

Scattering by Dielectric Sphere Near a Dielectric Interface

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1 Scalar Helmholtz equation in Spherical Coordinates

The scalar Helmholtz equation forms the basis of the entire analysis as its solutions generate the basis functions for solving the wave equations for spherically symmetric systems. In coordinate free form, the equation is,

$$\nabla^2 u(\mathbf{r}) + k^2 u(\mathbf{r}) = 0. \quad (1.1)$$

This document uses spherical coordinates (r, θ, ϕ) , with vectorial definitions,

$$\begin{aligned} \hat{\mathbf{r}} &= \sin \theta \cos \phi \hat{\mathbf{x}} + \sin \theta \sin \phi \hat{\mathbf{y}} + \cos \theta \hat{\mathbf{z}}, \\ \hat{\boldsymbol{\theta}} &= \cos \theta \cos \phi \hat{\mathbf{x}} + \cos \theta \sin \phi \hat{\mathbf{y}} - \sin \theta \hat{\mathbf{z}}, \\ \hat{\boldsymbol{\phi}} &= -\sin \phi \hat{\mathbf{x}} + \cos \phi \hat{\mathbf{y}}. \end{aligned}$$

This obeys the cross product rule,

$$\hat{\mathbf{r}} \times \hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\phi}}.$$

An important vector operator used below is the angular momentum operator,

$$\mathbf{L} = \frac{1}{i} \mathbf{r} \times \nabla. \quad (1.2)$$

In terms of $L^2 = \mathbf{L} \cdot \mathbf{L}$, the Laplacian is given by

$$\nabla^2 f = \frac{1}{r} \frac{\partial^2}{\partial r^2} (rf) - \frac{1}{r^2} L^2 f. \quad (1.3)$$

Thus an alternative form for the Helmholtz equation is

$$\frac{1}{r} \frac{\partial^2}{\partial r^2} (ru) - \frac{1}{r^2} L^2 u + k^2 u = 0, \quad (1.4)$$

so that solutions to this equation satisfy the following property (which I make use of below),

$$L^2(ru) = \frac{\partial^2}{\partial r^2} (ru) - k^2(ru).$$

The solutions to (1.4) can be obtained by separation of variables. The spherical harmonic functions are defined as,

$$Y_{lm}(\theta, \phi) = \left[\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} P_{lm}(\cos \theta) e^{im\phi}, \quad (1.5)$$

where $P_{lm}(x)$ are the associated Legendre polynomials, and solve the eigenvalue problem for the squared angular momentum operator

$$L^2 Y_{lm} = l(l+1) Y_{lm}. \quad (1.6)$$

(l, m)	0	± 1	± 2	± 3
0	$\frac{1}{\sqrt{4\pi}}$			
1	$\sqrt{\frac{3}{4\pi}} \cos \theta$	$\sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}$		
2	$\sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$	$\sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\phi}$	$\sqrt{\frac{15}{8\pi}} \sin^2 \theta e^{\pm 2i\phi}$	

Table 1: First few Spherical Harmonics

The angular momentum components are written conveniently in terms of,

$$\begin{aligned}
L_{\pm} = L_x \pm iL_y &= e^{\pm i\phi} \left(\pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right), \\
L_z &= -i \frac{\partial}{\partial \phi}.
\end{aligned}$$

The angular momentum operator acting on Y_{lm} yields the following

$$\begin{aligned}
LY_{lm} &= \hat{x} \frac{1}{2} \left(\sqrt{(l-m)(l+m+1)} Y_{l,m+1} + \sqrt{(l+m)(l-m+1)} Y_{l,m-1} \right) \\
&+ \hat{y} \frac{1}{2i} \left(\sqrt{(l-m)(l+m+1)} Y_{l,m+1} - \sqrt{(l+m)(l-m+1)} Y_{l,m-1} \right) \\
&+ \hat{z} m Y_{lm}.
\end{aligned} \tag{1.7}$$

In terms of the spherical basis,

$$L_r =$$

A few low order spherical Harmonics are tabulated here for easy reference in Table 1. Note that $Y_{lm}(\theta, \phi) = 0$ at $\theta = 0, \pi$ for $l = 1, 2, 3$.

For the radial dependence, we first introduce the Bessel Function Notation

$$\text{First Kind: } \mathcal{J}_n^{(1)}(x) = J_n(x), \tag{1.8}$$

$$\text{Second Kind: } \mathcal{J}_n^{(2)}(x) = N_n(x), \tag{1.9}$$

$$\text{Hankel: } \mathcal{J}_n^{(3)}(x) = H_n^{(1)}(x) = J_n(x) + iN_n(x), \tag{1.10}$$

$$\mathcal{J}_n^{(4)}(x) = H_n^{(2)}(x) = J_n(x) - iN_n(x). \tag{1.11}$$

We will refer to the superscript of $\mathcal{J}^{(\alpha)}$ as the Bessel type denoting the type of Bessel function as defined above. Spherical Bessel Functions

$$j_l^{(\alpha)}(x) = \sqrt{\frac{\pi}{2x}} \mathcal{J}_{l+1/2}^{(\alpha)}(x). \tag{1.12}$$

Riccati Bessel Functions

$$\psi_l^{(i)}(x) = x j_l^{(i)}(x). \tag{1.13}$$

In more explicit terms,

$$j_l^{(1)}(x) = (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\sin x}{x}, \quad (1.14)$$

$$j_l^{(2)}(x) = -(-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\cos x}{x}, \quad (1.15)$$

$$j_l^{(3)}(x) = (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{e^{ix}}{ix}, \quad (1.16)$$

$$j_l^{(4)}(x) = (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{e^{-ix}}{-ix}. \quad (1.17)$$

Following identity for the spherical Bessel function plays an important simplifying role,

$$j_l^{(1)}(x) j_l^{(2)'}(x) - j_l^{(1)'}(x) j_l^{(2)}(x) = \frac{1}{x^2}. \quad (1.18)$$

As a result of this identity, Riccati functions obey

$$\psi_l^{(1)}(x) \psi_l^{(3)'}(x) - \psi_l^{(1)'}(x) \psi_l^{(3)}(x) = i. \quad (1.19)$$

General series solution in terms of spherical harmonic and spherical Bessel functions

$$u^{(\alpha)}(k\mathbf{r}) = \sum_{l,m} a_{lm} j_l^{(\alpha)}(kr) Y_{lm}(\theta, \phi). \quad (1.20)$$

The choice of Bessel function is dictated by the boundary conditions (finite at origin and vanishing at infinity etc.) or convenience in other cases. For use in the formulation below, I define a single basis function above as

$$u_{lm}^{(\alpha)}(k\mathbf{r}) = j_l^{(\alpha)}(kr) Y_{lm}(\theta, \phi). \quad (1.21)$$

Converting between plane wave and spherical harmonics plays an important role in the analysis and the computational algorithm below. For this purpose, I collect some useful results in relating the two bases. A scalar plane wave can be represented in spherical harmonics as

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{l=0}^{\infty} \sum_{m=-l}^l 4\pi i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}), \quad (1.22)$$

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^l 4\pi i^l j_l(kr) Y_{lm}(\hat{\mathbf{k}}) Y_{lm}^*(\hat{\mathbf{r}}) \quad (1.23)$$

Note that the complex conjugation can be interchanged. Multiplication with $Y_{lm}(\hat{\mathbf{k}})$ and integration over the sphere in $\hat{\mathbf{k}}$ gives the inverse relation,

$$j_l(kr) Y_{lm}(\hat{\mathbf{r}}) = \frac{1}{4\pi i^l} \int d\Omega e^{i\mathbf{k}\cdot\mathbf{r}} Y_{lm}(\hat{\mathbf{k}}). \quad (1.24)$$

2 Vector Helmholtz equation

The vector Helmholtz equation is satisfied by vector fields such that each component satisfies (1.1). Thus for a vector field $\mathbf{U}(\mathbf{r})$,

$$\nabla^2 \mathbf{U} + k^2 \mathbf{U} = 0. \quad (2.1)$$

Of course, the solutions to each scalar component of \mathbf{U} can be written using (1.20) with separate coefficients a_{lm} for each direction. However, more elegant formulation is possible that can be extended to other coordinate systems as well.

