1 Mie scattering, or scattering by a spherical particle(lecture 7)

An exact solution for scattering by electromagnetic waves by a spherical particle was presented by Mie and this kind of scattering is commonly called Mie scattering. Lately, the contribution by Lorenz has also been recognized, but his solution was not based on Maxwell's equations.

The solution of the scattering problem is composed of several fundamental stages. To start with, the scalar Helmholtz equation is solved in spherical coordinates, introducing the spherical harmonics and Bessel, Neumann, and Hankel special functions of fractional order (the so-called spherical Bessel functions, etc.).

In solving the vector Helmholtz wave equation, a general expansion in electric and magnetic multipoles is introduced and, in particular, the vector spherical harmonics. The energy and angular distributions of multipole fields are illustrated with examples, underscoring the power of the multipole analysis. To cope with the boundary conditions in the spherical geometry, the original incident plane wave field must be presented as a multipole expansion.

The actual scattering problem for a spherical particle can then be solved in a straightforward way. With the help of the multipole exansion, we can have a look at the boundary conditions for a nonspherical particle. In this case, the coefficients of the vector spherical harmonics can no longer be obtained analytically.

2 Scalar wave equation in spherical geometry

In order to prepare for the treatment of the vector wave equation, we consider the scalar wave equation for scalar field $\Psi(\mathbf{x}, t)$,

$$\nabla^2\Psi(\mathbf{x}, t) - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Psi(\mathbf{x}, t) = 0 \tag{1}$$

We can Fourier-transform the wave equation with respect to time,

$$\Psi(\mathbf{x}, t) = \int_{-\infty}^{\infty} d\omega \Psi(\mathbf{x}, \omega)e^{-i\omega t}, \tag{2}$$

in which case each Fourier-component fulfils the wave equation

$$(\nabla^2 + k^2)\Psi(\mathbf{x}, \omega) = 0, \qquad k^2 = \omega^2/c^2 \tag{3}$$

In the case of a single small particle, it is advantageous to search for the solution of the wave equation in the spherical coordinate system. Scattering extends to the full solid angle 4π and the small particle is located in a constrained region near the origin. In the spherical coordinates r, θ, φ, the wave equation is of the form (see Arfken, Jackson)

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\Psi}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\Psi}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\varphi^2} + k^2\Psi = 0 \tag{4}$$

The scalar wave equation can be solved by separating the variables so that the part including the angular coordinates is represented by the scalar spherical harmonics functions and the part including the radial dependence is represented by the spherical Bessel, Neumann, and Hankel functions,

$$\Psi(\mathbf{x},\omega) = \sum_{l,m} f_{lm}(r) Y_{lm}(\theta,\varphi) \tag{5}$$

The radial part ($f_{lm}(r)$) fulfils its differential equation independently of the index m,

$$\Big[\frac{d^2}{dr^2}\frac{2}{r}\frac{d}{dr} + k^2 - \frac{l(l+1)}{r^2}\Big] f_l(r) = 0. \tag{6}$$

By writing

$$f_l(r) = \frac{1}{\sqrt{r}} u_l(r) \tag{7}$$

we obtain

$$\Big[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} + k^2 - \frac{(l+\frac{1}{2})^2}{r^2}\Big] u_l(r) = 0, \tag{8}$$

which is the Bessel equation with order $l+\frac{1}{2}$. Then, in the most general way,

$$\begin{aligned} f_{lm}(r) &= A_{lm} j_l(kr) + B_{lm} n_l(kr) \\ &= \tilde{A}_{lm} h_l^{(1)}(kr) + \tilde{B}_{lm} h_l^{(2)}(kr), \end{aligned}$$

$$h_l^{(1)}(x) = j_l(x) + i n_l(x), \qquad h_l^{(2)}(x) = j_l(x) - i n_l(x), \tag{9}$$

where $j_l, n_l, h_l^{(1)}$ and $h_l^{(2)}$ are the spherical Bessel, Neumann, and Hankel functions. For example,

