Lecture 15.

Light scattering and absorption by atmospheric particulates.

Part 3: Scattering and absorption by nonspherical particles.

Objectives:

1. Types of nonspherical particles in the atmosphere.
2. Ray-tracing method.
3. T-Matrix method.
4. FDTD method.
5. DDA method.

Required Reading:

L02: 5.3, 5.5

Advanced/Additional Reading:

L02: 5.4

Mishchenko, Hovenier, and Travis (Eds.), Light scattering by nonspherical particles. Academic Press. 2000.

Good website with information on various methods and numerical codes for scattering by nonspherical particles: http://www.t-matrix.de/

1. Types of nonspherical particles in the atmosphere:

Aerosols:

Dry salts (e.g., dry sulfates, nitrates, sea-salt) (cube- or rectangular-like shapes)

Dust (various shapes)

Carbonaceous (chain-like aggregates)

Bio aerosols (various shape)

Ice crystals: several typical habits (can be predicted as a function of T and environmental conditions)

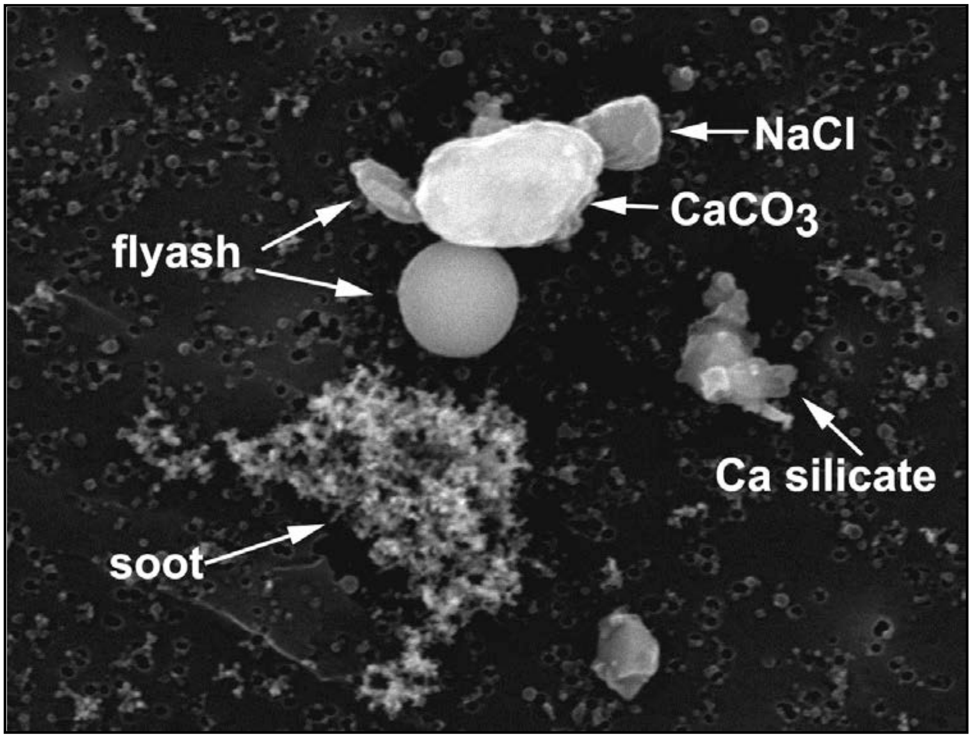


Figure 15.1 Examples of aerosol particle shapes.

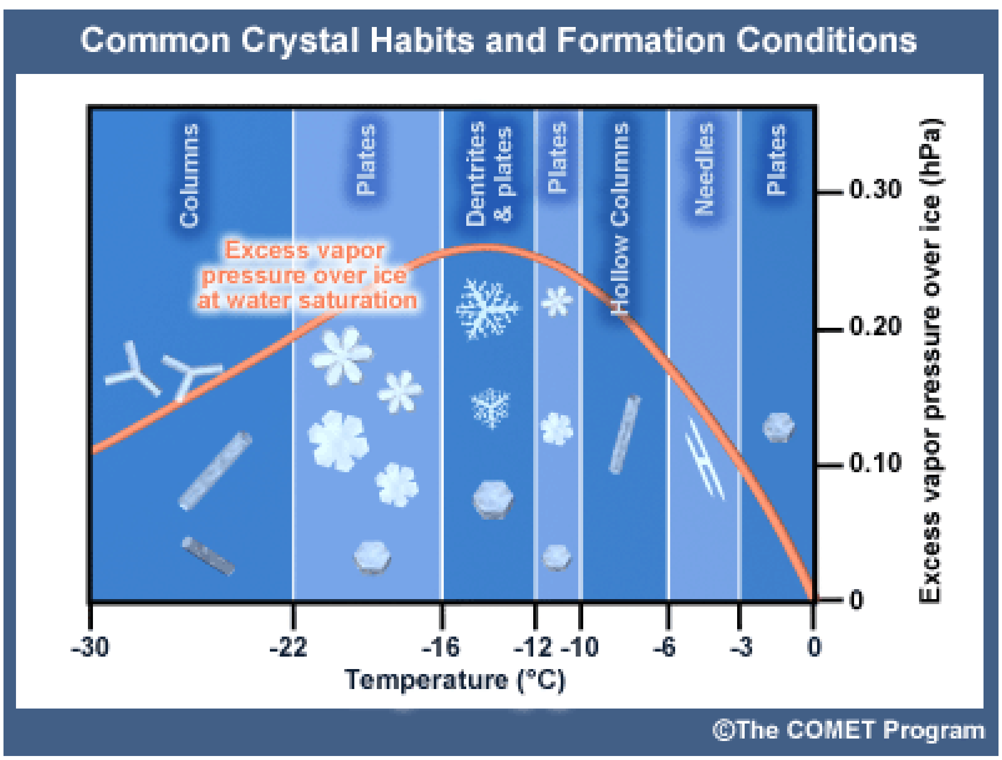
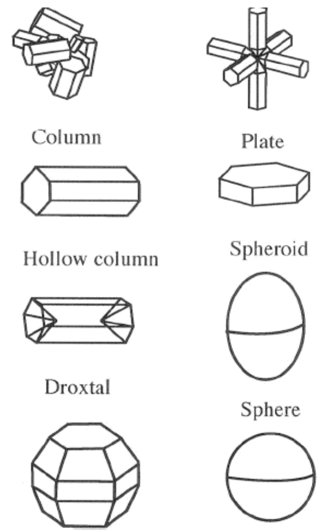


