Chapter 6

Dust scattering off particles

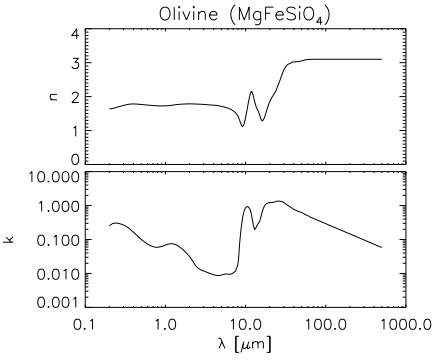
6.1 Overview

The theory of scattering off dust particles is a quite advanced topic. There are entire books devoted to this topic. The most famous of these books are:

- H.C. van de Hulst, "Light Scattering by Small Particles", Dover Books on Physics
- C.F. Bohren and D.R. Huffman, "Absorption and Scattering of Light by Small Particles", John Wiley and Sons

The main objective is to calculate the scattering and absorption cross sections at a given wavelength, for a particle of a given size and shape, made from a given type of material. In addition to this, the scattering cross section is angle-dependent, and tends to polarize the light.

The calculation of these quantities requires us to solve the classical equations of electrodynamics inside and outside of the dust grain. The dust grain is assumed to be made of dielectric material, so the material reacts to the presence of an electromagnetic field by becoming polarized. In other words: we consider the material to be made up of an infinite number of infinitely small electric and magnetic dipoles who's dipole strengths are proportional to the imposed field strengths. The induced dipoles create their own field in return. If the imposed field is an electromagnetic wave, the induced field is also an electromagnetic wave, i.e. the dust partical emits its own waves in reaction to the imposed waves. This is the process that is called scattering.



The properties of the material (how strongly the electric and magnetic dipoles react to the imposed field) are fully given by the *complex index of refraction*

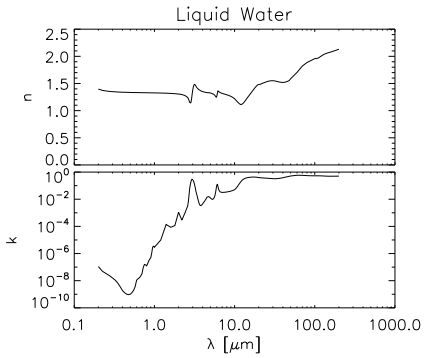
$$m(\lambda) = n(\lambda) - ik(\lambda) \tag{6.1}$$

where $n(\lambda)$ and $k(\lambda)$ are the real and the imaginary part of the complex index of refraction. They have to be given as a function of λ. Typically they are measured in the laboratory for a given material, and then provided to the community as a table for a finely sampled set of wavelengths. For common astrophysical materials you can find such tables at the Jena Optical Constants database[1].

Roughly one can interpret n and k as the scattering and absorption part of the refractive index. A particle with $k = 0$ (at some wavelength) will not absorb light, but it will scatter light. In reality k will never be exactly 0, because all materials absorb a bit. But k can easily be of order 10^{-8} or less for e.g. water or glass at visual wavelengths.

[1] http://www.astro.uni-jena.de/Laboratory/Database/databases.html

Material with $n = 1$ and $k = 0$ would be invisible, since it would have the same optical properties as vacuum. Typically n has values not much smaller than 1 and not much bigger than a few.



Another fundamental parameter is the ratio of the size of the particle over the wavelength:

$$x = \frac{2\pi a}{\lambda} \tag{6.2}$$

where a is the radius of the particle. Of course, this parameter is only well-defined for spherical particles, and in general particles can have very irregular shapes. Nevertheless, it gives a rough idea of how the particle size and the wavelength compare. We can distinguish three regimes:

- $x \ll 1$ (*the Rayleigh regime*): The particle is much smaller than the wavelength. The scattering process in this regime is called *Rayleigh scattering*, for which there is a simple theory.
- $x \simeq 1$: The particle size is similar to the wavelength. This is the most complex regime, and requires the full solution of the Mawell equations.
- $x \gg 1$ (*geometric optics regime*): The particle is much larger than the wavelength, so that it can be regarded in the geometric optics regime. This does not mean that its scattering is simple: reflection on the surface and refraction in the interior can still be quite complex (e.g. light passing through a rain drop), but it can be calculated using e.g. ray-tracing through the particle and off the particle's surface.

