Electromagnetic scattering 1: Mie theory

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Wave equations

Maxwell's equations (homogeneous and isotropic)

$$\nabla \times \mathbf{E} = i\omega\mu\mathbf{H} \tag{1}$$

$$\nabla \times \mathbf{H} = -i\omega\epsilon\mathbf{E} \tag{2}$$

$$\nabla \cdot \mathbf{E} = 0, \quad \nabla \cdot \mathbf{H} = 0 \tag{3}$$

Wave equations

$$\nabla \times \nabla \times \mathbf{E} = \omega^2\epsilon\mu\mathbf{E} \tag{4}$$

$$\nabla \times \nabla \times \mathbf{H} = \omega^2\epsilon\mu\mathbf{H} \tag{5}$$

Identity:

$$\nabla \times \nabla \times \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2\mathbf{A} \tag{6}$$

Helmholtz equations:

$$\nabla^2\mathbf{E} + k^2\mathbf{E} = 0 \tag{7}$$

$$\nabla^2\mathbf{H} + k^2\mathbf{H} = 0 \tag{8}$$

where $k = \omega\sqrt{\epsilon\mu}$

Spherical vector wave functions

Spherical coordinate system (θ, ϕ, r)

Let us introduce a vector function:

$$\mathbf{M}(\theta, \phi, r) = \nabla \times (\mathbf{c}\varphi(\theta, \phi, r)), \tag{9}$$

where φ is a scalar function and $\mathbf{c}$ is a constant "pilot" vector

Note that $\mathbf{M}$ is a solenoidal function, i.e., $\nabla \cdot \mathbf{M} = 0$

Applying $\nabla^2 + k^2$ operator to $\mathbf{M}$ we obtain

$$\nabla^2\mathbf{M} + k^2\mathbf{M} = \nabla \times [\mathbf{c}(\nabla^2\varphi + k^2\varphi)] \tag{10}$$

Now, we can see that $\mathbf{M}$ satisfies the vector Helmholtz equation if staisfies the scalar Helmholtz

$$\nabla^2\varphi + k^2\varphi = 0 \tag{11}$$

Spherical vector wave functions

Another solenoidal function that satisfies the vector Helmholtz equation can be generated by taking a curl of $\mathbf{M} = \nabla \times (\mathbf{c}\varphi)$

$$\mathbf{N} = \frac{1}{k}\nabla \times \mathbf{M} \tag{12}$$

We also note that

$$\mathbf{M} = k\nabla \times \mathbf{N} \tag{13}$$

The functions $\mathbf{M}$ and $\mathbf{N}$ are known as the vector spherical wave function (VSWF)

Third VSWF corresponds irrotational field (non-propagating component)

$$\mathbf{L} = \nabla\varphi \tag{14}$$

Next, we need to find φ

Scalar solution

Let the scalar function φ be a solution of

$$\nabla^2\varphi + k^2\varphi = 0 \tag{15}$$

In the spherical coordinate system, the above equation reads as

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\varphi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\varphi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\varphi}{\partial\phi^2} + k^2\varphi = 0 \tag{16}$$

We seek a solution of the form

$$\varphi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi) \tag{17}$$

Separation of variables: p.d.e $\rightarrow$ o.d.e

Scalar solution: angular part $\Phi(\phi)$

Substituting (17) into (16) and expressing R and Θ dependent terms with a separation constant m^2, we obtain

$$\frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0 \tag{18}$$

The solution reads as

$$\Phi = e^{\pm im\phi} \tag{19}$$

m is an integer since we require the solution to be periodic $\Phi(\phi) = \Phi(\phi + 2\pi)$

Scalar solution: angular part $\Theta(\theta)$

Substituting (17) and (19) into (16) and expressing R dependent term with a separation constant $l(l+1)$, we obtain

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[l(l+1)-\frac{m^2}{\sin^2\theta}\right]\Theta=0 \tag{20}$$

Solution: Associated Legendre functions of first kind

$$\Theta = P_l^m(\eta) = \frac{(1-\eta^2)^{m/2}}{2^l l!}\frac{d^{l+m}(\eta^2-1)^l}{d(\eta)^{l+m}} \tag{21}$$

where $\eta = \cos\theta$ (spherical coordinate)

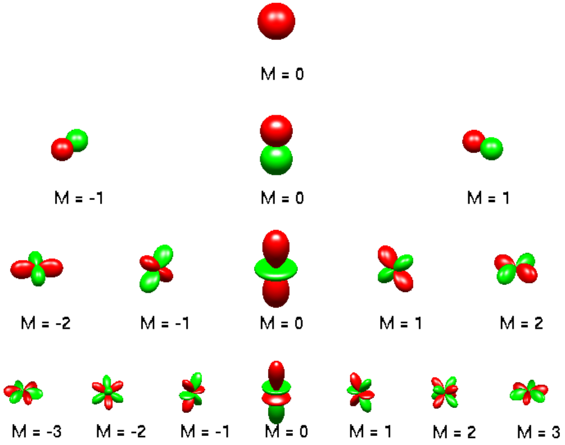
$l = 0, 1, 2, ..., L$ and $m = -l, ..., l$

