Mie theory for metal nanoparticles

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In this work, I aim at giving a clear and self-sufficient description of Mie theory. This famous theory is suited to compute accurately the optical cross sections of a spherical particle. One usually needs to spend some time and read a couple of papers or books, fighting with the cgs and SI units, before clearly understanding what the parameters mean and before making sure that one writes a proper code. This document may help you saving some time. A Matlab code is also provided.

This work in now described in J. Phys. Chem. C **119**, 28586–28596 (2015).

The reference document on this subject is the famous textbook from Bohren and Huffman but the information is not easy to extract.

Consider a spherical particle of radius r_0, complex electric permittivity $\varepsilon = n^2$ embedded in a dielectric medium of permittivity $\varepsilon_\mathsf{m} = n_\mathsf{m}^2$. This particle is illuminated by a plane wave of angular frequency $\omega = 2\pi\, c/\lambda_0 = k\, c/n_\mathsf{m}$.

Let us define from now on a set of useful dimensionless parameters:

$$\begin{aligned} m &= n/n_\mathsf{m} \\ v &= k\, r_0 \\ w &= m\, v \end{aligned}$$

In these conditions, the extinction, scattering and absorption cross sections are given by the formulae:

$$\sigma_\mathsf{ext} = \frac{2\pi}{k^2} \sum_{j=1}^{\infty} (2j+1)\, \mathsf{Re}(a_j + b_j) \tag{1}$$

$$\sigma_\mathsf{sca} = \frac{2\pi}{k^2} \sum_{j=1}^{\infty} (2j+1)\, (|a_j|^2 + |b_j|^2) \tag{2}$$

$$\sigma_\mathsf{abs} = \sigma_\mathsf{ext} - \sigma_\mathsf{sca} \tag{3}$$

where

$$a_j = \frac{m\,\psi_j(w)\,\psi_j'(v) \,-\, \psi_j(v)\,\psi_j'(w)}{m\,\psi_j(w)\,\xi_j'(v) \,-\, \xi_j(v)\,\psi_j'(w)} \tag{4}$$

$$b_j = \frac{\psi_j(w)\,\psi_j'(v) \,-\, m\,\psi_j(v)\,\psi_j'(w)}{\psi_j(w)\,\xi_j'(v) \,-\, m\,\xi_j(v)\,\psi_j'(w)} \tag{5}$$

In these expressions, ψ_j and ξ_j are Ricatti–Bessel functions defined as:

$$\begin{aligned} \psi_j(x) &= \sqrt{\frac{\pi\, x}{2}}\, J_{j+\frac{1}{2}}(x) \\ \xi_j(x) &= \sqrt{\frac{\pi\, x}{2}}\, \left[J_{j+\frac{1}{2}}(x) \,+\, i\, Y_{j+\frac{1}{2}}(x)\right] \end{aligned}$$

J_ν and Y_ν are the Bessel functions of first and second order respectively. They are standard Matlab functions, named respectively `besselj` and `bessely`. Note that these functions are solutions of the Bessel differential equation:

$$x^2 \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + 2x \frac{\mathrm{d}y}{\mathrm{d}x} + \left[x^2 - \nu(\nu+1)\right] y = 0$$

while ψ_j and ξ_j are solutions of the following differential equation:

$$x^2 \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + \left[x^2 - j(j+1)\right] y = 0$$

ψ_j and ξ_j can be expressed as a sum of sines and cosines. For instance, the first terms read:

$$\begin{aligned} \psi_0(x) &= \sin(x) \\ \xi_0(x) &= \sin(x) - i\cos(x) \\ \psi_1(x) &= \sin(x)/x - \cos(x) \\ \xi_1(x) &= \sin(x)/x \,-\, i\,(\cos(x)/x \,+\, \sin(x)) \end{aligned}$$

In Eqs. (1) and (2), the sum over j can be restricted to only a few terms, up to $j = N$. Bohren and Huffman proposed the value $N = v + 4\, v^{1/3} + 2$.

In Eqs. (4) and (5), the primes indicate differentiation with respect to the argument in parenthesis. The derivatives can be conveniently expressed as follows:

$$\begin{aligned} \psi_j'(x) &= \psi_{j-1}(x) - \frac{j}{x}\,\psi_j(x) \\ \xi_j'(x) &= \xi_{j-1}(x) - \frac{j}{x}\,\xi_j(x) \end{aligned}$$

I wrote a Matlab code that can be found in the next page. Free to use. Enjoy.

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[1] C. F. Bohren and D. R. Huffman, *Absorption and scattering of light by small particles* (Wiley interscience, 1983)