Figure 15.2 Ice crystal habits.

<u>Database of optical properties of ice crystals:</u>

Yang, P., H. Wei, H. L Huang, B. A. Baum, Y. X. Hu, M. I. Mishchenko, and Q. Fu, 2005: Scattering and absorption property database of various nonspherical ice particles in the infrared and far-infrared spectral region. Appl. Opt., 44, 5512-5523.

Shapes of ice crystals included in the database:



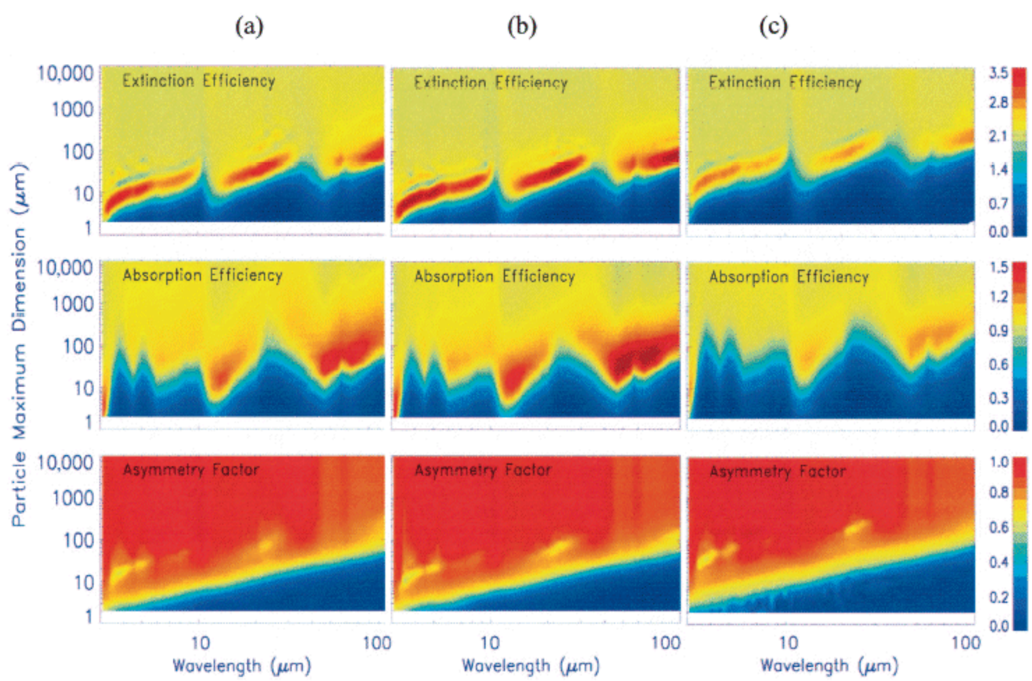


Figure 15. 3 Contours of the extinction efficiency, absorption efficiency, and asymmetry parameter for (a) solid columns, (b) droxtals and (c) aggregates.

2. Ray-tracing method.

The ray-tracing method (also called the geometrical optics approximation, or ray optics approximation) is an approximate method for computing light scattering by particles much larger than a wavelength (i.e., the smallest size parameter is about 80-100).

Basic principles: The ray-tracing method is based on the assumption that the incident EM wave can be represented as a collection of independent parallel rays. Ray tracing is commonly performed using a Monte Carlo approach.

Ray tracing consists of two parts:

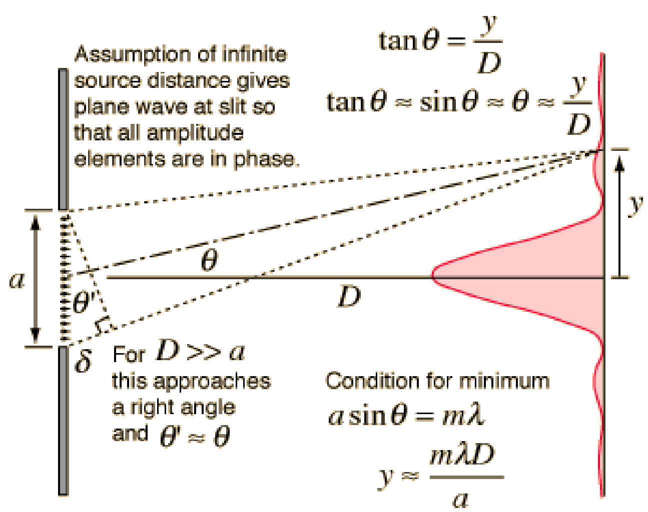
1) diffraction theory for the forward scattering peak; and
2) ray tracing using Fresnel reflection and transmission formulas.

Advantages: The ray-tracing method can be applied to any shape (spherical or non spherical)

Limitations: It is an approximate method (by definition);
Limited range of size parameters;
Absorbing particles require special treatment.

- ***Diffraction***

In geometric optics, 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.