Scalar solution: angular part

Scalar spherical harmonic

$$Y_l^m = c_l^m P_l^m(cos\theta)e^{im\phi} \quad (22)$$

where c_l^m is a normalization constant



l=0

l=1

l=2

l=3

Scalar solution: radial part

Case 3. $\varphi = R(r)$

$$r^2 \frac{d^2 R}{dr^2} + 2r \frac{dR}{dr} + (k^2 r^2 - l(l+1))R = 0 \quad (23)$$

defining $R(r) = Z(r)/\sqrt(kr)$ we get the Bessel equation of order$(l + 1/2)$

$$r^2 \frac{d^2 Z}{dr^2} + 2r \frac{dZ}{dr} + (k^2 r^2 - (l+1/2)^2)Z = 0 \quad (24)$$

Two solutions can be written as

$$R = j_l(kr) = \sqrt{\frac{\pi}{2kr}} J_{l+\frac{1}{2}}(kr) \quad (25)$$

$$R = h_l(kr) = \sqrt{\frac{\pi}{2kr}} H_{l+\frac{1}{2}}(kr) \quad (26)$$

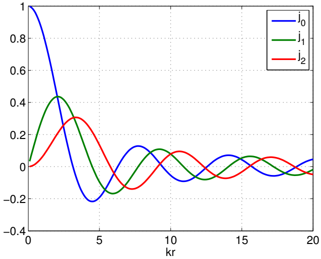
where $j_l(kr)$ the spherical Bessel function and $h_l(kr)$ is the first order Hankel function.

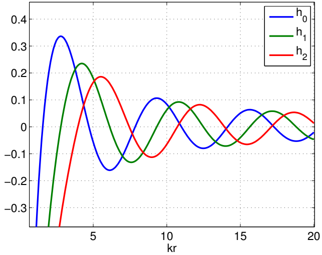
Full solution

Full solution for the scalar Helmholtz equation read as

$$\varphi_{l,m}(r,\theta,\phi) = c_l^m Y_l^m(\theta,\phi) z_l(kr) \tag{27}$$

where $z_l(kr)$ is spherical Bessel ($j_l(kr)$) or Hankel function ($h_l(kr)$)





$$h_l = j_l + i y_l \tag{28}$$

y_l is the spherical bessel of the second kind

Vector solution

Three independent vector solutions ($\nabla^2\mathbf{E} + k_m^2\mathbf{E} = 0$):

$$\mathbf{L}_{l,m} = \nabla\varphi_{l,m} \tag{29}$$

$$\mathbf{M}_{l,m} = \nabla \times \mathbf{r}\varphi_{l,m} \tag{30}$$

$$\mathbf{N}_{l,m} = \frac{1}{k_m}\nabla \times \mathbf{M}_{l,m} \tag{31}$$

$\mathbf{M}_{l,m}$ and $\mathbf{N}_{l,m}$ are solenoidal vector fields and are curl of each other

$\mathbf{L}_{m,l}$ is purely irrotational and represents longitudinal wave (can be omitted)

$\mathbf{M}_{l,m}$ and $\mathbf{N}_{l,m}$ are called as vector spherical harmonics

Solution for the wave equation in spherical coordinates

Find functions in spherical coordinates that satisfy the wave equation construction and forms a complete set, i.e.,

$$\nabla \times \nabla \times \mathbf{u}_n = k^2 \mathbf{u}_n,$$

and

$$\nabla \cdot \mathbf{u}_n = 0,$$

Due to a completeness of VSWFs, the electric field can be expressed as

$$\mathbf{E} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} (a_{nm}\mathbf{M}_{nm} + b_{nm}\mathbf{N}_{nm})$$

a_{nm} and b_{nm} are the expansion coefficients Truncation:

$$\mathbf{E} \approx \sum_{n=1}^{p} \sum_{m=-n}^{n} (a_{nm}\mathbf{M}_{nm} + b_{nm}\mathbf{N}_{nm})$$

Typically $p = 2 + kr + 4(kr)^{1/3}$

Solution for the wave equation in spherical coordinates

Scalar spherical harmonics

$$Y_{nm}(\theta,\phi) = P_n^{|m|}(\cos\theta)e^{im\phi}$$

$P_n^{|m|}$ is associated Legendre functions Vector spherical harmonics

$$\begin{aligned}
\mathbf{P}_{nm}(\theta,\phi) &= Y_{nm}(\theta,\phi)\hat{\mathbf{u}}_r \\
\mathbf{B}_{nm}(\theta,\phi) &= \frac{r}{\sqrt{n(n+1)}}\nabla Y_{nm}(\theta,\phi) \\
\mathbf{C}_{nm}(\theta,\phi) &= -\hat{\mathbf{u}}_r \times \mathbf{B}_{nm}(\theta,\phi)
\end{aligned}$$

