<u>Lecture 14</u>

<u>Scattering. Part 2: Scattering and absorption by aerosol particles.</u>

<u>Objectives:</u>

1. Underlying physics of scattering and absorption of an individual particle.

2. Mie-Debye theory.

<u>Required Reading</u>:

L80: 5.4

<u>Additional/advanced Reading</u>:

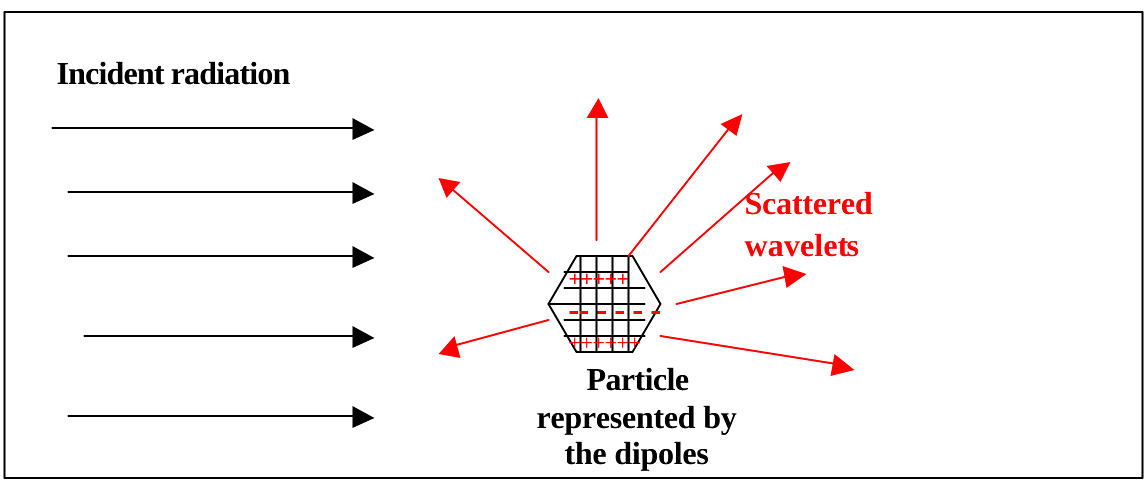
Le93: 12.3/G&Y:7.6

<u>Recommended reading:</u>

Bohren, G.F., and D.R. Huffmn, Absorption and scattering of light by small particles. John Wiley&Sons, 1983.

<u>1. Underlying physics of scattering and absorption of an individual particle.</u>

Consider a single arbitrary particle. The incident electromagnetic field induces dipole oscillations. The dipoles oscillate at the frequency of the incident field and therefore scatter radiation in all directions. In a given direction of observation, the total scattered field is a superposition of the scattered wavelets of these dipoles, accounting for their phase difference: scattering by the dipoles is coherent (i.e., there is a definite relation between phases). In general, these phase relations vary with the scattering direction.



NOTE: The phase relations between scattered wavelets depend on scattering direction, and size and shape of a particle. But the amplitude and phase of the induced dipole depend on the material of the particle.

NOTE: If a particle is much smaller than the wavelength of the incident field (Rayleigh scattering), all the secondary wavelets are approximately in phase so there is little variation of scattered field with direction (see Lecture 13 and Laboratory 6).

2. Mie-Debye theory.

NOTE: Mie-Debye theory is often called **Mie theory**.

Mie theory outline:

Assumptions:

i) Particle is a **sphere** of radius a;

ii) Particle is **homogeneous** (therefore it is characterized by a **single refractive index** $m = m_r - i m_i$ at a given wavelength);

NOTE: Mie theory requires the relative refractive index = refractive index of a particle/refractive index of a medium. But for air m is about 1, so one needs to know the refractive index of the particle (i.e., refractive index of the material of which the particle is composed).

Strategy:

Seek a solution of a vector wave equation (which follows from the Maxwell equations) for $\vec{E}$ and $\vec{H}$

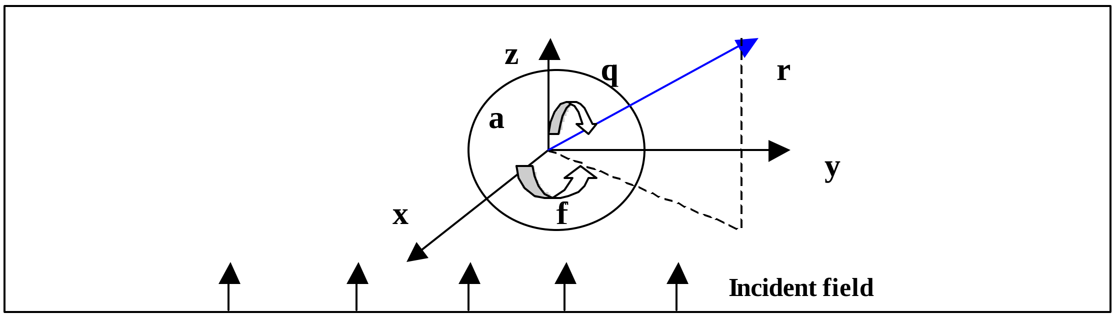
$$\nabla^2 \vec{E} + k^2 m^2 \vec{E} = 0$$

with the boundary condition that the tangential component of $\vec{E}$ and $\vec{H}$ be continuous across the spherical surface of a particle. Here k is the propagation (or wave) constant, $\mathbf{k = 2\pi/\lambda = \omega/c}$

NOTE: Mie theory calculates the electromagnetic field at all points in the particle (called internal field) and at all points of the homogeneous medium in which the particle is embedded. For all practical applications in the atmosphere, light scattering observations are carried out in the far-field zone (i.e., at the large distances from a sphere):

NOTE: Assumption on the spherical surface of a particle allows solving the vector equation analytically.