Calculating the scattering and absorption cross sections for all wavelength regimes is complicated. For homogeneous spheres this was first done in its full complexity by Gustav Mie. This calculational method is called *Mie theory*. For the $x \ll 1$ regime Mie theory produces the same scattering cross sections as Rayleigh theory, as it should. For $x \gg 1$ the theory becomes, however, more and more difficult to apply, since it involves a series expansion that requires ever more terms. Therefore, for $x \gg 1$ it, at some point, becomes more practical to use geometric optics.

Mie Theory is only applicable to spherical particles. The *T-matrix method* is its extension to non-spherical particles, though this method works best for still relatively simple shapes such as ellipsoids. A book that describes this method in detail is:

- Mishchenko, Travis & Lacis "Scattering, absorption and emission of light by small particles", Cambridge Univ Press[2]

For complex-shaped particles a fully numerical method has to be employed to solve the Maxwell equations. One such method is the *Discrete Dipole Approximation (DDA)*. For a list of publicly available codes see e.g. the Wikipedia page on DDA codes[3].

To give a complete overview of scattering theory, even of the basics, would require far too much time for this lecture. We will therefore keep this chapter very summary.

6.2 Rayleigh scattering

For small particles ($2\pi a \ll \lambda$) we can calculate the scattering cross sections according to Rayleigh scattering theory. We will not derive it, but instead quote the results from the books.

[2] http://www.giss.nasa.gov/staff/mmishchenko/books.html
[3] http://en.wikipedia.org/wiki/Discrete_dipole_approximation_codes

The scattering efficiency factor for Rayleigh scattering is

$$Q_{\rm sca,Ray} = \frac{8}{3}\left(\frac{2\pi a}{\lambda}\right)^4 \left|\frac{m^2-1}{m^2+2}\right|^2 \tag{6.3}$$

where m is the complex index of refraction. This means that the scattering cross section of a single particle is

$$\sigma_{\rm sca,Ray} = \frac{2}{3}\pi^5 \frac{(2a)^6}{\lambda^4} \left|\frac{m^2-1}{m^2+2}\right|^2 \tag{6.4}$$

The scattering opacity of small particles in the Rayleigh regime therefore goes roughly as $1/\lambda^4$, modulo the wavelength-dependence of m.

The scattering phase function (see Section 5.1.5) is given by

$$\Phi(\cos\Theta) = \frac{3}{4}(1+\cos^2\Theta) \tag{6.5}$$

(normalized such that $\frac{1}{2}\int_{-1}^{+1}\Phi(\mu)d\mu = 1$. Note that this is the same scattering phase function as for electron scattering.

The absorption efficiency factor is

$$Q_{\rm abs,Ray} = 4\left(\frac{2\pi a}{\lambda}\right) {\rm Im}\left(\frac{m^2-1}{m^2+2}\right) \tag{6.6}$$

meaning that the absorption cross section of a single particle is

$$\sigma_{\rm abs,Ray} = \pi\left(\frac{(2a)^3}{\lambda}\right) {\rm Im}\left(\frac{m^2-1}{m^2+2}\right) \tag{6.7}$$

The absorption opacity of small particles in the Rayleigh regime therefore goes roughly as $1/\lambda$, modulo the wavelength-dependence of m.

6.3 Mie Theory

Understanding Mie theory is not an easy task, and the derivation of the equations is somewhat elaborate. Here I merely discuss the basic idea behind it, and I refer to the book by Bohren & Huffman (see above) for details.

We consider a plane electromagnetic wave in vacuum with a wavelength λ, incident on a sphere of radius a with a complex refractive index m. The interaction of this wave with the sphere causes the sphere to radiate electromagnetic waves of itself. These waves are not isotropic in general. We can expand this outgoing wave using *vector spherical harmonics*. The idea is the same as for expanding a scalar field in spherical harmonics, but now for a vector field. Like with spherical harmonics, this involves Legendre polynomials and Bessel functions. The expansion coefficients are written as a_n and b_n, where n is the expansion index going from $n = 1$ to $n \to \infty$. These a_n and b_n are called the *scattering coefficients*.