I first introduce the general statement that if a function f solves the scalar equation (1.1), then

$$\mathbf{M}_f(\mathbf{r}) = \nabla \times (\mathbf{r}f), \quad (2.2)$$

$$\mathbf{N}_f(\mathbf{r}) = \frac{1}{k} \nabla \times \mathbf{M}_f, \quad (2.3)$$

solve the vector equation (2.1). Moreover, it is easy to show that

$$\mathbf{M}_f(\mathbf{r}) = \frac{1}{k} \nabla \times \mathbf{N}_f. \quad (2.4)$$

I now apply this to the specific case of solutions in spherical coordinates. I begin with the solutions $u_{lm}^{(\alpha)}(k\mathbf{r})$ defined in (1.21) and define

$$\begin{aligned} \mathbf{M}_{lm}^{(\alpha)}(k\mathbf{r}) &= \frac{1}{\sqrt{l(l+1)}} \nabla \times [\mathbf{r} u_{lm}^{(\alpha)}(k\mathbf{r})] \\ &= \frac{1}{\sqrt{l(l+1)}} \nabla u_{lm}^{(\alpha)}(k\mathbf{r}) \times \mathbf{r} \\ &= \frac{j_l^{(\alpha)}(kr)}{\sqrt{l(l+1)}} \nabla Y_{lm}(\hat{\mathbf{r}}) \times \mathbf{r} \end{aligned}$$

At this point, it is convenient to write the above expression in terms of the Riccati Bessel functions defined in (1.13), and to introduce a vector function to write

$$\mathbf{M}_{lm}^{(\alpha)}(k\mathbf{r}) = \frac{\psi_l^{(\alpha)}(kr)}{kr} \mathbf{A}_{1lm}(\hat{\mathbf{r}}),$$

where,

$$\mathbf{A}_{1lm}(\hat{\mathbf{r}}) = -\mathbf{r} \times \nabla Y_{lm}(\hat{\mathbf{r}}) = \frac{-i\mathbf{L}}{\sqrt{l(l+1)}} Y_{lm} = \frac{1}{\sqrt{l(l+1)}} \left[\frac{\partial_\phi Y_{lm}}{\sin \theta} \hat{\boldsymbol{\theta}} - (\partial_\theta Y_{lm}) \hat{\boldsymbol{\phi}} \right]. \quad (2.5)$$

I now compute $\mathbf{N}_{lm}^{(\alpha)}(\mathbf{r})$ directly from (2.3). Using the curl operator in spherical coordinates

$$\begin{aligned} \mathbf{N}_{lm}^{(\alpha)}(k\mathbf{r}) &= \frac{1}{k} \nabla \times \mathbf{M}_{lm}^{(\alpha)}(k\mathbf{r}) = \frac{1}{k} \nabla \times \left(\psi_l^{(\alpha)}(kr) \frac{1}{kr} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) \right) \\ &= \frac{1}{k} \nabla \times \left(j_l^{(\alpha)}(kr) \mathbf{A}_{1lm}(\hat{\mathbf{r}}) \right) \\ &= \frac{1}{kr} \frac{\partial}{\partial kr} \left(\psi_l^{(\alpha)}(kr) \right) \hat{\mathbf{r}} \times \mathbf{A}_{1lm}(\hat{\mathbf{r}}) + \frac{\psi_l^{(\alpha)}(kr)}{(kr)^2} r^2 \nabla \times \left(\frac{1}{r} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) \right). \end{aligned}$$

I now introduce two additional vector functions

$$\begin{aligned}\mathbf{A}_{2lm}(\hat{\mathbf{r}}) &= \hat{\mathbf{r}} \times \mathbf{A}_{1lm}(\hat{\mathbf{r}}), \\ \mathbf{A}_{3lm}(\hat{\mathbf{r}}) &= \frac{r^2}{\sqrt{l(l+1)}} \nabla \times \left[\frac{1}{r} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) \right].\end{aligned}$$

Computation of \mathbf{A}_{2lm} is straightforward,

$$\mathbf{A}_{2lm}(\hat{\mathbf{r}}) = \frac{1}{\sqrt{l(l+1)}} \left[(\partial_\theta Y_{lm}) \hat{\boldsymbol{\theta}} + \frac{\partial_\phi Y_{lm}}{\sin \theta} \hat{\boldsymbol{\phi}} \right].$$

To compute \mathbf{A}_{3lm} , I note that the $\hat{\mathbf{r}}$ component of the curl operator produces L^2 term, , while the $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ components vanish.

$$\begin{aligned}\nabla \times \left[\frac{1}{r} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) \right] &= \hat{\mathbf{r}} \frac{1}{r^2} \frac{-1}{\sqrt{l(l+1)}} \left[\frac{\partial}{\partial \theta} (\sin \theta \partial_\theta Y_{lm}) \frac{\partial^2 Y_{lm}}{\partial \phi^2} \right] \\ &= \frac{\sqrt{l(l+1)}}{r^2} Y_{lm}.\end{aligned}$$

The vanishing of $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ components can be seen from the fact that $\mathbf{A}_{1lm} \cdot \hat{\mathbf{r}} = 0$ so that the only terms that contribute to the curl along those components are of the form

$$\frac{\partial}{\partial r} \left(r \frac{1}{r} A \right) = 0,$$

since A does not depend on r .

For the tangential components, we define $x = kr$, and write the derivative as

$$\frac{1}{kr} \frac{1}{k} \frac{\partial}{\partial r} \left(\psi_l^{(\alpha)}(kr) \right) = \frac{1}{x} \psi_l^{(\alpha)'}(x), \quad x \equiv kr.$$

With these simplifications, and $\partial_\phi Y_{lm} = im Y_{lm}$, the functions $\mathbf{M}^{(\alpha)}, \mathbf{N}^{(\alpha)}$ can be written as product of radial component and *vector spherical harmonics*,

$$\mathbf{M}_{lm}^{(\alpha)}(k\mathbf{r}) = \frac{\nabla_{\mathbf{r}} \times [\mathbf{r} u_{lm}^{(\alpha)}(k\mathbf{r})]}{\sqrt{l(l+1)}} = \frac{\psi_l^{(\alpha)}(kr)}{kr} \mathbf{A}_{1lm}(\hat{\mathbf{r}}), \quad (2.6)$$

$$\mathbf{N}_{lm}^{(\alpha)}(k\mathbf{r}) = \frac{\nabla_{\mathbf{r}} \times \nabla_{\mathbf{r}} \times [\mathbf{r} u_{lm}^{(\alpha)}(k\mathbf{r})]}{k\sqrt{l(l+1)}} = \frac{\psi_l^{(\alpha)'}(kr)}{kr} \mathbf{A}_{2lm}(\hat{\mathbf{r}}) + \sqrt{l(l+1)} \frac{\psi_l^{(\alpha)}(kr)}{(kr)^2} \mathbf{A}_{3lm}(\hat{\mathbf{r}}) \quad (2.7)$$

From the Hankel function definitions, and for $\mathbf{Q} = \mathbf{M}, \mathbf{N}$,

$$\mathbf{Q}_{lm}^{(3,4)}(k\mathbf{r}) = \mathbf{Q}_{lm}^{(1)}(k\mathbf{r}) \pm i \mathbf{Q}_{lm}^{(2)}(k\mathbf{r}).$$

Also, by symmetry it follows that the curl-relations also apply in \mathbf{k} space,

$$\begin{aligned}\nabla_{\mathbf{r}} \times \mathbf{M}^{(\alpha)}(k\mathbf{r}) &= k \mathbf{N}^{(\alpha)}(k\mathbf{r}), \\ \nabla_{\mathbf{k}} \times \mathbf{M}^{(\alpha)}(k\mathbf{r}) &= r \mathbf{N}^{(\alpha)}(k\mathbf{r}),\end{aligned}$$

These two vector functions are *linearly independent*. It is also apparent that \mathbf{M} is purely tangential while \mathbf{N} has a radial component. Since $\nabla \times \hat{\mathbf{r}} = 0$, the latter is a purely rotational field as well.

