Diffraction and Scattering in Electrodynamics by Prof. Kun Din

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As was said in the previous lecture, there is no rigid distinction between scattering and diffraction. We can say scattering reflects the particle nature of light, while diffraction reflects the wave nature of light, but scattering can be derived from the "medium in light" picture, which utilizes Maxwell equations about *waves*, while diffraction involves things like aperture, i.e. boundary conditions, which may be seen as scattering.

In the previous lecture we derived scattering, absorption and extinction cross sections, the optical theorem from the conservation of energy, and we also discussed scattering and absorption efficiency. We discussed the geometrical optics.

1 Mie scattering

We continue the discussion on Mie scattering. **Mie scattering** is among few examples that can be solved exactly. It studies a sphere made of dielectric. The scattered fields at infinity are expanded using spherical functions:

$$\boldsymbol{E}_{\mathrm{s}} = \sum_{n=1}^{\infty} E_n (\mathrm{i} a_n \boldsymbol{N}_{e1n}^{(3)} - b_n \boldsymbol{M}_{o1n}^{(3)}), \quad \boldsymbol{H}_{\mathrm{s}} = \frac{k}{\omega\mu} \sum_{n=1}^{\infty} E_n (\mathrm{i} b_n \boldsymbol{N}_{o1n}^{(3)} + a_n \boldsymbol{M}_{e1n}^{(3)}). \tag{1}$$

The coefficients a_n and b_n are called **Mie coefficients**. We will find that the a_n coefficients give the response of electric n-poles while the b_n coefficients give the response of magnetic n-poles. The input light beam is described by

$$\boldsymbol{E}_{\mathrm{i}} = E_0 \sum_{n=1}^{\infty} \mathrm{i}^n \frac{2n+1}{n(n+1)} (\boldsymbol{M}^{(1)}). \tag{2}$$

We label the electric and magnetic fields inside the sphere as $\boldsymbol{E}_1$ and $\boldsymbol{B}_1$, respectively.

We introduce several notations. First we introduce the Legendre polynomials

$$\mathrm{P}_n^m(x) = (1-x)^{m/2} \frac{\mathrm{d}^m \mathrm{P}_n(x)}{\mathrm{d}x^m}. \tag{3}$$

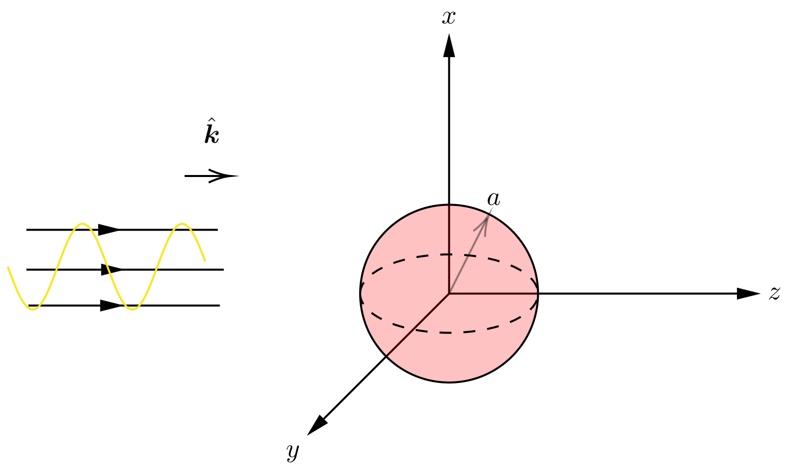

Figure 1: Mie scattering

Note that Jackson, Zangwill and Mathematica add an additional $(-1)^m$ factor to the definition. Furthermore we define

$$\pi_n(\cos\theta) = \frac{\mathrm{P}_n(\cos\theta)}{\sin\theta}, \quad \tau_n(\cos\theta) = \frac{\mathrm{d}\,\mathrm{P}_n(\cos\theta)}{\mathrm{d}\theta}. \tag{4}$$

We have several useful formulae about these functions. First are recurrence formulae:

$$\pi_n(\nu) = \frac{2n-1}{n-1}\nu\pi_{n-1}(\nu) - \frac{n}{n-1}\pi_{n-2}(\nu), \tag{5}$$

$$\tau_n(\nu) = n\nu\pi_n(\nu) - (n+1)\pi_{n-1}(\nu), \tag{6}$$

and

$$\pi_0 = 0, \quad \pi_1 = 1. \tag{7}$$

We also have

$$\pi_n(-\nu) = (-1)^{n-1}\pi_n(\nu), \quad \tau_n(-\nu) = (-1)^n\tau_n(\nu). \tag{8}$$

The orthogonality relations are

$$\int_0^\pi \sin\theta\,\mathrm{d}\theta\,(\tau_n + \pi_n)(\tau_m + \pi_m) = 0, \quad \int_0^\pi \sin\theta\,\mathrm{d}\theta \tag{9}$$

We compare (2) and (1) on the $r = a$ surface. The boundary conditions are

$$(\boldsymbol{E}_\mathrm{i} + \boldsymbol{E}_\mathrm{s} - \boldsymbol{E}_1) \times \hat{\boldsymbol{e}}_r = 0, \quad (\boldsymbol{H}_\mathrm{i} + \boldsymbol{H}_\mathrm{s} - \boldsymbol{H}_1) \times \hat{\boldsymbol{e}}_r = 0.$$