Vector spherical wave functions:

$$\begin{aligned}
\mathbf{M}_{nm}(r,\theta,\phi) = {} & c_{nm}\mathbf{C}_{nm}(\theta,\phi)z_n(kr) \\
\mathbf{N}_{nm}(r,\theta,\phi) = {} & c_{nm}\frac{\sqrt{n(n+1)}}{kr}\mathbf{P}_{nm}(\theta,\phi)z_n(kr) \\
& +c_{nm}\left(\frac{n+1}{kr}z_n(kr) - z_{n+1}(kr)\right)\mathbf{B}_{nm}(\theta,\phi)
\end{aligned}$$

z_n are spherical bessel or hankel functions, and c_{nm} are normalization coefficients

Scattering by a sphere

Incident field:

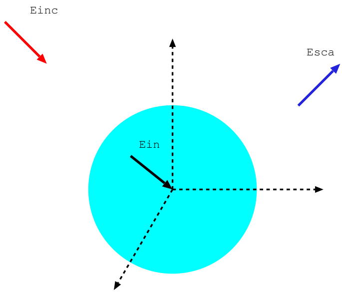
$$\mathbf{E}^{inc} \approx \sum_{l=1}^{L} \sum_{m=-l}^{l} a_{l,m}^{inc}\mathbf{M}_{l,m} + b_{l,m}^{inc}\mathbf{N}_{l,m} \tag{32}$$

Scattered field:

$$\mathbf{E}^{sca} \approx \sum_{l=1}^{L} \sum_{m=-l}^{l} a_{l,m}^{sca}\mathbf{M}_{l,m} + b_{l,m}^{sca}\mathbf{N}_{l,m} \tag{33}$$

Field inside the sphere:

$$\mathbf{E}^{in} \approx \sum_{l=1}^{L} \sum_{m=-l}^{l} a_{l,m}^{in}\mathbf{M}_{l,m} + b_{l,m}^{in}\mathbf{N}_{l,m} \tag{34}$$



Enforce boundary conditions $\mathbf{n} \times (\mathbf{E}^{sca} + \mathbf{E}^{inc}) = \mathbf{n} \times \mathbf{E}^{in}$

$$a_{l,m}^{sca} = a_{l,m} * a_{l,m}^{inc}, \quad b_{l,m}^{sca} = b_{l,m} * b_{l,m}^{inc} \tag{35}$$

Expansion of fields

Expansion coefficients for a particular incident wave

$$A_{l,m} = \int_{\Omega} \mathbf{M}^*_{l,m} \mathbf{E}^{inc} \, \mathrm{d}\Omega \tag{36}$$

$$B_{l,m} = \int_{\Omega} \mathbf{N}^*_{l,m} \mathbf{E}^{inc} \, \mathrm{d}\Omega \tag{37}$$

where $\Omega = 4\pi r^2$
These can be written as

$$A_{l,m} = -i^{l+1} \frac{2l+1}{l(l+1)} \frac{(l-m)!}{(l+m)!} \Pi_{l,m} E_0 \tag{38}$$

$$B_{l,m} = -i^{l+2} N_m \frac{2l+1}{l(l+1)} \frac{(l-m)!}{(l+m)!} T_{l,m} E_0 \tag{39}$$

Expansion of incident fields

Expansion coefficients for a plane-wave $\theta = 0$

All terms vanish except when $m = 1$

$$\Pi_{l,1} = 1 \tag{40}$$

and

$$T_{l,1} = \frac{1}{2} l(l+1) \tag{41}$$

The coefficients are

$$A_{l,1} = i^{l-1} E_0 \frac{2l+1}{l(l+1)} \tag{42}$$

$$B_{l,1} = i A_{l,1} \tag{43}$$

Determination of coefficients

Applying interface conditions to the vector spherical harmonics

$$
\begin{aligned}
j_l(N\chi)c_l + h_l(\chi)b_l &= j_l(\chi) \\
[N\chi j_l(N\chi)]' \, c_l + [\chi h_l(\chi)]' b_l &= [\chi j_l(\chi)]' \\
N j_l(N\chi)d_l + h_l(\chi)a_l &= j_l(\chi) \\
[N\chi j_l(N\chi)]' \, d_l + [\chi h_l(\chi)]' a_l &= [\chi j_l(\chi)]'
\end{aligned}
\tag{44}
$$

evaluated at $r = a$. Now we can solve coefficients for the scattered fields

$$
\begin{aligned}
a_l &= \frac{N^2 j_l(N\chi)\,[\chi j_l(\chi)]' - j_l(\chi)\,[N\chi j_l(N\chi)]'}{N^2 j_l(N\chi)\,[\chi h_l(\chi)]' - h_l(\chi)\,[N\chi j_l(N\chi)]'} \\
b_l &= \frac{j_l(N\chi)\,[\chi j_l(\chi)]' - j_l(\chi)\,[N\chi j_l(N\chi)]'}{j_l(N\chi)\,[\chi h_l(\chi)]' - h_l(\chi)\,[N\chi j_l(N\chi)]'}
\end{aligned}
\tag{45}
$$