The notation above is fairly common, but slightly different from that used in Kristensson's book. Since I use that book quite often, the following describe the relationship to his notation. First, he uses real-valued spherical harmonics and puts an extra index to indicate even ($\cos m\phi$) and odd ($\sin m\phi$) terms. Second, he switches the order of l and m indices, and third, he uses the symbol \mathbf{u} to describe Hankel function variety of spherical harmonics, and \mathbf{v} for the Bessel function of the first kind. Dropping his σ , indices,

$$\begin{aligned}\mathbf{u}_{1ml}(k\mathbf{r}) &= \mathbf{M}_{lm}^{(3)}(k\mathbf{r}), \\ \mathbf{u}_{2ml}(k\mathbf{r}) &= \mathbf{N}_{lm}^{(3)}(k\mathbf{r}), \\ \mathbf{v}_{1ml}(k\mathbf{r}) &= \mathbf{M}_{lm}^{(1)}(k\mathbf{r}), \\ \mathbf{v}_{2ml}(k\mathbf{r}) &= \mathbf{N}_{lm}^{(1)}(k\mathbf{r}).\end{aligned}$$

For completeness, Kristensson augments this zero-divergence set with $\mathbf{u}_3 = \nabla u^{(3)}$, $\mathbf{v}_3 = \nabla u^{(1)}$, which have zero-curl. These waves do not arise in homogeneous source free regions, and so are not used in this document.

3 Properties of Vector Spherical Harmonics

The vector spherical harmonics are defined as,

$$\mathbf{A}_{1lm}(\hat{\mathbf{r}}) = \frac{-iLY_{lm}}{\sqrt{l(l+1)}} \quad (3.1)$$

$$= \frac{1}{\sqrt{l(l+1)}} \left[\left(\frac{1}{\sin\theta} \partial_\phi Y_{lm} \right) \hat{\boldsymbol{\theta}} - (\partial_\theta Y_{lm}) \hat{\boldsymbol{\phi}} \right], \quad (3.2)$$

$$\mathbf{A}_{2lm}(\hat{\mathbf{r}}) = \frac{r\nabla Y_{lm}}{\sqrt{l(l+1)}} \quad (3.3)$$

$$= \frac{1}{\sqrt{l(l+1)}} \left[(\partial_\theta Y_{lm}) \hat{\boldsymbol{\theta}} + \left(\frac{1}{\sin\theta} \partial_\phi Y_{lm} \right) \hat{\boldsymbol{\phi}} \right],$$

$$\mathbf{A}_{3lm}(\hat{\mathbf{r}}) = Y_{lm}(\theta, \phi) \hat{\mathbf{r}}. \quad (3.4)$$

where the derivatives of Y_{lm} are,

$$\frac{dY_{lm}}{d\theta} = \left[m \cot\theta Y_{lm}(\theta, \phi) + \sqrt{(l+m+1)(l-m)} e^{-i\phi} Y_{l,m+1}(\theta, \phi) \right]. \quad (3.5)$$

$$\frac{dY_{lm}}{d\phi} = imY_{lm}. \quad (3.6)$$

Note that we have the triad and orthogonality, such that

$$\begin{aligned}\hat{\mathbf{r}} \times \mathbf{A}_{1lm} &= \mathbf{A}_{2lm}, \\ \hat{\mathbf{r}} \times \mathbf{A}_{3lm} &= 0,\end{aligned}\tag{3.7}$$

and

$$\int d\Omega \mathbf{A}_{qlm}^*(\hat{\mathbf{r}}) \cdot \mathbf{A}_{q'l'm'}(\hat{\mathbf{r}}) = \delta_{qq'} \delta_{ll'} \delta_{mm'}.$$

Note also that under inversion, $\hat{\mathbf{r}} \rightarrow -\hat{\mathbf{r}}$, the spherical harmonics acquire l dependent sign, $Y_{lm}(\pi - \theta, \phi + \pi) = (-1)^l Y_{lm}(\theta, \phi)$. Since \mathbf{L} does not change the parity,

$$\begin{aligned}\mathbf{A}_{1lm}(-\hat{\mathbf{r}}) &= (-1)^l \mathbf{A}_{1lm}(\hat{\mathbf{r}}), \\ \mathbf{A}_{2lm}(-\hat{\mathbf{r}}) &= (-1)^{l+1} \mathbf{A}_{2lm}(\hat{\mathbf{r}}).\end{aligned}$$

The second equation can be derived using 3.7,

$$\mathbf{A}_{2lm}(-\hat{\mathbf{r}}) = -\hat{\mathbf{r}} \times \mathbf{A}_{1lm}(-\hat{\mathbf{r}}) = (-1)^{l+1} \hat{\mathbf{r}} \times \mathbf{A}_{1lm}(\hat{\mathbf{r}}) = (-1)^{l+1} \mathbf{A}_{2lm}(\hat{\mathbf{r}}).$$

At $l = 0$,

$$\begin{aligned}\mathbf{A}_{1lm}(\hat{\mathbf{r}}) = \mathbf{A}_{2lm}(\hat{\mathbf{r}}) &= 0 \\ \mathbf{A}_{3lm}(\hat{\mathbf{r}}) &= \frac{1}{\sqrt{4\pi}} \hat{\mathbf{r}}.\end{aligned}$$

Following are some useful properties of the vector spherical harmonics. First, since \mathbf{A}_{qlm} do not depend on r , and $\nabla(1/r) = -\hat{\mathbf{r}}/r^2$,

$$\nabla \times \left(\frac{1}{r} \mathbf{A}_{qlm} \right) = \frac{1}{r} \nabla \times \mathbf{A}_{qlm} - \frac{1}{r^2} \hat{\mathbf{r}} \times \mathbf{A}_{qlm} = \frac{1}{r} \nabla \times \mathbf{A}_{qlm} - \frac{1}{r^2} \begin{cases} \mathbf{A}_{2lm} & q = 1 \\ -\mathbf{A}_{1lm} & q = 2 \\ 0 & q = 3 \end{cases}.$$

which follow directly or using the definitions of \mathbf{M} and \mathbf{N} functions above

$$\begin{aligned}\nabla \times \mathbf{A}_{1lm} &= \frac{\mathbf{A}_{2lm}(\hat{\mathbf{r}}) + \sqrt{l(l+1)} \mathbf{A}_{3lm}(\hat{\mathbf{r}})}{r}, \\ \nabla \times \mathbf{A}_{2lm} &= -\frac{\mathbf{A}_{1lm}(\hat{\mathbf{r}})}{r}, \\ \nabla \times \mathbf{A}_{3lm} &= \frac{\sqrt{l(l+1)}}{r} \mathbf{A}_{1lm}(\hat{\mathbf{r}}).\end{aligned}$$

Thus the double curl operation is,

$$\begin{aligned}\nabla \times (\nabla \times \mathbf{A}_{1lm}) &= \frac{l(l+1) \mathbf{A}_{1lm}}{r^2}, \\ \nabla \times (\nabla \times \mathbf{A}_{2lm}) &= -\frac{\sqrt{l(l+1)} \mathbf{A}_{2lm}(\hat{\mathbf{r}})}{r^2}, \\ \nabla \times (\nabla \times \mathbf{A}_{3lm}) &= \frac{l(l+1) \mathbf{A}_{3lm}(\hat{\mathbf{r}})}{r^2}.\end{aligned}$$