We have We get the final results

$$\begin{aligned} a_n &= \frac{\mu m^2 j_n(mx)(xj_n(x))' - \mu_1 j_n(x)(mxj_n(mx))'}{\mu m^2 j_n(mx)(xh_n^{(1)}(x))' - \mu_1 h_n^{(1)}(x)(mxj_n(mx))'}, \\ b_n &= \frac{\mu_1 j_n(mx)(xj(x))' - \mu j_n(x)(mxj_n(mx))'}{\mu_1 j_n(mx)(xh_n^{(1)}(x))' - \mu h_n^{(1)}(x)(mxj_n(mx))'}. \end{aligned} \tag{10}$$

We find that the denominator of a_n may be zero, which gives the eigenmodes of the system. Finding these modes is extremely hard. The behavior around poles is highly nonlinear, and ordinary gradient descent methods have severe divergence problems. Sometimes the poles are close to each other and it is almost impossible to distinguish them. Even when these problems are solved, whether we have already found a complete set of eigenmodes is still a question hard to answer. This topic - finding the poles of a scattering matrix - is still a frontline nowadays.

In the $ka \ll 1$ limit, $x \ll 1$, and the denominator of a_n is

$$\begin{aligned} f_E(\omega, n) &= \frac{\epsilon_1\mu_1}{\epsilon}\frac{(mx)^n}{(2n+1)!!}\mathrm{i}\frac{(2n-1)!!}{x^{n+1}}n + \mu_1\mathrm{i}\frac{(2n-1)!!}{x^{n+1}}\frac{(mx)^n}{(2n+1)!!}(1+n) \\ &= \frac{\mu_1}{\epsilon}\frac{\mathrm{i}m^n}{(2n+1)x}(\epsilon_1 n + \epsilon(n+1)), \end{aligned} \tag{11}$$

and its zero point is given by

$$\frac{\epsilon_1(\omega, n)}{\epsilon} = -\frac{n+1}{n}. \tag{12}$$

This equation gives the "electric" eigenmodes. For example, for a metal sphere, we have

$$\omega_1 = \frac{\omega_\mathrm{p}}{\sqrt{3}}. \tag{13}$$

This is called **local surface plasmon polariton**. The term "plasmon" comes from the fact that this mode involves charge fluctuation in the metal, and "plasmon polariton" means the exciton formed by coupling between plasmon and photon. The term **surface plasmon polariton (SPP)** means a plasmon polariton propagating on some surface, and the word "local" means SPP in this case is restricted to the sphere and cannot propagate to infinity.

Now we derive the energy flow in Mie scattering. Since we need to handle the fields directly, we define **Riccati-Bessel functions** as follows:

$$\begin{aligned}
\psi_n(\rho) &= \rho j_n(\rho) = S_n(\rho), \\
\chi_n(\rho) &= -\rho y_n(\rho) = C_n(\rho), \\
\xi_n(\rho) &= \rho h_n^{(1)}(\rho) = \psi_n - \mathrm{i}\chi_n, \\
\zeta_n(\rho) &= \rho h_n^{(2)}(\rho) = \psi_n + \mathrm{i}\chi_n,
\end{aligned} \tag{14}$$

and now the scattering field can be written in one line as

$$E_{\mathrm{s},\theta} = \frac{\cos\phi}{\rho} \sum_n E_n (\mathrm{i} a_n \xi_n' \tau_n - b_n \chi_n \pi_n), \tag{15}$$

where the $'$ superscript means the argument is r and the special functions without prime superscript have θ as arguments.

$$C_{\mathrm{sca}} = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} (2n+1)(|a_n|^2 + |b_n|^2), \tag{16}$$

$$C_{\mathrm{ext}} = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} (2n+1) \operatorname{Re}(a_n + b_n). \tag{17}$$

After calculating everything numerically, we find that Mie scattering agrees with Rayleigh scattering when $ka \ll 1$, which, in the language of Mie scattering, can be described as throwing away all b_n's and only keep a_1, or in other words treating the sphere as an electric dipole. In this case we have

$$Q_{\mathrm{sca}} = \frac{8}{3}(ka)^4 \left(\frac{\epsilon_1 - \epsilon}{\epsilon + 1 + 2\epsilon_2} \right)^2. \tag{18}$$

The $(ka)^4$ dependence is the typical feature of Rayleigh scattering. This can be seen as

$$\alpha = 4\pi\epsilon_0 a^3 \frac{\epsilon_1 - \epsilon}{\epsilon_1 + 2\epsilon}. \tag{19}$$

On the other limit we have geometrical optics.

The cross sections can also be evaluated via **partial-wave expansion**, which is often used in quantum mechanical scattering problems.

$$2\delta_k = \Delta \sin\alpha. \tag{20}$$

$$f(0) = 2\pi a^2 \left(1 - \frac{2}{\Delta} \sin\Delta + \frac{2}{\Delta^2}(1 - \cos\Delta) \right). \tag{21}$$

We find that the large oscillating period can be easily captured if we consider the phase of each partial wave. In other words, the large oscillating period is almost simply the interference of the components in the scattering beam. On the other hand, the small oscillating period comes from the details of the sphere, or to be exact from the eigenmodes of the system. If we change a, there will not be significant change on the large oscillating period, because we will only see change on Δ.