Consider a spherical coordinate system centered on a spherical particles of radius ***a*** and with the incident radiation propagating in z-direction.



In the far-field zone (i.e., at the large distances from a sphere), the solution of the vector wave equation can be obtained as

$$E_r^s = H_r^s \approx 0$$

$$E_\theta^s = H_\varphi^s \approx \frac{-i}{kr} e^{-ikr} \cos(\varphi) \sum_1^\infty \frac{2n+1}{n(n+1)} \left[a_n \frac{dP_n^1(\cos\theta)}{d\theta} + b_n \frac{P_n^1(\cos\theta)}{\sin\theta} \right]$$

$$-E_\varphi^s = H_\theta^s \approx \frac{-i}{kr} e^{-ikr} \sin(\varphi) \sum_1^\infty \frac{2n+1}{n(n+1)} \left[a_n \frac{dP_n^1(\cos\theta)}{\sin\theta} + b_n \frac{P_n^1(\cos\theta)}{d\theta} \right]$$

[14.1]

where P_n^1 are the associated Legendre polynomials, and a_n and b_n are **Mie coefficients** which don't depend on the angles but depend on size parameter $\mathbf{x = 2\pi a/\lambda}$ (*a* is the radius of the particle) and variable $\mathbf{y = x\, m}$ (*m* is relative refractive index of the particle). The expression for a_n and b_n are given by Eq.[5.74] in L80.

Let’s define two **Mie scattering functions**:

$$S_1(q) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left[a_n p_n(\cos q) + b_n t_n(\cos q) \right]$$

$$S_2(q) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left[b_n p_n(\cos q) + a_n t_n(\cos q) \right] \qquad [14.2]$$

where $\mathbf{p_n}$ and $\mathbf{t_n}$ are so-called **angular functions**

$$p_n(\cos q) = \frac{1}{\sin(q)} P_n^1(\cos q)$$

$$t_n(\cos q) = \frac{d}{dq} P_n^1(\cos q) \qquad [14.3]$$

thus we may re-write Eq.[14.1]

$$E_q^s = \frac{-i}{kr} e^{-ikr} \cos(j) S_2(q)$$

$$-E_j^s = \frac{-i}{kr} e^{-ikr} \sin(j) S_1(q) \qquad [14.4]$$

Let’s define the perpendicular and parallel components of the electric field as

$$E_r^s = -E_j^s \qquad \text{and} \qquad E_l^s = E_q^s$$

and decompose the incident electric vector into the perpendicular and parallel components as

$$E_r^i = \exp(-ikz) \sin j \qquad \text{and} \qquad E_l^i = \exp(-ikz) \cos j$$

Then Eq.[14.4] can be expressed as

$$\begin{bmatrix} E_l^s \\ E_r^s \end{bmatrix} = \frac{\exp(-ikr + ikz)}{ikr} \begin{bmatrix} S_2(q) & 0 \\ 0 & S_1(q) \end{bmatrix} \begin{bmatrix} E_l^i \\ E_r^i \end{bmatrix} \qquad [14.5]$$

Eq.[14.5] is a fundamental equation of scattered radiation by a sphere including polarization.

Now the scattered intensity components in the far field are

$$I_l^s = I_l^i \frac{i_2}{k^2 r^2}$$

$$I_r^s = I_r^i \frac{i_1}{k^2 r^2}$$

where $\boldsymbol{i_1}$ and $\boldsymbol{i_2}$ are so-called the **intensity function** for the perpendicular and parallel components, respectively, $i_1(q) = |S_1(q)|^2$ and $i_2(q) = |S_2(q)|^2$

From Mie theory it follows that the **extinction cross-section** of a particle is

$$s_e = \frac{4p}{k^2}\mathrm{Re}[S(0^0)] \qquad [14.6]$$

But for the forward direction (i.e. θ =0^0) from Eq.[14.2], we have

$$S_1(0^0) = S_2(0^0) = \frac{1}{2}\sum_{n=1}^{\infty}(2n+1)(a_n + b_n)$$

Let’s introduce the **efficiencies (or efficiency factors)** for extinction, scattering and absorption as

$$Q_e = \frac{s_e}{pa^2} \qquad Q_s = \frac{s_s}{pa^2} \qquad Q_a = \frac{s_a}{pa^2}$$

where $\boldsymbol{pa^2}$ is the particle area projected onto the plane perpendicular to the incident beam