Integrate the far field contribution of incident wave over the aperture

$$E = -\frac{iE_0}{R\lambda}\int_A \exp(-ikR)dA \qquad [15.1]$$

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

For sphere (circular aperture), the diffraction pattern is

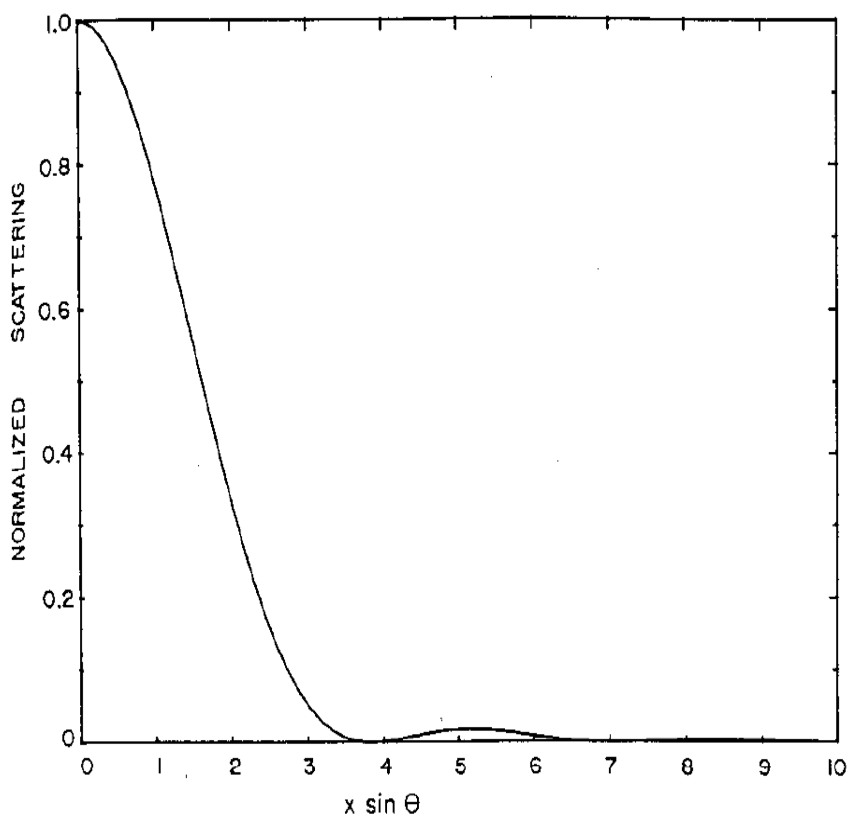
$$I(\Theta) = -\frac{I_o}{R^2k^2}\frac{x^4}{4}\left[\frac{2J_1(x\sin\Theta)}{x\sin\Theta}\right]^2 \qquad [15.2]$$

where k = 2π/λ, and $\boldsymbol{J}_1$ is the Bessel function.

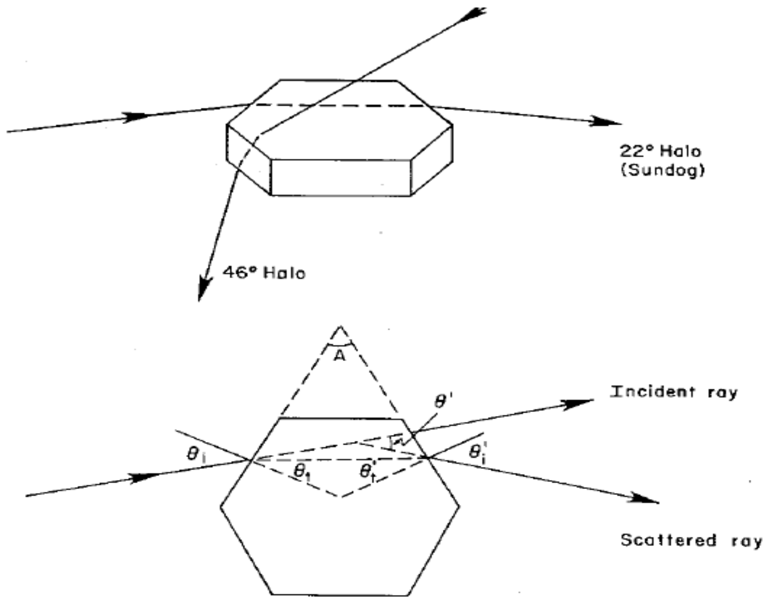
Example: Scattering diagram for diffraction by a circular disk.

Diffraction peak in the phase function: width Θ ~1/x, height P(0) ~x^2

First zero at x sinΘ = 3.83 and max at x sinΘ = 5.14



➢ ***<u>Fresnel reflection and transmission</u>***



Snell's law gives the refraction angle θ_t:

$$\mathbf{\sin\theta_i = m \sin\theta_t} \qquad [15.3]$$

Fresnel formula for polarized reflection amplitude coefficients:

$$r_r = \frac{\cos\theta_i - \sqrt{m^2 - \sin^2\theta_i}}{\cos\theta_i + \sqrt{m^2 - \sin^2\theta_i}} \qquad [15.4]$$

$$r_l = \frac{\sqrt{m^2 - \sin^2\theta_i} - m^2\cos\theta_i}{\sqrt{m^2 - \sin^2\theta_i} + m^2\cos\theta_i} \qquad [15.5]$$

Reflectivity and transmission coefficient for intensity:

$$R_r = \left|r_r\right|^2, \quad R_l = \left|r_l\right|^2, \quad T_r = 1 - R_r, \quad T_l = 1 - R_l \qquad [15.6]$$

