radiance from path ds is then $J(\Omega)\, \beta ds$.

The scattering source function has units of intensity.
Plays the role of the Planck function in thermal radiative transfer.

General Radiative Transfer Equation

Using the gradient operator for the streaming term $\Omega \cdot \nabla I$ the RTE is

$$\Omega \cdot \nabla I(\mathbf{x}, \Omega) = \beta \left[-I(\mathbf{x}, \Omega) + J(\mathbf{x}, \Omega) \right]$$

where $\mathbf{x}$ is the space coordinate.

The source function including scattering and thermal emission is

$$J(\Omega) = \frac{\omega}{4\pi} \int_{4\pi} P(\Omega, \Omega')\, I(\Omega')\, d\Omega' \; + \; (1-\omega) B(T)$$

where $B(T)$ is the Planck function, ω is the single scattering albedo, $P(\Omega, \Omega')$ is the phase function from incident direction Ω' to scattered direction Ω.

Plane-Parallel Solar Radiative Transfer Equation

Mostly we will ignore horizontal variability (assume a plane-parallel atmosphere) and omit thermal emission in the shortwave.

The monochromatic solar radiative transfer equation is then

$$\mu \frac{dI(\mu, \phi)}{dz} = -\beta \left[I(\mu, \phi) - \frac{\omega}{4\pi} \int_0^{2\pi} \int_{-1}^{1} P(\Theta)\, I(\mu', \phi')\, d\mu' d\phi' \right]$$

The first term on right is the extinction and the second is the scattering source.

Usually the phase function depends only on the scattering angle Θ:

$$\cos\Theta = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi' - \phi)$$

Often we use optical depth as the vertical coordinate:

$$\mu\frac{dI(\mu,\phi)}{d\tau} = I(\mu,\phi) - J(\mu,\phi)$$

Diffuse and Direct Separation

The top boundary condition is incident collimated solar radiation $I(\infty,\Omega) = S_0\delta(\Omega + \Omega_0)$, where the direction of solar radiation is $-\Omega_0$ and S_0 is the monochromatic solar flux.

For convenience we can divide the solar radiation into the unscattered *direct* beam and the once or more scattered *diffuse* radiation.

Beer's Law provides the solution for the direct beam flux

$$F(z) = S_0 e^{-\tau/\mu_0}$$

Scattering of the direct beam is the *source* of diffuse radiation:

$$J_{dif} = \frac{\omega}{4\pi}P(\mu,\phi;-\mu_0,\phi_0+\pi)\; S_0 e^{-\tau/\mu_0}$$

The boundary condition for diffuse radiation is $I(\infty,\mu,\phi) = 0$ for $\mu < 0$.

First Order Scattering Solution

In optically thin atmosphere ($\tau^* \ll 1$) most photons are scattered once.

The only source of first ordered scattered light is the diffuse source J_{dif}.

As before, integrate the source function for upwelling radiance:

$$I^{\uparrow}(\tau,\mu,\phi) \; = \int_{\tau}^{\tau_*} J_{dif}(\tau',\mu,\phi)\; e^{-(\tau'-\tau)/\mu}\; d\tau'/\mu$$

assuming no surface reflection. Substitute in the source function

$$I^{\uparrow}(\tau,\mu,\phi) \; = S_0\frac{\omega P(\Theta)}{4\pi}\int_{\tau}^{\tau_*}\exp\left[-(\tau'-\tau)/\mu - \tau'/\mu_0\right]\; d\tau'/\mu$$

The first order scattering solution at $\tau = 0$ is

$$I_1^{\uparrow}(\mu,\phi) \; = S_0\frac{\omega P(\Theta)}{4\pi}\;\frac{\mu_0}{\mu+\mu_0}\left[1 - e^{-\left(\frac{1}{\mu_0}+\frac{1}{\mu}\right)\tau^*}\right]$$

where τ^* is the optical depth of the atmosphere.