The next step is to also expand the incoming plane wave into the same set of vector spherical harmonics. These expansion coefficients are usually written as c_n and d_n.

The goal is now to link a_n and b_n (the outgoing wave) to c_n and d_n (the incoming wave). This can be done by applying the usual boundary conditions for the electric and magnetic fields at the edge of the sphere, with which we are familiar from our lectures on electromagnetism. This can be done for each value of n separately. The result is:

$$a_n = \frac{m\psi_n(mx)\psi_n'(x) - \psi_n(x)\psi_n'(mx)}{m\psi_n(mx)\xi_n'(x) - \xi_n(x)\psi_n'(mx)} \tag{6.8}$$

$$b_n = \frac{\psi_n(mx)\psi_n'(x) - m\psi_n(x)\psi_n'(mx)}{\psi_n(mx)\xi_n'(x) - m\xi_n(x)\psi_n'(mx)} \tag{6.9}$$

where ψ and ξ are the *Riccati-Bessel functions*[4].

Now that we know the full expansion of the outgoing wave, we can calculate the scattering cross section, and find:

$$\sigma_{\rm scat} = \frac{2\pi}{k^2}\sum_{n=1}^{\infty}(2n+1)\left(|a_n|^2+|b_n|^2\right) \tag{6.10}$$

where $k = 2\pi/\lambda$ is the wave number of the incident wave. The full extinction coefficient (scattering + absorption) is:

$$\sigma_{\rm ext} = \frac{2\pi}{k^2}\sum_{n=1}^{\infty}(2n+1){\rm Re}\left\{a_n+b_n\right\} \tag{6.11}$$

From this you can calculate the absorption cross section as

$$\sigma_{\rm abs} = \sigma_{\rm ext} - \sigma_{\rm sca} \tag{6.12}$$

The larger the particle is compared to the wavelength, the more terms have to be included in the sum. Typically, for $x \gtrsim 1$, one needs $n \simeq x$ terms. For large particles ($x \gg 1$) this may require a lot of computing time. Good Mie codes take particular care of various possible numerical problems arising due to finite precision of the computer, which could lead to wrong results for large sums of terms. A good code is the BHMIE code of Bohren & Huffman, a version of which can be downloaded from the website of B. Draine[5].

6.4 Describing polarized light with a Stokes vector

Scattering tends to polarize light. Also, the scattering cross sections may be different for differently polarized light. So we must, for a more accurate study of scattering, introduce a method for describing polarized light. To do this we introduce the *Stokes vector*. Let us do this step by step, starting from the electromagnetic wave description of light.

Perfectly coherent light propagating into a direction $\mathbf{n}$ can be described by its frequency ν, the amplitudes of the left- and right- polarized components (or equivalently the horizontal- and vertical- polarized components) and their phase difference. The absolute phase (which varies on a time scale $1/\nu$) is for our purpose irrelevant. To make this quantitative we must introduce $\mathbf{e}_{x'}$ and $\mathbf{e}_{y'}$ basis vectors perpendicular to $\mathbf{n}$. In doing so we have various choices. Most importantly: we choose globally a right-handed coordinate system. We choose $\mathbf{e}_{x'}$ and $\mathbf{e}_{y'}$ such that

$$\mathbf{e}_{x'} \times \mathbf{e}_{y'} = \mathbf{n} \tag{6.13}$$

This means that if we look into the beam of radiation (the radiation coming toward us) we can define the x'-direction to be "right" and the y'-direction to be "up". The $\mathbf{n}$ vector can also be written as $\mathbf{e}_{z'}$.