Fourier integrals over unit sphere (see Appendix) follow from substitution of (1.22). Using the fact that $i^l(-1)^l = i^{-l}$ and $A_{1lm}(-\hat{\mathbf{k}}) = (-1)^l A_{1lm}(\hat{\mathbf{k}})$, it is shown in Appendix B on page 17,

$$\int d\Omega e^{-i\mathbf{k}\cdot\mathbf{r}} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) = 4\pi i^{-l} \mathbf{M}_{lm}^{(1)}(r\mathbf{k}) = 4\pi i^l \mathbf{M}_{lm}^{(1)}(-r\mathbf{k}), \quad (3.8)$$

and for \mathbf{A}_{2lm} ,

$$\int d\Omega e^{-i\mathbf{k}\cdot\mathbf{r}} \mathbf{A}_{2lm}(\hat{\mathbf{r}}) = 4\pi i^{-l+1} \mathbf{N}_{lm}^{(1)}(r\mathbf{k}) = 4\pi i^{l+1} \mathbf{N}_{lm}^{(1)}(-r\mathbf{k}). \quad (3.9)$$

4 Electromagnetic fields in source free regions

I now apply the above formalism to general solutions of *source free* Maxwell equations in spherical coordinates. The Faraday and Ampere laws give

$$\mathbf{E} = \frac{i\eta_0}{k} \nabla \times \mathbf{H}. \quad (4.1)$$

$$\mathbf{H} = \frac{1}{i\eta_0 k} \nabla \times \mathbf{E}, \quad (4.2)$$

Here $\eta_0 = \sqrt{\mu_0/\varepsilon_0}$ is the free space impedance. In free space $\nabla \cdot \mathbf{E} = 0$ and without longitudinal component of magnetization, $\nabla \cdot \mathbf{H} = 0$. In a particular region, I pick Bessel variants that are appropriate for fields in that region and write the electric field as

$$\mathbf{E}(\mathbf{r}) = \sum_{lm} a_{lm} \mathbf{M}_{lm}^{(\alpha)}(k\mathbf{r}) + b_{lm} \mathbf{N}_{lm}^{(\alpha)}(k\mathbf{r}).$$

From (4.2),

$$\mathbf{H}(\mathbf{r}) = \frac{n}{i\eta_0 k} \sum_{lm} a_{lm} \nabla \times \mathbf{M}_{lm}^{(\alpha)}(k\mathbf{r}) + b_{lm} \nabla \times \mathbf{N}_{lm}^{(\alpha)}(k\mathbf{r}).$$

Here n is the refractive index of the medium, and it comes from the factor $k/\omega = n/c$. I now apply the general relationships (2.3) and (2.4), and write the following pair of equations for the electric and magnetic fields

$$\mathbf{E}(\mathbf{r}) = \sum_{lm} a_{lm} \mathbf{M}_{lm}^{(\alpha)}(k\mathbf{r}) + b_{lm} \mathbf{N}_{lm}^{(\alpha)}(k\mathbf{r}) \quad (4.3)$$

$$\mathbf{H}(\mathbf{r}) = \frac{n}{i\eta_0 k} \sum_{lm} a_{lm} \mathbf{N}_{lm}^{(\alpha)}(k\mathbf{r}) + b_{lm} \mathbf{M}_{lm}^{(\alpha)}(k\mathbf{r}). \quad (4.4)$$

Since $\mathbf{r} \cdot \mathbf{M} = 0$ and $\mathbf{r} \cdot \mathbf{N} \sim \mathbf{r} \cdot \mathbf{A}_3$, and using the relation (2.4), we have for any vector field $\mathbf{F}(\mathbf{r})$,

$$\begin{aligned}\mathbf{F}(\mathbf{r}) &= \sum_{lm} a_{lm} \mathbf{M}_{lm}^{(\alpha)}(\mathbf{r}) + b_{lm} \mathbf{N}_{lm}^{(\alpha)}(\mathbf{r}), \\ \mathbf{r} \cdot \mathbf{F}(\mathbf{r}) &= \sum_{lm} b_{lm} \sqrt{l(l+1)} \frac{\psi_l^{(\alpha)}(kr)}{(kr)^2} Y_{lm}(\theta, \phi) r,\end{aligned}$$

Multiplying by Y_{lm}^* and using the orthogonality properties of scalar spherical harmonics, and using the relationships (4.3) and (4.4), the orthogonality relations for \mathbf{A}_{1lm} yield,

$$a_{lm} \frac{\psi_l^{(\alpha)}(kr)}{kr} = \frac{k}{\sqrt{l(l+1)}} \int d\Omega \mathbf{A}_{1lm}^*(\hat{\mathbf{r}}) \cdot \mathbf{E}(\mathbf{r}), \quad (4.5)$$

$$b_{lm} \frac{\psi_l^{(\alpha)}(kr)}{kr} = \frac{i\eta_0 k}{n\sqrt{l(l+1)}} \int d\Omega \mathbf{A}_{1lm}^*(\hat{\mathbf{r}}) \cdot \mathbf{H}(\mathbf{r}). \quad (4.6)$$

I now write a vector plane wave as, $\mathbf{E}_0 e^{i\mathbf{k} \cdot \mathbf{r}}$ for an arbitrary complex vector \mathbf{E}_0 such that $\mathbf{E}_0 \cdot \mathbf{k} = 0$. I plug this into the expression for the coefficients a_{lm} , (4.6), and use 3.8 on the previous page to write

$$\begin{aligned}a_{lm} j_l(kr) &= \mathbf{E}_0 \cdot \left[\int d\Omega e^{-i\mathbf{k} \cdot \mathbf{r}} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) \right]^*, \\ &= \mathbf{E}_0 \cdot 4\pi i^l \mathbf{M}_{lm}^{(1)*}(r\hat{\mathbf{k}})\end{aligned}$$

I apply this same derivation to the corresponding magnetic field. Collecting the above derivations, I summarize the plane wave expansion in the following set of relations,

$$a_{lm} = 4\pi i^l \mathbf{A}_{1lm}^*(\hat{\mathbf{k}}) \cdot \mathbf{E}_0 = 4\pi i^l \mathbf{A}_{2lm}^*(\hat{\mathbf{k}}) \cdot (\hat{\mathbf{k}} \times \mathbf{E}_0) \quad (4.7)$$

$$b_{lm} = -4\pi i^{l+1} \mathbf{A}_{2lm}^*(\hat{\mathbf{k}}) \cdot \mathbf{E}_0 = 4\pi i^{l+1} \mathbf{A}_{1lm}^*(\hat{\mathbf{k}}) \cdot (\hat{\mathbf{k}} \times \mathbf{E}_0). \quad (4.8)$$

5 Dielectric Sphere in Vacuum

I now apply the formalism of the previous section to compute the scattered field of a dielectric sphere in vacuum. I let the refractive index of the sphere be n , so that outside, $k = 2\pi/\lambda$ and inside, $k_{sph} = nk$. I will keep the externally imposed incident field in general form, and will specialize to specific cases later. This is convenient since the incident field itself is defined as the field without the presence of the sphere, and therefore can be considered as the field from many other scattering sources, as will be done in the second part with an interface below the sphere. The field outside the sphere consists of the

incident field and the scattered field. In order to compute the scattered field, I write them separately as

$$\mathbf{E}_{inc}(\mathbf{r}) = \sum_{lm} a_{lm} \mathbf{M}_{lm}^{(1)}(k\mathbf{r}) + b_{lm} \mathbf{N}_{lm}^{(1)}(k\mathbf{r}), \quad (5.1)$$

$$\mathbf{E}_{sca}(\mathbf{r}) = \sum_{lm} e_{lm} \mathbf{M}_{lm}^{(3)}(k\mathbf{r}) + f_{lm} \mathbf{N}_{lm}^{(3)}(k\mathbf{r}). \quad (5.2)$$

The field inside the sphere contains the origin, and therefore I use Bessel functions of the first kind and write

$$\mathbf{E}_{sph}(\mathbf{r}) = \sum_{lm} c_{lm} \mathbf{M}_{lm}^{(1)}(n k \mathbf{r}) + d_{lm} \mathbf{N}_{lm}^{(1)}(n k \mathbf{r}). \quad (5.3)$$