$$\begin{aligned} j_0(x) &= \frac{\sin x}{x}, \\ j_1(x) &= \frac{\sin x}{x^2} - \frac{\cos x}{x}, \\ j_2(x) &= (\frac{3}{x^3} - \frac{1}{x})\sin x - \frac{3\cos x}{x^2}, \\ n_0(x) &= -\frac{\cos x}{x}, \\ n_1(x) &= -\frac{\cos x}{x^2} - \frac{\sin x}{x}, \\ n_2(x) &= -(\frac{3}{x^3} - \frac{1}{x})\cos x - \frac{3\sin x}{x^2}, \\ h_0^{(1)}(x) &= \frac{e^{ix}}{ix}, \end{aligned}$$

$$
\begin{aligned}
h_1^{(1)}(x) &= -\frac{e^{ix}}{x}(1+\frac{i}{x}), \\
h_2^{(1)}(x) &= \frac{ie^{ix}}{x}(1+\frac{3i}{x}-\frac{3}{x^2}).
\end{aligned} \tag{10}
$$

The functions j_l and n_l can be analytically generated using the so-called Rodriques' formulae

$$
j_l(x) = (-x)^l(\frac{1}{x}\frac{d}{dx})^l(\frac{\sin x}{x}) \tag{11}
$$

$$
n_l(x) = -(-x)^l(\frac{1}{x}\frac{d}{dx})^l(\frac{\cos x}{x}) \tag{12}
$$

In the limit $x << 1, l$, the functions can be calculated using the leading terms of their series expansions,

$$
\begin{aligned}
j_l(x) &= \frac{x^l}{(2l+1)!!}\Big(1-\frac{x^2}{2(2l+3)}+\dots\Big), \\
n_l(x) &= -\frac{(2l-1)!!}{x^{l+1}}\Big(1-\frac{x^2}{2(1-2l)}+\dots\Big).
\end{aligned} \tag{13}
$$

Correspondingly, in the limit $x >> l$, we obtain

$$
\begin{aligned}
j_l(x) &\approx \frac{1}{x}\sin(x-\frac{l\pi}{2}), \\
n_l(x) &\approx -\frac{1}{x}\cos(x-\frac{l\pi}{2}), \\
h_l^{(1)}(x) &\approx (-i)^{l+1}\frac{e^{ix}}{x}.
\end{aligned} \tag{14}
$$

The functions obey the recursive relations

$$
\begin{aligned}
\frac{2l+1}{x}z_l(x) &= z_{l-1}(x)+z_{l+1}(x), \\
z_l'(x) &= \frac{1}{2l+1}[lz_{l-1}(x)-(l+1)z_{l+1}(x)], \\
\frac{d}{dx}[xz_l(x)] &= xz_{l-1}(x)-lz_l(x),
\end{aligned} \tag{15}
$$

where $z_l(x)$ can be any of the functions j_l, n_l, $h_l^{(1)}$ or $h_l^{(2)}$. In practical numerical computations, special attention needs to paid to numerical stability, for example, to the direction the recursive relations are utilized. The Wronskian determinants are, pair-wise,

$$
W(j_l,n_l) = \frac{1}{i}W(j_l,h_l^{(1)}) = -W(n_l,h_l^{(1)}) = \frac{1}{x^2}. \tag{16}
$$

Thus, the general solution of the scalar wave equation in spherical coordinates can be presented in the form

$$\Psi(\mathbf{x}) = \sum_{l,m} \left[A_{lm}^{(1)} h_l^{(1)}(kr) + A_{lm}^{(2)} h_l^{(2)}(kr) \right] Y_{lm}(\theta, \varphi) \tag{17}$$

that is, as a sum of outgoing and incoming waves.