At some fixed point P in space the electric field components for a perfectly coherent plane wave can be written as

$$E_{x'}(P,t) = E_{x',0}\cos(\omega t - \Delta_{x'}) \tag{6.14}$$
$$E_{y'}(P,t) = E_{y',0}\cos(\omega t - \Delta_{y'}) \tag{6.15}$$

where $\Delta_{x'}$ and $\Delta_{y'}$ are phase lags. The phase lag between the y' and x'-fields is $\Delta = \Delta_{y'} - \Delta_{x'}$, meaning that for positive Δ the y'-field lags behind the x'-field. The full

[4] The Riccati-Bessel function ψ_n is also often written as S_n, and is given by $\psi_n(x) = x j_n(x)$ in terms of the spherical bessel function $j_n(x)$.

[5] http://www.astro.princeton.edu/~draine/scattering.html

plane wave can be written as:

$$E_{x'}(\mathbf{x},t) = E_{x',0}\cos(\omega t - \mathbf{k}\cdot\mathbf{x} - \Delta_{x'}) \quad (6.16)$$
$$E_{y'}(\mathbf{x},t) = E_{y',0}\cos(\omega t - \mathbf{k}\cdot\mathbf{x} - \Delta_{y'}) \quad (6.17)$$

where $\mathbf{x}$ is the position vector, $\mathbf{k}$ is the wave vector such that $c = \omega/|\mathbf{k}|$ (with c the light speed). The full electric field vector is then

$$\mathbf{E}(\mathbf{x},t) = E_{x'}(\mathbf{x},t)\mathbf{e}_{x'} + E_{y'}(\mathbf{x},t)\mathbf{e}_{y'} \quad (6.18)$$

The magnetic field $\mathbf{H}$ is then

$$\mathbf{H}(\mathbf{x},t) = \mathbf{n}\times\mathbf{E}(\mathbf{x},t) \quad (6.19)$$

The average Poynting vector of this plane wave is equal to the flux vector $\mathbf{F}$

$$\mathbf{F} = \langle\mathbf{E}(\mathbf{x},t)\times\mathbf{H}(\mathbf{x},t)\rangle \quad (6.20)$$

The intensity $I(\mathbf{n}')$ is

$$I(\mathbf{n}') = |\mathbf{F}|\delta(\mathbf{n}'-\mathbf{n}) \quad (6.21)$$

meaning it is infinity in the direction $\mathbf{n}' = \mathbf{n}$ and zero for $\mathbf{n}' \neq \mathbf{n}$. This is because a perfectly plane wave corresponds to radiation from an infinitely small solid angle Ω, yet with finite total power, meaning that the power per solid angle diverges.

A perfectly coherent plane wave is fully described by its direction $\mathbf{n}$, its frequency ν, its amplitudes $E_{x',0}$, $E_{y',0}$ and the phase difference $\Delta \equiv \Delta_{y'} - \Delta_{x'}$.

In many applications radiation is not perfectly coherent. In those cases just $\mathbf{n}$, ν, $E_{x',0}$, $E_{y',0}$ and Δ are not enough to describe the radiation fully. A complete description can, however, be given by the Stokes parameters, which, for coherent radiation read:

$$I = E_{x',0}^2 + E_{y',0}^2 \quad (6.22)$$
$$Q = E_{x',0}^2 - E_{y',0}^2 \quad (6.23)$$
$$U = 2E_{x',0}E_{y',0}\cos\Delta \quad (6.24)$$
$$V = 2E_{x',0}E_{y',0}\sin\Delta \quad (6.25)$$

but they are also applicable to non-coherent radiation. These Stokes parameters are often conveniently written in terms of a column vector:

$$\begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} \quad (6.26)$$

Note that the Stokes parameters can be used to describe the flux, as is done here, but can also be used for intensity. This can lead to some confusion, in particular when we write I for the 1st Stokes parameter of the flux rather than the intensity. We will stick to this notation, however, because it is convention. The meaning will be made clear in the context.