I now match the tangential components of \mathbf{E} and \mathbf{H} at the sphere boundary, $\mathbf{r} = a\hat{\mathbf{r}}$. From (2.6) and (2.7) it is clear that the angular functions are identical in each region and therefore, only there coefficients play a role. Also, since \mathbf{M} and \mathbf{N} are linearly independent, their coefficients are matched separately. Matching E_θ ,

$$\psi_l^{(1)}(ka) a_{lm} + \psi_l^{(3)}(ka) e_{lm} = \frac{1}{n} \psi_l^{(1)}(nka) c_{lm} \quad (5.4)$$

$$\psi_l^{(1)'}(ka) b_{lm} + \psi_l^{(3)'}(ka) f_{lm} = \frac{1}{n} \psi_l^{(1)'}(nka) d_{lm}, \quad (5.5)$$

and matching H_θ

$$\psi_l^{(1)'}(ka) a_{lm} + \psi_l^{(3)'}(ka) e_{lm} = \psi_l^{(1)'}(nka) c_{lm}, \quad (5.6)$$

$$\psi_l^{(1)}(ka) b_{lm} + \psi_l^{(3)}(ka) f_{lm} = \psi_l^{(1)}(nka) d_{lm}. \quad (5.7)$$

Eliminating c_{lm} from (5.4) and (5.6), and d_{lm} from (5.5) and (5.7), I get the following. The factors of i arise from the Wronskian (1.19) (see Appendix C on page 19)

$$c_{lm} = \frac{-i}{\beta_{1l}(ka)} a_{lm}, \quad (5.8)$$

$$d_{lm} = \frac{-in}{\beta_{2l}(ka)} b_{lm}, \quad (5.9)$$

$$e_{lm} = -\frac{\alpha_{1l}(ka)}{\beta_{1l}(ka)} a_{lm} = -i\alpha_{1l}(ka) c_{lm}, \quad (5.10)$$

$$f_{lm} = -\frac{\alpha_{2l}(ka)}{\beta_{2l}(ka)} b_{lm} = -\frac{i}{n} \alpha_{2l}(ka) d_{lm}. \quad (5.11)$$

Here the numerator and denominator are functions of ka and defined as follows,

$$\begin{aligned}
\alpha_{1l}(x) &= \psi_l^{(1)}(x)\psi_l^{(1)'}(nx) - \frac{1}{n}\psi_l^{(1)'}(x)\psi_l^{(1)}(nx), \\
\alpha_{2l}(x) &= \psi_l^{(1)}(x)\psi_l^{(1)'}(nx) - n\psi_l^{(1)'}(x)\psi_l^{(1)}(nx), \\
\beta_{1l}(x) &= \psi_l^{(3)}(x)\psi_l^{(1)'}(nx) - \frac{1}{n}\psi_l^{(3)'}(x)\psi_l^{(1)}(nx), \\
\beta_{2l}(x) &= \psi_l^{(3)}(x)\psi_l^{(1)'}(nx) - n\psi_l^{(3)'}(x)\psi_l^{(1)}(nx).
\end{aligned}$$

This completes the derivation of the standard Mie theory for a dielectric sphere. In the next section, I describe the scattering by the interface. Before moving on, note that the Hankel functions $\psi_l^{(3)}(z)$ are extremely rapidly diverging with l at a fixed z . Note that the smallest argument is ka where largest value occurs. It is better to write the coefficients by pulling these terms out, and dividing them into \mathbf{M} and \mathbf{N} functions if necessary. I introduce the logarithmic derivative

$$D^{(\alpha)}(x) = \frac{\psi^{(\alpha)'}(x)}{\psi^{(\alpha)}(x)}.$$

Then

$$e_{lm} = -\frac{\psi_l^{(1)}(ka) D_l^{(1)}(nka) - \frac{1}{n}D_l^{(1)}(ka)}{\psi_l^{(3)}(ka) D_l^{(1)}(nka) - \frac{1}{n}D_l^{(3)}(ka)} a_{lm}, \quad (5.12)$$

$$f_{lm} = -\frac{\psi_l^{(1)}(ka) D_l^{(1)}(nka) - nD_l^{(1)}(ka)}{\psi_l^{(3)}(ka) D_l^{(1)}(nka) - nD_l^{(3)}(ka)} b_{lm}. \quad (5.13)$$

Thus I will write the numerically stable form for the scattered field as follows,

$$\mathbf{E}_{sca}(\mathbf{r}) = \sum_{lm} \tilde{e}_{lm} \tilde{\mathbf{M}}_{lm}^{(3)}(k\mathbf{r}) + \tilde{f}_{lm} \tilde{\mathbf{N}}_{lm}^{(3)}(k\mathbf{r}),$$

where

$$\begin{aligned}
\tilde{e}_{lm} &= \psi_l^{(3)}(ka) e_{lm}, \\
\tilde{f}_{lm} &= \psi_l^{(3)}(ka) f_{lm},
\end{aligned}$$

$$\begin{aligned}
\tilde{\mathbf{M}}_{lm}^{(3)}(k\mathbf{r}) &= \frac{1}{kr} \frac{\psi_l^{(3)}(kr)}{\psi_l^{(3)}(ka)} \mathbf{A}_{1lm}(\hat{\mathbf{r}}), \\
\tilde{\mathbf{N}}_{lm}^{(3)}(k\mathbf{r}) &= \frac{1}{kr} \frac{\psi_l^{(3)'}(kr)}{\psi_l^{(3)}(ka)} \mathbf{A}_{2lm}(\hat{\mathbf{r}}) + \sqrt{l(l+1)} \frac{\psi_l^{(3)}(kr)}{(kr)^2 \psi_l^{(3)}(ka)} \mathbf{A}_{3lm}(\hat{\mathbf{r}}).
\end{aligned}$$

6 Integrals for scattering matrix

6.1 Surface Integration over a circumscribing sphere

The far field is obtained from surface integral over an imaginary sphere in the background medium that encloses the sphere being studied. Thus setting $b > a$ to be the radius of this sphere, the far field in the direction $\hat{\mathbf{k}}$ is given by

$$\begin{aligned} \mathbf{F}(\hat{\mathbf{k}}) &= \frac{ikb^2}{4\pi} \hat{\mathbf{k}} \times \int d\hat{\mathbf{r}}' e^{-ikR\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}'} \left[\hat{\mathbf{r}}' \times \mathbf{E}_s(b\hat{\mathbf{r}}') - \eta_0 \hat{\mathbf{k}} \times \left(\hat{\mathbf{r}}' \times \mathbf{H}_s(b\hat{\mathbf{r}}') \right) \right] \\ &= \frac{ikb^2}{4\pi} \sum_{lm} \hat{\mathbf{k}} \times \int d\hat{\mathbf{r}}' e^{-ikR\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}'} \left[\hat{\mathbf{r}}' \times \mathbf{M}_{lm}^{(3)}(kb\hat{\mathbf{r}}') + i\hat{\mathbf{k}} \times \left(\hat{\mathbf{r}}' \times \mathbf{N}_{lm}^{(3)}(kb\hat{\mathbf{r}}') \right) \right] e_{lm} + \\ &\quad \frac{ikb^2}{4\pi} \sum_{lm} \hat{\mathbf{k}} \times \int d\hat{\mathbf{r}}' e^{-ikR\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}'} \left[\hat{\mathbf{r}}' \times \mathbf{N}_{lm}^{(3)}(kb\hat{\mathbf{r}}') + i\hat{\mathbf{k}} \times \left(\hat{\mathbf{r}}' \times \mathbf{M}_{lm}^{(3)}(kb\hat{\mathbf{r}}') \right) \right] f_{lm} \end{aligned}$$

Consider the first term (drop the A_3) term

$$\int d\hat{\mathbf{r}}' e^{-ikb\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}'} \hat{\mathbf{r}}' \times \mathbf{M}^{(3)}(kb\hat{\mathbf{r}}') = \frac{\psi^{(3)}(kb)}{kb} \int d\hat{\mathbf{r}}' e^{-ikR\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}'} \hat{\mathbf{r}}' \times \mathbf{A}_{1lm}(\hat{\mathbf{r}}') = \frac{\psi^{(3)}(kb)\psi^{(1)'}(kb)}{kb} 4\pi i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}).$$