NOTE: For $\theta = 0^0$, reflection is $R = \left|\frac{m-1}{m+1}\right|^2$ => reflectivity increases with refractive index

➢ ***Diffraction + reflection and refraction***

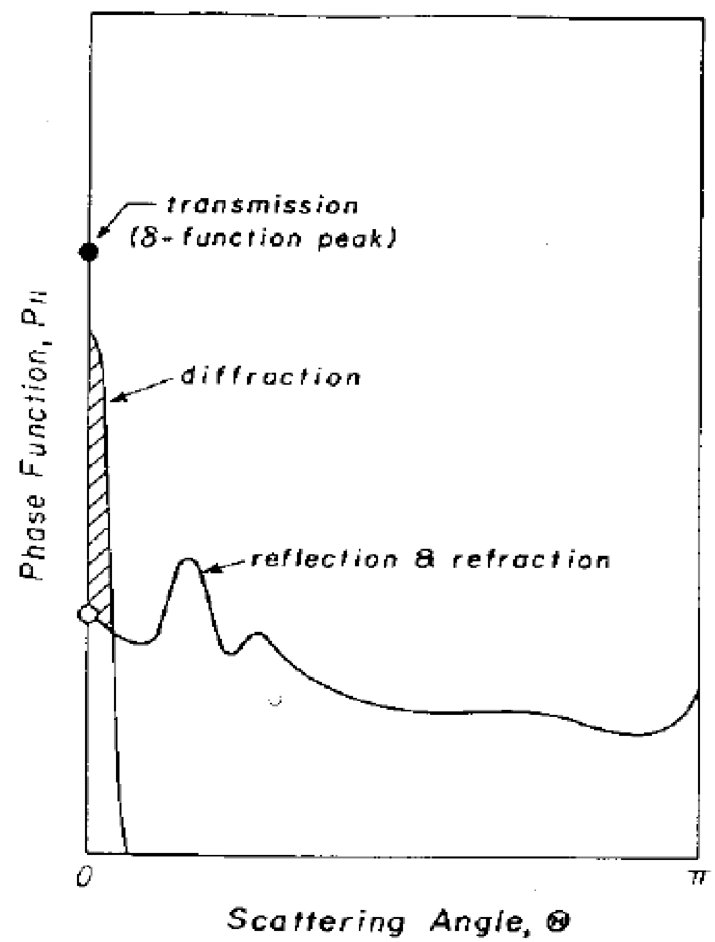


Figure 15.4 A schematic representation of the components of the phase function for randomly oriented hexagonal ice crystals (from Liou, 1992).

3. T-Matrix method.

T-Matrix method, TMM, enables calculation of optical properties of particles with rotationally symmetric shape (such as spheroids, circular cylinders, Chebyshev shapes, etc.)

NOTE: T-matrix FORTRAN code is available at

http://www.giss.nasa.gov/staff/mmishchenko/t_matrix.html

Basic principles: TMM is based on expanding the incident EM and scattered fields in vector spherical wave functions. The T matrix transforms the expansion coefficients of the incident field into those of scattered field and, if known, can be used to compute any scattering characteristic of a nonspherical particle. The elements of the T matrix are independent of the incident and scattering fields and depend only on the shape, size parameter, and refractive index of the scattering particle and on its orientation with respect to the reference frame.

Advantages: TTM is highly accurate and computationally fast

Limitations: Limited types of particle shapes;
Limited range of size parameters ($x < 30$).

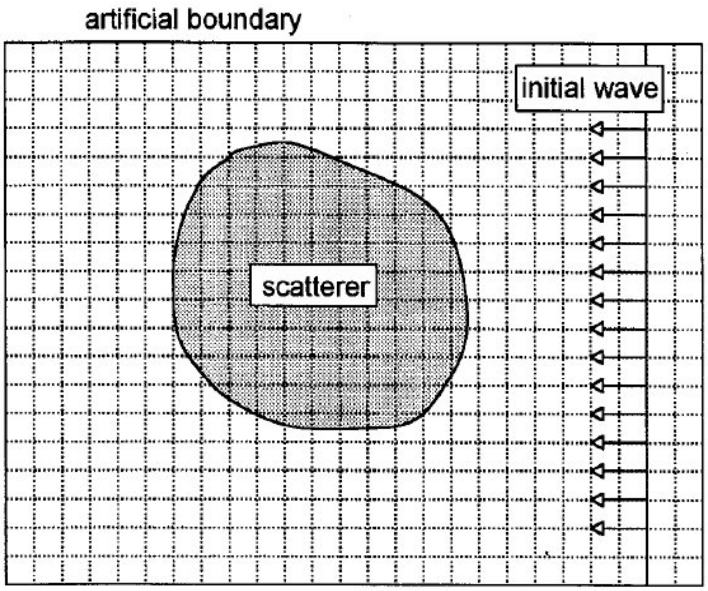
For large size parameters:

Improved geometric optics method (IGOM) (e.g., Yang P. and K. N. Liou, "Geometric-optics-integral-equation method for light scattering by nonspherical ice crystals," Appl. Opt. 35, 6568–6584 , 1996).

4. FDTD method.

Finite Difference Time Domain, FDTD, method enables calculations of optical properties of particles of complicated geometries and compositions.

Basic principles: FDTD solves the Maxwell's curl equations in the time-domain by introducing a finite difference analog. The space containing a scattering particle is dicretized by using a grid mesh. The existence of the particle is represented by assigning suitable electromagnetic constants in terms of permittivity, permeability and conductivity (depending on particle properties) over the grid points.



Advantages: FDTD can be applied to particles having any shape and composition.