The meaning of the Stokes parameters is as follows. I is the total flux (or intensity, depending on the context). The Q, U and V have the same dimension as I but only describe the polarization state. If $Q = U = V = 0$ the light is unpolarized, meaning it is not coherent. Perfectly coherent light has $Q^2 + U^2 + V^2 = I^2$. In general we have $0 \leq Q^2 + U^2 + V^2 \leq I^2$. For $V = I$ ($\Delta = \pi/2$, i.e. the $E_{y'}$ lags $\pi/2$ behind $E_{x'}$) we have *right-handed* circularly polarized light, meaning that the tip of the $\mathbf{E}$ field at a fixed point in space, when looking into the light (the propagation of light is toward the reader) rotates counter-clockwise (when the x-coordinate points right, and the y'-coordinate points up). The 3-D helix of his field will be *left-handed* (when the

z-coordinate points into the propagation direction of the light, i.e. toward the reader, i.e. a right-handed coordinate system). For $Q = I$ we have linearly polarized light in which the **E**-field lies in the x-direction. For $U = I$ we have linearly polarized light in which **E** lies along the $x' = y'$ line (when looking into the light). These definitions are consistent with the IAU 1974 definitions (Hamaker & Bregman 1996, A&AS 117, pp.161).

Important note: In order to be able to make sense of a Stokes vector in problems of radiative transfer, we must always specify a reference coordinate system. Since light may travel in any direction we cannot define this reference coordinate system apriori. So far we are used to specifying the direction of propagation **n** if we talk about the intensity. Let us call this the *polarization reference vector*. Now, if we talk about the polarized intensity in terms of a Stokes vector, we must, in addition to specifying **n**, also specify some additional unit vector **S**, which we *define* to point along the positive y' direction, as defined above. Clearly it must hold that $\mathbf{S} \cdot \mathbf{n} = 0$. The **S** vector gives the direction of the **E** field for radiation polarized with $Q = -I$ and $U = V = 0$.

If, for whatever reason, we need to do a rotation coordinate transformation from the (x', y')-basis to an (x'', y'')-basis according to

$$\begin{pmatrix} x'' \\ y'' \end{pmatrix} = \begin{pmatrix} \cos\psi & \sin\psi \\ -\sin\psi & \cos\psi \end{pmatrix} \begin{pmatrix} x' \\ y' \end{pmatrix} \tag{6.27}$$

(e.g. when rotating the direction of the polariation reference vector **S**), we must change the Stokes vectors with the following transformation:

$$\begin{pmatrix} I'' \\ Q'' \\ U'' \\ V'' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(2\psi) & \sin(2\psi) & 0 \\ 0 & -\sin(2\psi) & \cos(2\psi) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} I' \\ Q' \\ U' \\ V' \end{pmatrix} \tag{6.28}$$

Matrices that manipulate Stokes vectors are called *Müller matrices*. This particular example is the Müller matrix of rotation in the (x', y')-plane. But we will later encounter scattering Müller matrices.

6.5 The scattering matrix

Using the Stokes vector description of radiation, let us look again at the scattering problem. Let us describe the incoming plane wave as a flux Stokes vector $F = (F_I, F_Q, F_U, F_V)$, and the outgoing semi-spherical wave as $W = (W_I, W_Q, W_U, W_V)$, where W is a function of distance r from the particle, and roughly goes as $1/r^2$. Let us focus on the scattering into some direction θ and ϕ. We can now describe the relation between W and F with a *scattering matrix*:

$$\begin{pmatrix} W_I \\ W_Q \\ W_U \\ W_V \end{pmatrix} = \frac{1}{r^2} \begin{pmatrix} Z_{11} & Z_{12} & Z_{13} & Z_{14} \\ Z_{21} & Z_{22} & Z_{23} & Z_{24} \\ Z_{31} & Z_{32} & Z_{33} & Z_{34} \\ Z_{41} & Z_{42} & Z_{43} & Z_{44} \end{pmatrix} \begin{pmatrix} F_I \\ F_Q \\ F_U \\ F_V \end{pmatrix} \tag{6.29}$$

which is written under the assumption $r \gg \lambda/2\pi$. The elements Z_{ij} are the elements of the scattering matrix. Note that the scattering matrix is dependent on angle: $S_{ij}(\theta, \phi)$. By definition the total scattering cross section is the angle-integrated cross section:

$$\sigma_{\rm scat} = \int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\phi \, Z_{11}(\theta, \phi) \tag{6.30}$$