From the cross product relations, and setting $i^{-l+1}i = -i^{-l}$

$$i\hat{\mathbf{k}} \times \int d\hat{\mathbf{r}}' e^{-ikb\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}'} \hat{\mathbf{r}}' \times \mathbf{M}^{(3)}(kb\hat{\mathbf{r}}') = \frac{\psi^{(3)}(kb)\psi^{(1)'}(kb)}{kb} \left(4\pi i^{-l} \mathbf{A}_{1lm}(\hat{\mathbf{k}}) \right).$$

The second variety is

$$\int d\hat{\mathbf{r}}' e^{-ikb\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}'} \hat{\mathbf{r}}' \times \mathbf{N}^{(3)}(kb\hat{\mathbf{r}}') = -\frac{\psi_l^{(3)'}(kb)}{kb} \int d\hat{\mathbf{r}}' e^{-ikb\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}'} \mathbf{A}_{1lm}(\hat{\mathbf{r}}') = \frac{\psi_l^{(3)'}(kb)\psi_l^{(1)}(kb)}{kb} \left(-4\pi i^{-l} \mathbf{A}_{1lm}(\hat{\mathbf{k}}) \right).$$

From the cross product relations, we also have

$$i\hat{\mathbf{k}} \times \int d\hat{\mathbf{r}}' e^{-ikb\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}'} \hat{\mathbf{r}}' \times \mathbf{N}^{(3)}(kb\hat{\mathbf{r}}') = \frac{\psi_l^{(3)'}(kb)\psi_l^{(1)}(kb)}{kb} \left(-4\pi i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) \right).$$

The far field integral now looks like:

$$\begin{aligned} \mathbf{F}(\hat{\mathbf{k}}) &= \frac{i}{4\pi k} \sum_{lm} \hat{\mathbf{k}} \times \left[\psi^{(3)}(kb)\psi^{(1)'}(kb) - \psi_l^{(3)'}(kb)\psi_l^{(1)}(kb) \right] 4\pi i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) e_{lm} + \\ &\quad \frac{i}{4\pi k} \sum_{lm} \hat{\mathbf{k}} \times \left[\psi_l^{(3)'}(kb)\psi_l^{(1)}(kb) - \psi^{(3)}(kb)\psi^{(1)'}(kb) \right] \left(-4\pi i^{-l} \mathbf{A}_{1lm}(\hat{\mathbf{k}}) \right). \end{aligned}$$

Using the Wronskian (1.19)

$$\begin{aligned}
\mathbf{F}(\hat{\mathbf{k}}) &= \frac{i}{k} \sum_{lm} (-ii^{-l+1}) \hat{\mathbf{k}} \times \mathbf{A}_{2lm}(\hat{\mathbf{k}}) e_{lm} + (-ii^{-l}) \hat{\mathbf{k}} \times \mathbf{A}_{1lm}(\hat{\mathbf{k}}) f_{lm} \\
&= \frac{i}{k} \sum_{lm} (i^2 i^{-l}) \mathbf{A}_{1lm}(\hat{\mathbf{k}}) e_{lm} - ii^{-l} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) f_{lm}.
\end{aligned}$$

Thus we finally get

$$\mathbf{F}(\hat{\mathbf{k}}) = \frac{1}{ik} \sum_{lm} \left[i^{-l} \mathbf{A}_{1lm}(\hat{\mathbf{k}}) e_{lm} + i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) f_{lm} \right]. \quad (6.1)$$

6.2 Volume Integrals over the Sphere

The volume formulation of the far field (see my paper and Krisstenson book pages 111, 190, and 278) gives,

$$\begin{aligned}
\mathbf{F}(\hat{\mathbf{k}}) &= (I - \hat{\mathbf{k}}\hat{\mathbf{k}}) \cdot \mathbf{W}(\hat{\mathbf{k}}) \\
\text{where, } \mathbf{W}(\hat{\mathbf{k}}) &= \frac{k^2}{4\pi} (n^2 - 1) \int d^3\mathbf{r}' e^{-i\mathbf{k} \cdot \mathbf{r}'} \mathbf{E}(\mathbf{r}').
\end{aligned} \quad (6.2)$$

The last integral is already in the form that would be implied by reciprocity. The far field vector $\mathbf{F}(\hat{\mathbf{k}})$ is consistent with the formalism that leads to the expression on the current page, and to the series solution for the S-matrix. I will now evaluate $\mathbf{W}(\hat{\mathbf{k}})$,

$$\begin{aligned}
\mathbf{W}(\hat{\mathbf{k}}) &= \sum_{lm} c_{lm} \frac{(n^2 - 1)}{4\pi k} \int_0^{ka} dx x^2 \frac{\psi_l^{(1)}(nx)}{nx} \int d\hat{\mathbf{r}} e^{-ix\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) + \\
&\quad \sum_{lm} d_{lm} \frac{(n^2 - 1)}{4\pi k} \int_0^{ka} dx x^2 \frac{\psi_l^{(1)'}(nx)}{nx} \int d\hat{\mathbf{r}} e^{-ix\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}} \mathbf{A}_{2lm}(\hat{\mathbf{r}}) + \\
&\quad \sum_{lm} d_{lm} \sqrt{l(l+1)} \frac{(n^2 - 1)}{4\pi k n^2} \int_0^{ka} dx \psi_l^{(1)}(nx) \int d\hat{\mathbf{r}} e^{-ix\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}} \mathbf{A}_{3lm}(\hat{\mathbf{r}}).
\end{aligned} \quad (6.3)$$

Substituting the results (3.8) and (3.9), the first term proportional to c_{lm} becomes,

$$\begin{aligned}
&\frac{1}{k} i^{-l} \mathbf{A}_{1lm}(\hat{\mathbf{k}}) c_{lm} (n^2 - 1) \int_0^{ka} dx x^2 j_l^{(1)}(nx) j_l^{(1)}(x) \\
&= \frac{1}{k} i^{-l} \mathbf{A}_{1lm}(\hat{\mathbf{k}}) (-\alpha_{1l}(ka)) c_{lm} \\
&= \frac{1}{k} i^{-l} \mathbf{A}_{1lm}(\hat{\mathbf{k}}) (-ie_{lm}).
\end{aligned}$$

The middle equality follows from

$$\alpha_{1l}(z) = (1 - n^2) \int_0^z dx x^2 j_l^{(1)}(nx) j_l^{(1)}(x).$$

This equality follows from the analytical evaluation of the integral on the right hand side,

$$\begin{aligned} (1 - n^2) \int_0^z dx x^2 j_l^{(1)}(nx) j_l^{(1)}(x) &= nz^2 \left[j_{l-1}(nz) j_l(z) - \frac{1}{n} j_{l-1}(z) j_l(nz) \right] \\ &= \alpha_{1l}(z). \end{aligned}$$

The last equality is verified analytically using Mathematica. From 3.9, the angular integral in the middle term in (6.3) is,

$$\int d\hat{\mathbf{r}} e^{-ix\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}} \mathbf{A}_{2lm}(\hat{\mathbf{r}}) = 4\pi i^{-l+1} \frac{\psi_l^{(1)'}(x)}{x} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) + \sqrt{l(l+1)} 4\pi i^{-l+1} \frac{\psi_l^{(1)}(x)}{x^2} \mathbf{A}_{3lm}(\hat{\mathbf{k}}).$$

Since only the orthogonal projection $(I - \hat{\mathbf{k}}\hat{\mathbf{k}}) \cdot \mathbf{W}(\hat{\mathbf{k}})$ enters the final expression (6.2), the \mathbf{A}_{3lm} term in the above result drops out eventually. Finally, the third term in (6.3) is

$$\begin{aligned} \int d\hat{\mathbf{r}} e^{-ix\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}} \mathbf{A}_{3lm}(\hat{\mathbf{r}}) &= 4\pi i^{-l+1} \frac{1}{r} \nabla_{\mathbf{k}} [j_l(kr) Y_{lm}(\hat{\mathbf{k}})] \\ &= 4\pi i^{-l+1} \frac{j_l(kr)}{r} \nabla_{\mathbf{k}} Y_{lm}(\hat{\mathbf{k}}) + 4\pi i^{-l+1} j_l'(kr) Y_{lm}(\hat{\mathbf{k}}) \hat{\mathbf{k}} \\ &= 4\pi i^{-l+1} \frac{j_l(kr)}{r} \frac{\sqrt{l(l+1)}}{k} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) + 4\pi i^{-l+1} j_l'(kr) \mathbf{A}_{3lm}(\hat{\mathbf{k}}) \\ &= 4\pi i^{-l+1} \frac{j_l(x)}{x} \sqrt{l(l+1)} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) + 4\pi i^{-l+1} j_l'(kr) \mathbf{A}_{3lm}(\hat{\mathbf{k}}). \end{aligned}$$