From Eq.[14.6] we have that

$$\boxed{Q_e = \frac{s_e}{pa^2} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)\,\mathrm{Re}[a_n + b_n]} \qquad [14.7]$$

From Mie theory it follows that the **scattering cross-section** of a particle is

$$Q_s = \frac{s_s}{pa^2} = \frac{2}{x^2}\int_0^p [i_1(q) + i_2(q)]\sin(q)\,dq \qquad [14.8]$$

Using the recurrence properties of the associated Legendre polynomials (see L80: Appendix E), we can express [14.8] as

$$\boxed{Q_s = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)[|a_n|^2 + |b_n|^2]} \qquad [14.9]$$

Finally, the absorption efficiency can be calculated as

$$\boxed{Q_a = Q_e - Q_s} \qquad [14.10]$$

Recall definition of Stokes parameters (see Lecture 13), which uniquely characterize the electromagnetic waves. Let ***I_0***, ***Q_0***, ***U_0*** and ***V_0*** be the Stokes parameters of incident field and I, Q, U and V be the Stokes parameters of scattered radiation

$$\begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} = M \begin{bmatrix} I_o \\ Q_o \\ U_0 \\ V_o \end{bmatrix}$$

where ***M*** is the **transformation matrix**

$$M = \begin{bmatrix} M_{11} & M_{12} & 0 & 0 \\ M_{12} & M_{11} & 0 & 0 \\ 0 & 0 & M_{33} & -M_{34} \\ & & M_{34} & M_{33} \end{bmatrix}$$

and

$$M_{11} = \frac{1}{2k^2r^2}\left[S_1(q)S_1^*(q) + S_2(q)S_2^*(q)\right]$$

$$M_{12} = \frac{1}{2k^2r^2}\left[S_2(q)S_2^*(q) - S_1(q)S_1^*(q)\right]$$

$$M_{33} = \frac{1}{2k^2r^2}\left[S_2(q)S_1^*(q) + S_1(q)S_2^*(q)\right]$$

$$-M_{34} = \frac{1}{2k^2r^2}\left[S_1(q)S_2^*(q) - S_2(q)S_1^*(q)\right]$$

Let's define the **scattering phase matrix** ***P(q)*** as

$$\boldsymbol{M(q) = C\ P(q)}$$

and that

$$\frac{1}{4p}\int_{\Omega} P_{11}(q)d\Omega = \int_0^{2p}\int_0^{p}\frac{P_{11}(q)}{4p}\sin(q)dq\,dj = 1$$

Thus we have

$$C = \frac{1}{2}\int_0^{p} M_{11}(q)\sin(q)dq = \frac{1}{4k^2r^2}\int_0^{p}\left[i_1(q) + i_2(q)\right]\sin(q)dq$$

Using the definition of the scattering cross section Eq.[14.8], ***C*** becomes

$$C = \frac{s_s}{4p\,r^2}$$

Therefore the elements of the **scattering phase matrix** ***P(q)*** can be expressed as

$$\frac{P_{11}}{4p} = \frac{1}{2k^2 s_s}(i_1 + i_2) = \frac{1}{2}\left(\frac{P_1}{4p} + \frac{P_2}{4p}\right) \qquad [14.11]$$

$$\frac{P_{12}}{4p} = \frac{1}{2k^2 s_s}(i_2 - i_1) = \frac{1}{2}\left(\frac{P_2}{4p} - \frac{P_1}{4p}\right)$$

$$\frac{P_{33}}{4\pi} = \frac{1}{2k^2\sigma_s}(i_3 + i_4)$$

$$-\frac{P_{34}}{4\pi} = \frac{1}{2k^2\sigma_s}(i_4 - i_3)$$

and the scattering phase matrix for a spherical particle is

$$P = \begin{bmatrix} P_{11} & P_{12} & 0 & 0 \\ P_{12} & P_{11} & 0 & 0 \\ 0 & 0 & P_{33} & -P_{34} \\ & & P_{34} & P_{33} \end{bmatrix}$$

NOTE: In general, for a particle of any shape, the **scattering phase matrix *P(θ)*** consists of 16 independent elements, but for a sphere this number reduces to four.

Thus, Mie theory gives the extinction, scattering and absorption cross-sections of a single spherical particle and the scattering phase matrix.

NOTE: Laboratory 6 deals with the modeling of aerosol optics using Mie theory.

Recall Lecture 4 where we discussed the aerosol article size distributions.

If the particles characterized by a size distribution N(r), the extinction, scattering and absorption coefficients (in units LENGTH^{-1}) are calculated as

$$b_e = \int_{r_1}^{r_2} s_e(r) N(r) dr$$

$$b_s = \int_{r_1}^{r_2} s_s(r) N(r) dr$$

$$b_a = \int_{r_1}^{r_2} s_a(r) N(r) dr$$

The **single scattering albedo** if defined as

$$v_0 = \frac{b_s}{b_e} \qquad [14.12]$$

- The **single scattering albedo** gives the percentage of light which will be scattered in a single scattered event.