Determination of coefficients

and for the internal fields

$$c_l = \frac{j_l(\chi)\,[\chi h_l(\chi)]' - h_l(\chi)\,[\chi j_l(\chi)]'}{j_l(N\chi)\,[\chi h_l(\chi)]' - h_l(\chi)\,[N\chi j_l(N\chi)]'}$$
$$d_l = \frac{N j_l(\chi)\,[\chi h_l(\chi)]' - N h_l(\chi)\,[\chi j_l(\chi)]'}{N^2 j_l(N\chi)\,[\chi h_l(\chi)]' - h_l(\chi)\,[N\chi j_l(N\chi)]'} \tag{46}$$

where χ is the size parameter

$$\chi = \frac{2\pi r_{sph}}{\lambda} \tag{47}$$

and N is the refractive index
Derivates:

$$j_l(x)' = j_{l-1}(x) - \frac{l+1}{x} j_l(x) \tag{48}$$

$$h_l(x)' = \frac{1}{2}[h_{l-1}(x) - \frac{h_l(x) + x h_{l+1}}{x}] \tag{49}$$

Scattering coefficient

Complex Poynting vector

$$\mathbf{S} = \frac{1}{2}\mathbf{E} \times \mathbf{H}^* \tag{50}$$

where $\mathbf{H}^*$ denotes complex conjugate of $\mathbf{H}$ Scattered energy

$$W_{sca} = \frac{1}{2} Re \int_S \hat{\mathbf{n}} \cdot \mathbf{E}_{sca} \times \mathbf{H}^*_{sca} \, \mathrm{d}S, \tag{51}$$

where S is a closed surface enclosing the particle

Scattering cross section:

$$C_{sca} = \frac{W_{sca}}{I_{inc}} \tag{52}$$

I_{inc} denotes the intensity of the incident field

For a plane wave incident, it can be shown that

$$C_{sca} = \frac{2\pi}{k^2} \sum_{l=1}^{\infty} (2l+1)(|a_l|^2 + |b_l|^2) \tag{53}$$

Extinction coefficient

Extincted energy

$$W_{ext} = \frac{1}{2} Re \int_S \hat{\mathbf{n}} \cdot \mathbf{E}_{inc} \times \mathbf{H}^*_{sca} \, \mathrm{d}S, \tag{54}$$

where S is a closed surface enclosing the particle

Scattering cross section:

$$C_{ext} = \frac{W_{ext}}{I_{inc}} \tag{55}$$

I_{inc} denotes the intensity of the incident field

For a plane wave incident, it can be shown that

$$C_{ext} = Re \frac{2\pi}{k^2} \sum_{l=1}^{\infty} (2l+1)(a_l + b_l) \tag{56}$$

Absorption coefficient

$$C_{abs} = C_{ext} - C_{sca} \tag{57}$$

Scattering amplitudes

$$S_1(\theta) = \sum_{l=1} \frac{2l+1}{l(l+1)}(a_l \pi_l(cos\theta) + b_n \tau_l(cos\theta)) \tag{58}$$

$$S_2(\theta) = \sum_{l=1} \frac{2l+1}{l(l+1)}(b_l \pi_l(cos\theta) + a_n \tau_l(cos\theta)) \tag{59}$$

where angular function are defined as

$$\pi_l(cos\theta) = \frac{1}{sin\theta} P_l^1(cos\theta) \tag{60}$$

$$\tau_l(cos\theta) = \frac{d}{d\theta} P_l^1(cos\theta) \tag{61}$$

S_3 and S_4 are zeros for spheres

Scattering patterns

Recursive computations

$$\pi_l = \frac{2l-1}{l-1}\cos\theta\pi_{l-1} - \frac{l}{l-1}\pi_{l-2} \tag{62}$$

starting with $\pi_0 = 0$, $\pi_1 = 1$ and $\pi_2 = 3\cos\theta$

$$\tau_l = l\cos\theta\pi_l - (l+1)\pi_{l-1} \tag{63}$$

with $\tau_0 = 0$, $\tau_1 = \cos\theta$ and $\tau_2 = 3\cos(2\theta)$