6.5.1 Randomly oriented and/or spherical particles

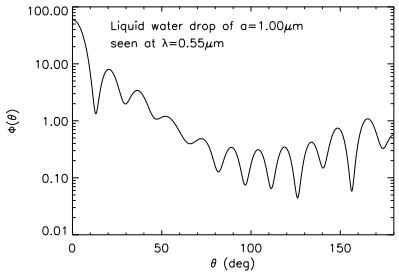
For spherical particles and/or for randomly oriented non-spherical particles the total angle-integrated scattering cross section is independent of the polarization state of

the incoming photon. This means that the scattering angular dependence becomes less complex. We can choose the polarization reference vector **S** such that $\phi = 0$, i.e. that the scattering occurs in the (x', z')-plane, i.e. the photon changes angle by rotation around the **S**-vector, such that it moves, afterward, in positive x'-direction (if we look into the light, the photon gets scattered to the right). Then the scattering matrix becomes simpler:

$$\begin{pmatrix} Z_{11} & Z_{12} & 0 & 0 \\ Z_{12} & Z_{22} & 0 & 0 \\ 0 & 0 & Z_{33} & Z_{34} \\ 0 & 0 & -Z_{34} & Z_{44} \end{pmatrix} \tag{6.31}$$

If we use Mie theory (i.e. for spherical particles) it reduces to an even simpler form:

$$\begin{pmatrix} Z_{11} & Z_{12} & 0 & 0 \\ Z_{12} & Z_{11} & 0 & 0 \\ 0 & 0 & Z_{33} & Z_{34} \\ 0 & 0 & -Z_{34} & Z_{33} \end{pmatrix} \tag{6.32}$$



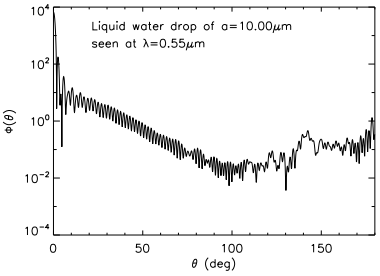
In conclusion: Mie theory gives four independent scattering matrix elements for each wavelength. They are:

$$S_{11} = \tfrac{1}{2}\left(|S_2|^2 + |S_1|^2\right) \tag{6.33}$$

$$S_{12} = \tfrac{1}{2}\left(|S_2|^2 - |S_1|^2\right) \tag{6.34}$$

$$S_{33} = \tfrac{1}{2}\left(S_2^* S_1 + S_2 S_1^*\right) \tag{6.35}$$

$$S_{34} = i\tfrac{1}{2}\left(S_2^* S_1 - S_2 S_1^*\right) \tag{6.36}$$



where

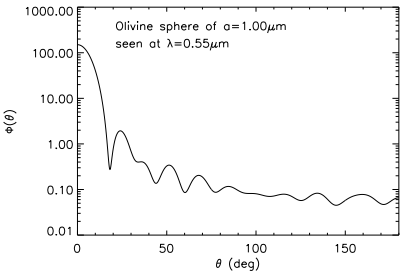
$$S_1 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)}(a_n \pi_n + b_n \tau_n) \tag{6.37}$$

$$S_2 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)}(a_n \tau_n + b_n \pi_n) \tag{6.38}$$

where

$$\pi_n(\theta) = \frac{P_n^1(\theta)}{\sin\theta} \qquad \text{and} \qquad \tau_n(\theta) = \frac{dP_n^1(\theta)}{d\theta} \tag{6.39}$$

with $P_n^1(\theta)$ the associated Legendre functions.



For unpolarized light the scattering phase function can now be calculated according to:

$$\Phi(\cos\theta) = \frac{1}{\sigma_{\text{scat}}} S_{11}(\cos\theta) \tag{6.40}$$

6.6 Some examples of real phase functions

In the margin figures we show some scattering phase functions computed with Mie theory. We show them for a water droplet and for a spherical olivine particle. The wavelenght is always $\lambda = 0.55\,\mu$m and we show the phase functions for particle radii of $a = 1\,\mu$m and $a = 10\,\mu$m.