Limitations: Known implementation problems (for instance, staircasing effect - due to selection of the Cartesian mesh grid)

Limited range of size parameters (up to x =15-20)

Applications (ice crystals):

Yang et al.: FDTD for size parameter ~15 and ray-tracing (for x >15)

NOTE: see Chapter 5.4 in L02 and

Yang, P., and K. N. Liou, 2000: Finite difference time domain method for light scattering by nonspherical particles. Chapter 7 in *Light scattering by nonspherical particles: theory, measurements, and geophysical applications*, Eds. M. I. Mishchenko, J. W. Hovenier, and L. D. Travis, Academic Press, pp.173-221.

5. DDA method.

Basics of dipole interactions:

In the Rayleigh limit, perpendicular and parallel components of scattered intensities in the far-field are

$$I_r = I_{0r} k^4 \alpha^2 / r^2$$

$$I_l = I_{0l} k^4 \alpha^2 \cos^2(\Theta) / r^2$$

where α is the polarizability of the particle and it relates to the refractive index via Lorentz-Lorentz formula (also known as Clausius-Mossotti formula) (see Lecture 15)

$$\alpha = \frac{3}{4\pi N_s}\left(\frac{m^2-1}{m^2+2}\right)$$

<u>EM field of two isolated dipoles:</u>

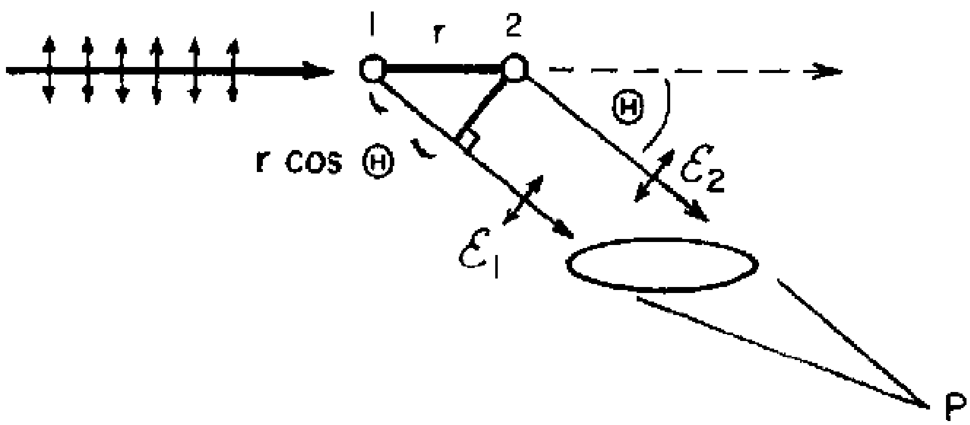


Figure 15.5 Two isolated dipoles scatter the incident EM field into all directions. An observer at point P will measure the superposition of scattered waves of two dipoles, propagating into the direction of observation (i.e., in scattering angle Θ). The interference of these two waves depends on the phase difference caused by the relative path difference.

The phase difference between two scattered waves at point P is the difference in path length of two waves

$$\Delta\delta = x(1-\cos\Theta) \qquad [15.7]$$

where x is the size parameter. Thus the scattered field is

$$E_{1+2} \sim E_1 \exp(-i\delta) + E_2 \exp(-i(\delta + \Delta\delta)) \qquad [15.8]$$

and the detected intensity (averaged over the full cycle)

$$I_{1+2} \sim E_1^2 + E_2^2 + 2E_1E_2 \cos(\Delta\delta) \qquad [15.9]$$

If $E_1=E_2$

$\Delta\delta = \pi, 3\pi, 5\pi \ldots$ => fields cancel (out of phase)

$\Delta\delta = 0, 2\pi, 4\pi, \ldots$ => fields reinforce (in phase)

NOTE: The forward scattering waves are always in phase.

- In general case for nonspherical particle represented by many dipoles, the phase difference depends on both the distance between dipoles and the direction of scattering (except for $\Theta = 0^0$, i.e. forward scattering) => the scattered radiation is a complex superposition of individual scattered waves of many different phase differences.
- The larger the particle, the higher intensity scattered in the forward direction and the greater the forward to backward asymmetry.