First Order Scattering Solution Example

First order scattering usually implies $\tau^* \ll 1$, so solution simplifies to

$$I_1^{\uparrow}(\mu,\phi) \; = S_0 \frac{\omega P(\Theta)}{4\pi} \, \frac{\tau^*}{\mu}$$

Molecular Rayleigh scattering at wavelength $\lambda = 0.7\ \mu$m.
Optical depth from molecular scattering formula is $\tau_{mol} = 0.037$.
TOA solar flux at $\lambda = 0.7\ \mu$m is $S_0 = 1400$ W m^{-2} μm^{-1}.
Solar geometry: $\theta_0 = 30°, \phi_0 = 180°\ \ (\mu_0 = 0.866)$
Viewing geometry: $\theta = 60°, \phi = 0°\ \ (\mu = 0.5)$.
Scattering angle is therefore $\Theta = 90°$. Rayleigh phase function is

$$P(\Theta) = \frac{3}{4}(1 + \cos^2\Theta) \; = 3/4$$

First order solution is then

$$I_1^{\uparrow}(\mu,\phi) = (1400 \text{ W m}^{-2}\mu\text{m}^{-1}) \frac{0.75}{4\pi} \frac{0.037}{0.5} \;\; = 6.2 \text{ W m}^{-2}\text{sr}^{-1}\mu\text{m}^{-1}$$

Order of Scattering Solution

If not optically thin, multiple scattering becomes important.
One method of solution is to calculate each order of scattering I_n:

$$I_n(\mathbf{x},\Omega) \; = \int_0^{s_{bnd}} J_n(\mathbf{x} - \Omega s, \Omega) \; \exp\left[- \int_0^s \beta(s')ds' \right] \; \beta(s) \; ds$$

$$J_{n+1}(\mathbf{x},\Omega) = \frac{\omega}{4\pi} \int_{4\pi} P(\Omega,\Omega') \; I(\mathbf{x},\Omega') \; d\Omega'$$

Iterate source function and radiance field for each point in space ($\mathbf{x}$) and all directions (Ω).
Total radiance is sum of all orders of scattering:

$$I(\mathbf{x},\Omega) = \sum_{n=1} I_n(\mathbf{x},\Omega)$$

Multiple scattering smooths the single scattering radiance field.

Legendre Series Expansion of Phase Functions

Standard RT models input phase functions as Legendre series:

$$P(\cos\Theta) = \sum_{l=0}^{N} \omega_l \mathcal{P}_l(\cos\Theta)$$

where $\mathcal{P}_l(x)$ are Legendre polynomials on $-1 \leq x \leq 1$.

$$\mathcal{P}_0 = 1 \quad \mathcal{P}_1 = x \quad \mathcal{P}_2 = (3x^2 - 1)/2 \qquad \mathcal{P}_n(1) = 1$$

More peaked phase function → more Legendre terms.

Legendre coefficients can be obtained from phase function by

$$\omega_l = \frac{2l+1}{2} \int_{-1}^{1} P(\cos\Theta)\, \mathcal{P}_l(\cos\Theta)\, d(\cos\Theta)$$

Standard phase function normalization implies $\omega_0 = 1$.

Phase Function Examples

Asymmetry parameter - measures degree of forward scattering

$$g = \frac{1}{2} \int_{-1}^{1} P(\cos\Theta) \cos\Theta d\cos\Theta \ = \omega_1/3$$

Rayleigh phase function:

$$\omega_0 = 1 \quad \omega_1 = 0 \quad \omega_2 = 1/2 \quad \omega_l = 0 \;\; l > 2$$