The term proportional to $\hat{\mathbf{k}}$ drops out in the final projection. Thus substituting these results into the middle and last sums of (6.3),

$$\begin{aligned} & i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) \frac{(n^2 - 1)}{k} \int_0^{ka} dx x^2 \frac{\psi_l^{(1)'}(nx)}{nx} \frac{\psi_l^{(1)'}(x)}{x} \\ & + i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) \frac{(n^2 - 1)}{kn^2} l(l+1) \int_0^{ka} dx \psi_l^{(1)}(nx) \frac{1}{x} j_l^{(1)}(x). \end{aligned}$$

Simplify

$$\begin{aligned} & \frac{1}{k} i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) d_{lm} \frac{1}{n} (n^2 - 1) \\ & \times \left[\int_0^{ka} dx \psi_l^{(1)'}(nx) \psi_l^{(1)'}(x) + l(l+1) \int_0^{ka} dx j_l^{(1)}(nx) j_l^{(1)}(x) \right] \\ & = \frac{1}{k} i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) \frac{1}{n} (-\alpha_{2l}(ka)) d_{lm} \\ & = \frac{1}{k} i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) \frac{1}{n} (-in f_{lm}) \\ & = \frac{1}{k} i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) (-i f_{lm}). \end{aligned}$$

The first equality follows from

$$\alpha_{2l}(z) = -(n^2 - 1) \int_0^z dx \left[\psi_l^{(1)'}(nx) \psi_l^{(1)'}(x) + l(l+1) j_l^{(1)}(nx) j_l^{(1)}(x) \right].$$

As far as I have searched, there is no analytical expression for the integral on the right. I verified the above result using two methods. First I verified that the series expansion for $ka \ll 1$ yields the exact same analytical expressions for the left and right sides at $l = 1, 2, 3$. I then performed numerical integration to verify that the result held for general ka and l . The calculation is available in the mathematica notebook `BesselIntegrals.nb`.

Put all the terms together,

$$\mathbf{F}(\hat{\mathbf{k}}) = \frac{1}{ik} \sum_{lm} i^{-l} \mathbf{A}_{1lm}(\hat{\mathbf{k}}) e_{lm} + i^{-l+1} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) f_{lm}.$$

This is the same the expression derived from surface integration (6.1). Note that the \mathbf{A}_{3lm} term plays a crucial role when deriving the correct radiation formula from the volume integral of the internal field. The surface integral drops this term from the outset. The internal field expressions must be updated in my code to include this term properly. This is the term that takes care of the discontinuity of the normal component of the field at the sphere boundary.

A Legendre Polynomials

Many different expressions exist for the derivative $P'_{lm}(z)$. The one I use below is (Lebedev, pg. 195)

$$\frac{dP_{lm}}{dz} = \frac{-1}{1-z^2} \left[mzP_{lm}(z) + (z^2-1)^{1/2}P_{l,m+1}(z) \right].$$

From this formula, it follows that

$$\begin{aligned} \frac{dY_{lm}}{d\theta} &= -\sin\theta \frac{dY_{lm}}{d\cos\theta} \\ &= \left[\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} e^{im\phi} \frac{1}{\sin\theta} [-i\sin\theta P_{l,m+1}(\cos\theta) + m\cos\theta P_{lm}(\cos\theta)] \\ &= \left[-i\sqrt{\frac{(l-m+1)!}{(l+m-1)!}} e^{-i\phi} Y_{l,m+1}(\theta, \phi) + m\cot\theta Y_{lm}(\theta, \phi) \right]. \end{aligned}$$

The factorial term in the last equality can be written as

$$\frac{(l-m+1)!}{(l+m-1)!} = (l-m+1)(l-m).$$

B Unit Sphere Integrals

Integrals of spherical Harmonics

$$\int d\Omega Y_{l'm'}^*(\hat{\mathbf{r}}) Y_{lm}(\hat{\mathbf{r}}) = \delta_{ll'} \delta_{mm'}.$$

From this equation, and [1.7](#),

$$\begin{aligned} \int d\Omega Y_{l'm'}^*(\hat{\mathbf{r}}) (\mathbf{L} Y_{lm}(\hat{\mathbf{r}})) &= \delta_{ll'} \delta_{m',m} m \hat{\mathbf{z}} + \\ &\quad \frac{1}{2} \delta_{ll'} \delta_{m',m+1} \sqrt{(l-m)(l+m+1)} (\hat{\mathbf{x}} - i\hat{\mathbf{y}}) + \\ &\quad \frac{1}{2} \delta_{ll'} \delta_{m',m-1} \sqrt{(l+m)(l-m+1)} (\hat{\mathbf{x}} + i\hat{\mathbf{y}}). \end{aligned} \tag{B.1}$$

Integral of A_{1lm}

$$\begin{aligned}
& \int d\Omega e^{-i\mathbf{k}\cdot\mathbf{r}} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) \\
&= \frac{1}{\sqrt{l(l+1)}} \sum_{l'm'} 4\pi i^{l'} j_{l'}(kr) Y_{l'm'}(-\hat{\mathbf{k}}) \int d\Omega Y_{l'm'}^*(\hat{\mathbf{r}}) (-i\mathbf{L} Y_{lm}(\hat{\mathbf{r}})) \\
&= \frac{-i}{\sqrt{l(l+1)}} \sum_{l'm'} 4\pi i^{l'} (-1)^{l'} j_{l'}(kr) Y_{l'm'}(\hat{\mathbf{k}}) \int d\Omega Y_{l'm'}^*(\hat{\mathbf{r}}) \mathbf{L} Y_{lm}(\hat{\mathbf{r}}) \\
&= \frac{-i}{\sqrt{l(l+1)}} 4\pi i^l (-1)^l j_l(kr) \left[m Y_{lm}(\hat{\mathbf{k}}) \hat{\mathbf{z}} \right. \\
&\quad \left. + \sqrt{(l-m)(l+m+1)} (\hat{\mathbf{x}} - i\hat{\mathbf{y}}) Y_{lm+1}(\hat{\mathbf{k}}) \right. \\
&\quad \left. + \sqrt{(l+m)(l-m+1)} (\hat{\mathbf{x}} - i\hat{\mathbf{y}}) Y_{lm-1}(\hat{\mathbf{k}}) \right] \\
&= 4\pi i^l (-1)^l j_l(kr) \left(\frac{-i\mathbf{L} Y_{lm}(\hat{\mathbf{k}})}{\sqrt{l(l+1)}} \right) \\
&= 4\pi i^l j_l(kr) (-1)^l \mathbf{A}_{lm}^{(1)}(\hat{\mathbf{k}}) \\
&= 4\pi i^l j_l(kr) \mathbf{A}_{lm}^{(1)}(-\hat{\mathbf{k}}).
\end{aligned}$$

Thus we have

$$\int d\Omega e^{-i\mathbf{k}\cdot\mathbf{r}} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) = 4\pi i^{-l} \mathbf{M}_{lm}^{(1)}(r\mathbf{k}) = 4\pi i^l \mathbf{M}_{lm}^{(1)}(-r\mathbf{k}).$$