Consider next the properties of the spherical-harmonics functions $Y_{lm}(\theta, \varphi)$. According to the definition,

$$\begin{aligned} Y_{lm}(\theta, \varphi) &= \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\varphi}, \\ l &= 0, 1, 2, \ldots, \\ m &= -l, -l+1, \ldots, 0, \ldots, l-1, l. \end{aligned} \tag{18}$$

The functions $P_l^m(x)$ are associated Legendre functions that can be derived from the Legendre polynomials $P_l(x)$ by the Rodriques' formula,

$$\begin{aligned} P_l^m(x) &= (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x) \\ &= (-1)^m \frac{1}{2^l l!} (1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (x^2-1)^l. \end{aligned} \tag{19}$$

For $P_l^m(x)$, it is generally true that

$$P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x) \tag{20}$$

so that

$$Y_{l,-m}(\theta, \varphi) = (-1)^m Y_{l,m}^*(\theta, \varphi) \tag{21}$$

The spherical-hamonics functions constitute a complete orthonormal set of functions,

$$\int_{4\pi} d\Omega Y_{l',m'}^*(\theta, \varphi) Y_{l,m}(\theta, \varphi) = \delta_{ll'} \delta_{mm'}, \tag{22}$$

with the closure relation

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{l,m}^*(\theta', \varphi') Y_{l,m}(\theta, \varphi) = \delta(\varphi - \varphi') \delta(\cos\theta - \cos\theta') \tag{23}$$

For example,

$$Y_{00} = \frac{1}{\sqrt{4\pi}},$$

$$
\begin{aligned}
Y_{10} &= \sqrt{\frac{3}{4\pi}}\cos\theta, \qquad Y_{11} = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi}, \\
Y_{20} &= \sqrt{\frac{5}{4\pi}}(\frac{3}{2}\cos^2\theta - \frac{1}{2}), \qquad Y_{21} = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\varphi}, \\
Y_{22} &= \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{i2\varphi}.
\end{aligned} \tag{24}
$$

For example, the following recursive relations can be derived for the associated Legendre functions:

$$
\begin{aligned}
& P_l^{m+1} - \frac{2mx}{\sqrt{1-x^2}}P_l^m + [l(l+1) - m(m-1)]P_l^{m-1} = 0 \\
(2l+1)xP_l^m &= (l+m)P_{l-1}^m + (l-m+1)P_{l+1}^m \\
(2l+1)\sqrt{1-x^2}P_l^m &= P_{l+1}^{m+1} - P_{l-1}^{m+1} \\
&= (l+m)(l+m-1)P_{l-1}^{m-1} - (l-m+1)(l-m+2)P_{l+1}^{m-1} \\
\sqrt{1-x^2}P_l^m &= \frac{1}{2}P_l^{m+1} - \frac{1}{2}(l+m)(l-m+1)P_l^{m-1}.
\end{aligned} \tag{25}
$$

Let us study the spherical wave expansion of the Green's function corresponding to an outgoing wave. The Green's function fulfils the inhomogeneous wave equation

$$
(\nabla^2 + k^2)G(\mathbf{x}, \mathbf{x}') = -\delta(\mathbf{x} - \mathbf{x}') \tag{26}
$$

and is of the form

$$
G(\mathbf{x}, \mathbf{x}') = \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x} - \mathbf{x}'|} \tag{27}
$$

Let us write

$$
G(\mathbf{x}, \mathbf{x}') = \sum_{lm} g_l(r, r')Y_{lm}^*(\theta', \varphi')Y_{lm}(\theta, \varphi) \tag{28}
$$

and insert this expression into the partial differential equation above. Then, we obtain

$$
\Big[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + k^2 - \frac{l(l+1)}{r^2}\Big]g_l = -\frac{1}{r^2}\delta(r - r') \tag{29}
$$

with the following wave solution that is finite at the origin and and outgoing wave at infinity,

$$
g_l(r, r') = Aj_l(kr_<)h_l^{(1)}(kr_>) \tag{30}
$$

where $r_> = \max(r, r')$ and $r_< = \min(r, r')$ and $A = ik$, so that the discontinuity of the derivatiuve is correct at $r = r'$. The spherical wave expansion of the Green's function is thus

$$
\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x} - \mathbf{x}'|} = ik\sum_{l=0}^{\infty} j_l(kr_<)h_l^{(1)}(kr_>)\sum_{m=-l}^{l} Y_{lm}^*(\theta', \varphi')Y_{lm}(\theta, \varphi) \tag{31}
$$