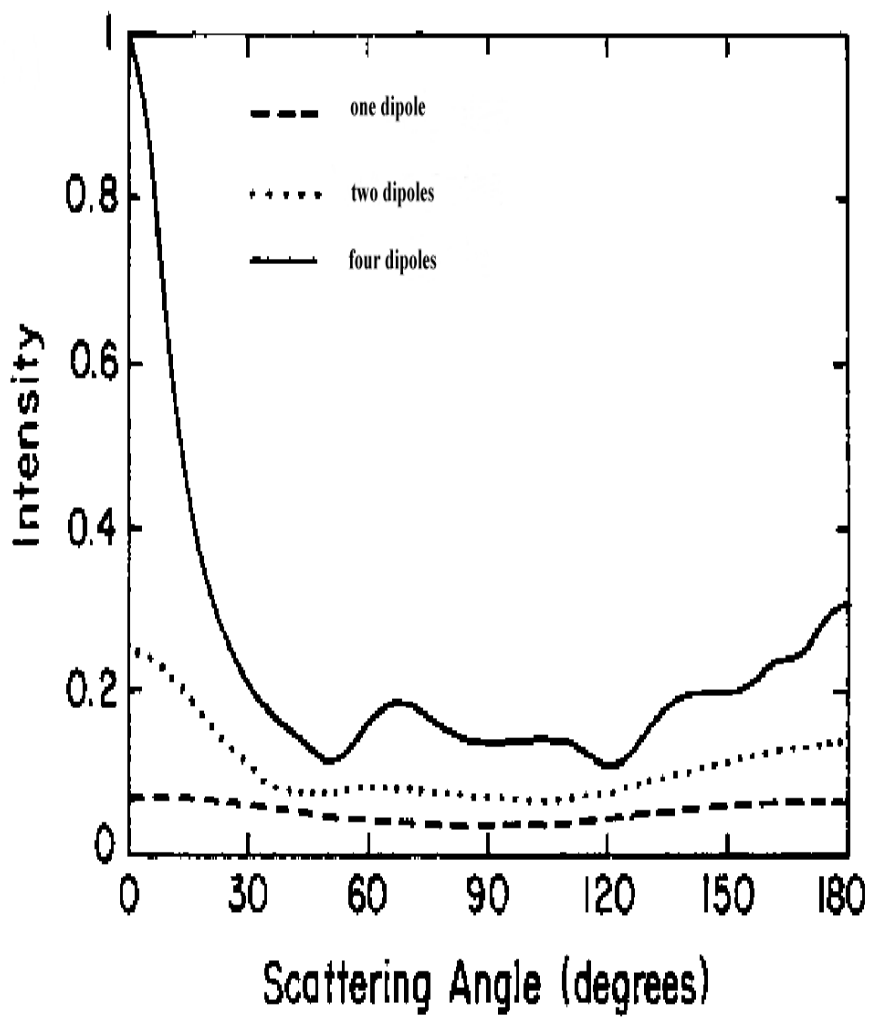


Figure 15.6 Intensity of dipoles lied on one line at the distance of one wavelength and interacted with each other (Bohren, 1987).

- In addition to phase differences, the scattered field is affected by interaction of dipoles with each other.

Consider a particle composed of many dipoles. The scattered field is incident field plus the fields produced by each dipole

$$E_{sc} = E_{inc} + \sum E_{dipoles} \quad [15.10]$$

The dipole moment of j-th dipole is

$$p_j = \alpha_j E_{dipole,j} \quad [15.11]$$

where α_j is the polarizability of the dipole and $E_{dipole,j}$ is the field acting on the dipole which is the superposition of incident field and the fields caused by other dipoles. Thus

$$p_j = \alpha_j [E_{inc,j} - \sum_{j \neq k} A_{jk} p_k] \quad [15.12]$$

where $-\sum_{j \neq k} A_{jk} p_k$ is the contribution from the electric field at j-th dipole from the k-th dipole.

NOTE: Solving Eqs.[15.10]-[15.12] for all p_j gives the basis of the Discrete Dipole Approximation (DDA) method.

<u>Outline of the DDA method:</u>

DDA (Discrete Dipole Approximation) method enables computation of optical properties of arbitrary shaped, inhomogeneous, and anisotropic particles.

NOTE: DDSCAT is a FORTRAN implementation of the DDA technique. The code and user guide are openly available at http://www.astro.princeton.edu/~draine/DDSCAT.html

<u>Basic principles</u>: In DDA, a particle is replaced by the array of polarizable points (dipoles), and then the electromagnetic scattering problem for an incident periodic wave interacting with this array of point dipoles is solved exactly.

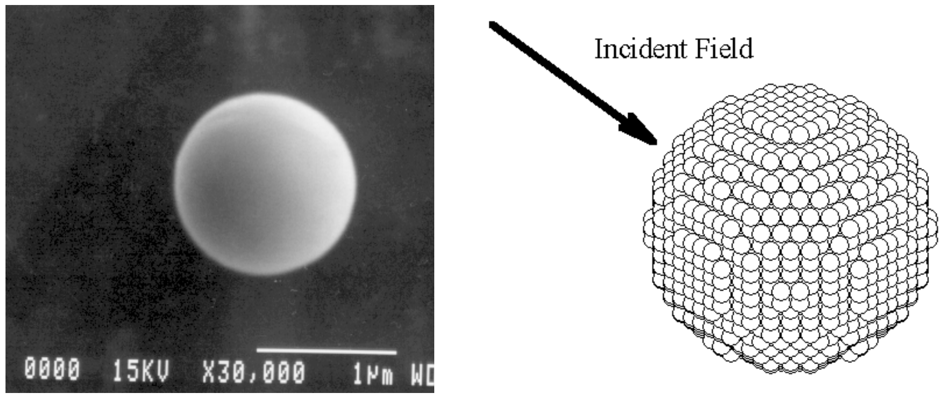


Figure 15.7 A spherical particle is represented by individual dipoles in DDA calculations.

<u>Advantages</u>: DDA can be applied to particles having any shape and composition (i.e., homogeneous or aggregates)

<u>Applicability and limitations of DDA:</u>

DDA is completely flexible regarding the geometry of a particle, being only limited by the need to use an interdipole distance ***d*** small to satisfy

$$\frac{2\pi}{\lambda}|m|d < 1 \qquad [15.13]$$

where m is the complex refractive index of the particle.

If a particle of volume V is represented by an array of N dipoles, located on a cubic lattice with lattice spacing ***d***, then

$$V = Nd^3 \qquad [15.14]$$

The size of the particle can be characterized by the "effective radius" $\boldsymbol{a_{eff}}$ as

$$a_{eff} = (3V/4\pi)^{1/3} \qquad [15.15]$$

i.e., $\boldsymbol{a_{eff}}$ is the radius of an equal volume sphere.

Then the size parameter is $x = \frac{2\pi}{\lambda}a_{eff}$

and it can be related to N as

$$x = \frac{2\pi}{\lambda} a_{eff} = \frac{62.04}{|m|} \left(\frac{N}{10^6} \right)^{1/3} |m| \frac{2\pi}{\lambda} d \qquad [15.16]$$

The number of dipoles N ~ $a_{eff}^{\ 3}$, so as particle size increases, the very large number of dipoles are required. Therefore, DDA is limited by the size parameter of about 15-20 (or the number of dipole is up to $N=10^6$).