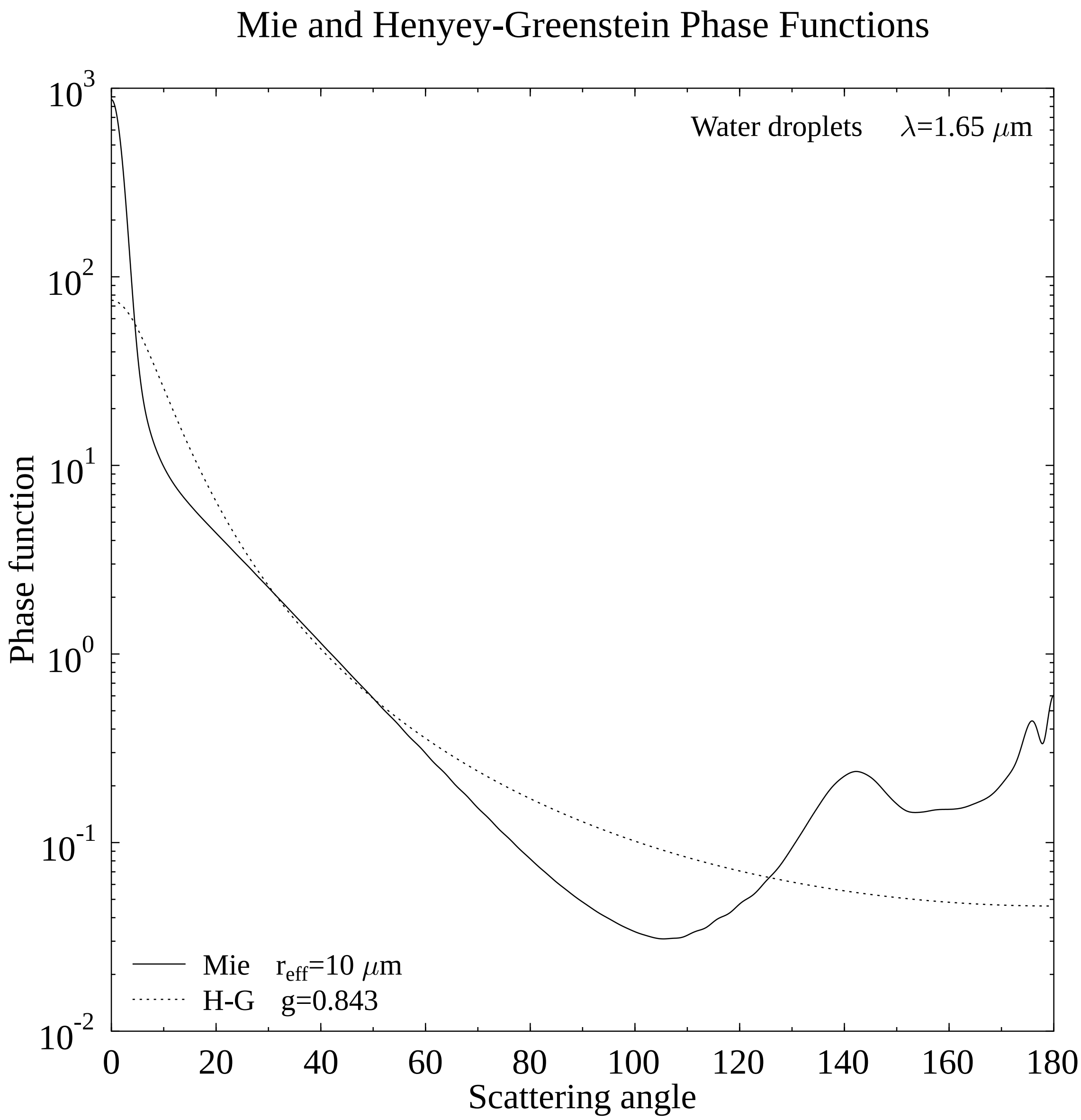
Henyey-Greenstein phase function - often used surrogate for Mie

$$P_{HG}(\Theta) = \frac{1 - g^2}{(1 + g^2 - 2g\cos\Theta)^{3/2}}$$

H-G phase function in forward direction: $P_{HG}(0^\circ) = (1+g)/(1-g)^2$.
H-G function in backward direction: $P_{HG}(180^\circ) = (1-g)/(1+g)^2$.
H-G phase function in Legendre polynomials:

$$\omega_l = (2l+1)g^l$$

The Henyey-Greenstein phase function is very different from the Mie phase function for backward directions ($\Theta > 90^\circ$), which means that it is not equivalent for radiance fields, although it usually adequate for flux calculations.



Comparison of Mie and Henyey-Greenstein phase function with same asymmetry parameter g.