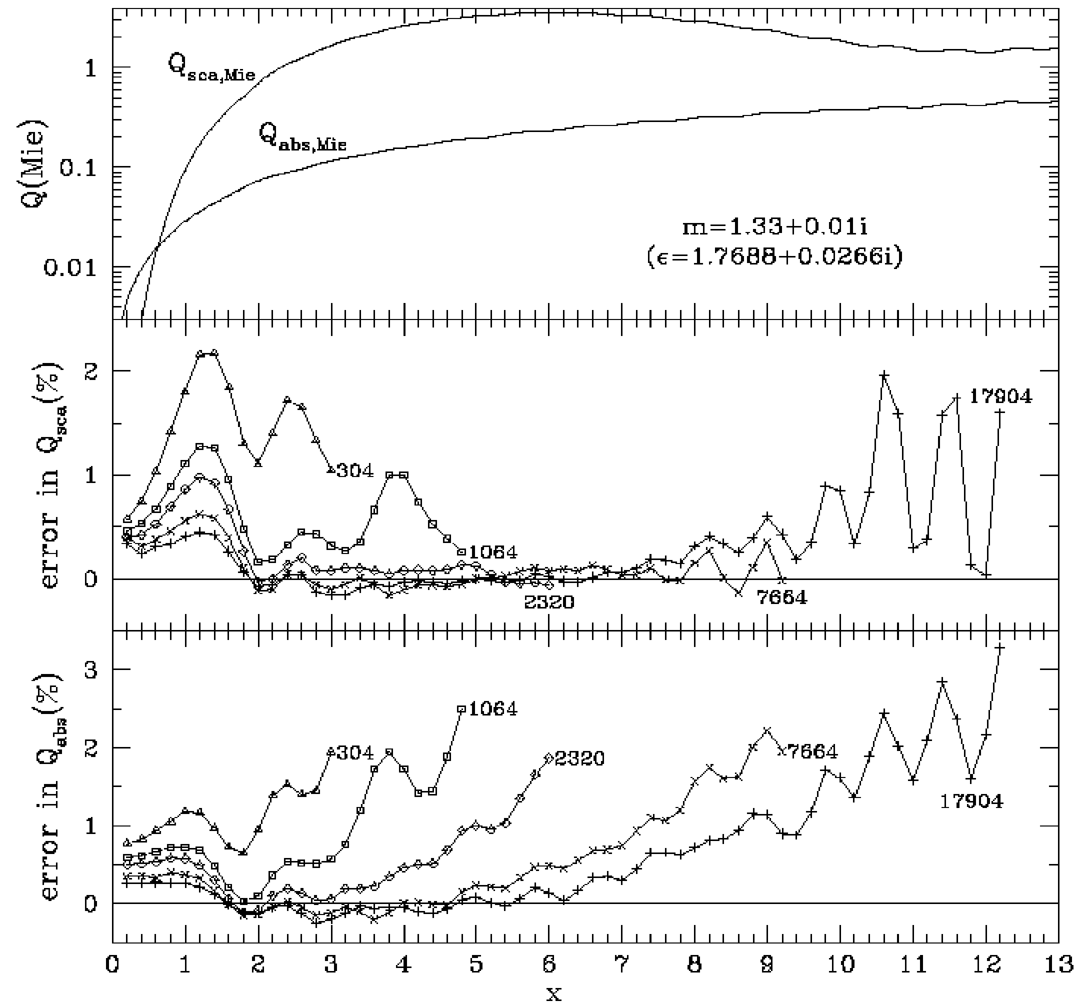


Figure 15.8 Scattering and absorption efficiencies for a sphere with m=1.33-0.01i. The upper panel shows exact calculations from Mie, whereas the middle and lower panels show fractional errors in Q_s and Q_e, calculated with DDSCAT for different numbers of dipoles N (Draine and Flatau, 1994).

Applications:

computations of optical properties of mineral dust particles

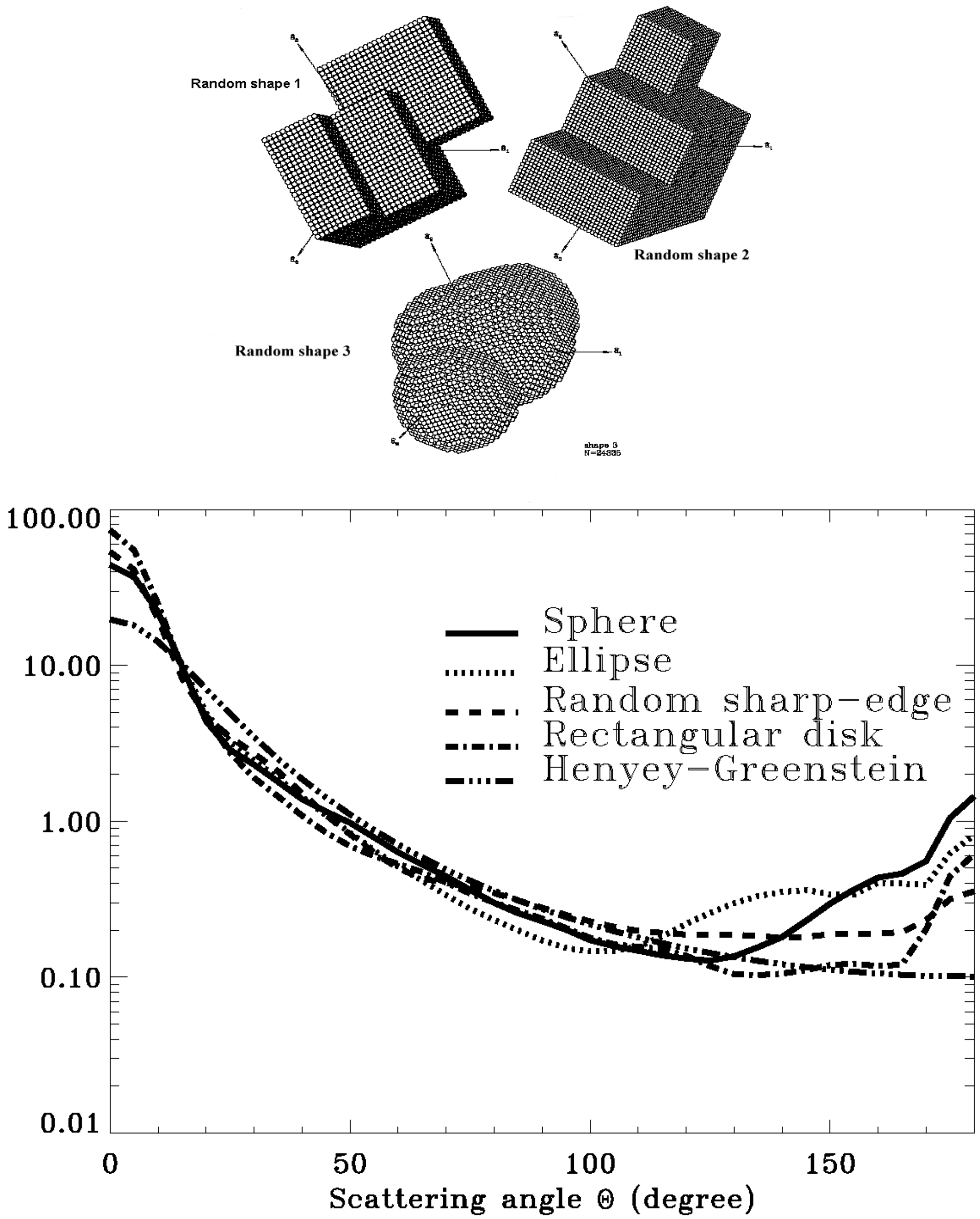


Figure 15.9 (Upper panel) Representation of different shapes of dust particles for DDA calculations. (Lower panel) Scattering phase function calculated with DDA for a log-normal size distribution with r_0= 0.5 μm, at λ = 0.5 μm , m = 1.51 -i0.002 (From Kalashnikova and Sokolik, 2004).

Extension of DDA to large size parameters:

ADDA (Amsterdam DDA)

http://code.google.com/p/a-dda/

Yurkin M.A., Maltsev V.P., and Hoekstra A.G. The discrete dipole approximation for simulation of light scattering by particles much larger than the wavelength. *J.Quant.Spectr.Radiat.Transf.* 106, 546-557, 2007.

Yurkin, M.A., and A. G. Hoekstra: The discrete dipole approximation: an overview and recent developments, J. Quant.Spectrosc. Radiat. Transfer 106, 558–589, 2007.

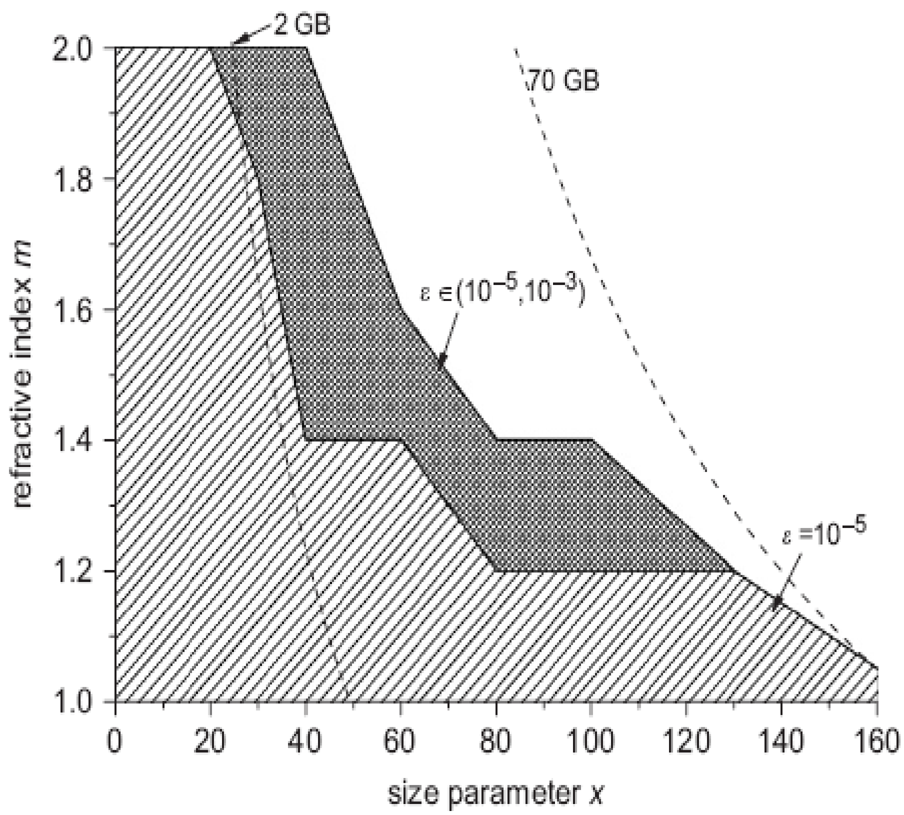


Figure 15.10 Current capabilities of ADDA for spheres with different x and m. The striped region corresponds to full convergence and densely hatched region to incomplete convergence. The dashed lines show two levels of memory requirements for the simulations (Yurkin et al., 2007)