Integral of A_{2lm}

$$\begin{aligned}
\int d\Omega e^{-i\mathbf{k}\cdot\mathbf{r}} \mathbf{A}_{2lm}(\hat{\mathbf{r}}) &= \int d\Omega e^{-i\mathbf{k}\cdot\mathbf{r}} \hat{\mathbf{r}} \times \mathbf{A}_{1lm}(\hat{\mathbf{r}}) \\
&= \left(\frac{i}{r} \partial_{\mathbf{k}} \right) \times \int d\Omega e^{-i\mathbf{k}\cdot\mathbf{r}} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) \\
&= 4\pi i^{-l} i \left(\frac{1}{r} \partial_{\mathbf{k}} \times \mathbf{M}_{lm}^{(1)}(r\mathbf{k}) \right) \\
&= 4\pi i^{-l+1} \mathbf{N}_{lm}^{(1)}(r\mathbf{k}).
\end{aligned}$$

Thus

$$\int d\Omega e^{-i\mathbf{k}\cdot\mathbf{r}} \mathbf{A}_{1lm}(\hat{\mathbf{r}}) = 4\pi i^{-l+1} \mathbf{N}_{lm}^{(1)}(r\mathbf{k}) = 4\pi i^{l+1} \mathbf{N}_{lm}^{(1)}(-r\mathbf{k}).$$

Integral of A_{3lm}

$$\begin{aligned}
& \int d\Omega e^{-i\mathbf{k}\cdot\mathbf{r}} \hat{\mathbf{r}} Y_{lm}(\hat{\mathbf{r}}) \\
&= \frac{i}{r} \partial_{\mathbf{k}} \int d\Omega e^{-i\mathbf{k}\cdot\mathbf{r}} Y_{lm}(\hat{\mathbf{r}}) \\
&= 4\pi i^{l*} \frac{i}{r} \partial_{\mathbf{k}} \left[j_l(kr) Y_{lm}(\hat{\mathbf{k}}) \right]
\end{aligned}$$

The inverse relation are,

$$\begin{aligned}
\int d\Omega e^{-i\mathbf{k}' \cdot \mathbf{r}} \mathbf{E}(\mathbf{r}; \mathbf{k}) &= \sum_{lm} a_{lm} \frac{\psi_{lm}^{(\alpha)}(k'r)}{k'r} 4\pi i^{l*} \mathbf{M}_{lm}^{(1)}(r\mathbf{k}) \\
&+ \sum_{lm} b_{lm} \frac{\psi_{lm}^{(\alpha)'}(k'r)}{k'r} 4\pi i^{l*} \mathbf{N}_{lm}^{(1)}(r\mathbf{k}) \\
&+ \sum_{lm} b_{lm} \sqrt{l(l+1)} \frac{\psi_{lm}^{(\alpha)*}(k'r)}{(k'r)^2} \left[\left(\frac{\partial j_l(kr)}{\partial kr} \right) \mathbf{A}_{3lm}(\hat{\mathbf{k}}) + \frac{j_l(kr)}{kr} \mathbf{A}_{2lm}(\hat{\mathbf{k}}) \right].
\end{aligned}$$

C Derivation of Mie coefficients

To eliminate \mathbf{M} coefficients

$$\begin{aligned}
\psi_l^{(1)}(ka) a_{lm} + \psi_l^{(3)}(ka) e_{lm} &= \frac{1}{n} \psi_l^{(1)}(nka) c_{lm} \\
\psi_l^{(1)'}(ka) a_{lm} + \psi_l^{(3)'}(ka) e_{lm} &= \psi_l^{(1)'}(nka) c_{lm}.
\end{aligned}$$

To eliminate c_{lm}

$$\begin{aligned}
n\psi_l^{(1)'}(nka) \psi_l^{(1)}(ka) a_{lm} + n\psi_l^{(1)'}(nka) \psi_l^{(3)}(ka) e_{lm} &= \psi_l^{(1)'}(nka) \psi_l^{(1)}(nka) c_{lm} \\
\psi_l^{(1)}(nka) \psi_l^{(1)'}(ka) a_{lm} + \psi_l^{(1)}(nka) \psi_l^{(3)'}(ka) e_{lm} &= \psi_l^{(1)}(nka) \psi_l^{(1)'}(nka) c_{lm},
\end{aligned}$$

Subtract the lower equation from the upper

$$\begin{aligned}
&\left[n\psi_l^{(1)'}(nka) \psi_l^{(3)}(ka) - \psi_l^{(1)}(nka) \psi_l^{(3)'}(ka) \right] e_{lm} \\
&= - \left[n\psi_l^{(1)'}(nka) \psi_l^{(1)}(ka) - \psi_l^{(1)}(nka) \psi_l^{(1)'}(ka) \right] a_{lm}.
\end{aligned}$$

To eliminate e_{lm} ,

$$\begin{aligned}
\psi_l^{(3)'}(ka) \psi_l^{(1)}(ka) a_{lm} + \psi_l^{(3)'}(ka) \psi_l^{(3)}(ka) e_{lm} &= \frac{1}{n} \psi_l^{(3)'}(ka) \psi_l^{(1)}(nka) c_{lm} \\
\psi_l^{(3)}(ka) \psi_l^{(1)'}(ka) a_{lm} + \psi_l^{(3)}(ka) \psi_l^{(3)'}(ka) e_{lm} &= \psi_l^{(3)}(ka) \psi_l^{(1)'}(nka) c_{lm}.
\end{aligned}$$

Subtract the top equation from lower

$$\begin{aligned}
&\left[\psi_l^{(3)}(ka) \psi_l^{(1)'}(ka) - \psi_l^{(3)'}(ka) \psi_l^{(1)}(ka) \right] a_{lm} \\
&= \left[\psi_l^{(3)}(ka) \psi_l^{(1)'}(nka) - \frac{1}{n} \psi_l^{(3)'}(ka) \psi_l^{(1)}(nka) \right] c_{lm}. \tag{C.1}
\end{aligned}$$

To eliminate \mathbf{N} coefficients

$$\begin{aligned}
\psi_l^{(1)'}(ka) b_{lm} + \psi_l^{(3)'}(ka) f_{lm} &= \frac{1}{n} \psi_l^{(1)'}(nka) d_{lm}, \\
\psi_l^{(1)}(ka) b_{lm} + \psi_l^{(3)}(ka) f_{lm} &= \psi_l^{(1)}(nka) d_{lm}.
\end{aligned}$$

To eliminate d_{lm}

$$\begin{aligned} & \left[n\psi_l^{(1)}(nka)\psi_l^{(3)'}(ka) - \psi_l^{(1)'}(nka)\psi_l^{(3)}(ka) \right] f_{lm} \\ = & - \left[n\psi_l^{(1)}(nka)\psi_l^{(1)'}(ka) - \psi_l^{(1)'}(nka)\psi_l^{(1)}(ka) \right] b_{lm}. \end{aligned}$$

To eliminate f_{lm}

$$\begin{aligned} & \left[\psi_l^{(3)'}(ka)\psi_l^{(1)}(ka) - \psi_l^{(3)}(ka)\psi_l^{(1)'}(ka) \right] b_{lm} \\ = & \left[\psi_l^{(3)'}(ka)\psi_l^{(1)}(nka) - \frac{1}{n}\psi_l^{(3)}(ka)\psi_l^{(1)'}(nka) \right] d_{lm}. \end{aligned} \quad (\text{C.2})$$

Using the identity (1.19), I set the coefficients of b_{lm} and a_{lm} in (C.1) and (C.2) as follows. First,

$$\psi_l^{(3)}(ka)\psi_l^{(1)'}(ka) - \psi_l^{(3)'}(ka)\psi_l^{(1)}(ka) = -i.$$

Then,

$$c_{lm} = \frac{-i}{\psi_l^{(3)}(ka)\psi_l^{(1)'}(nka) - \frac{1}{n}\psi_l^{(3)'}(ka)\psi_l^{(1)}(nka)} a_{lm},$$

and

$$d_{lm} = \frac{i}{\psi_l^{(3)'}(ka)\psi_l^{(1)}(nka) - \frac{1}{n}\psi_l^{(3)}(ka)\psi_l^{(1)'}(nka)} b_{lm},$$

D Translation of spherical harmonics

This is derived starting from (1.22), letting $\mathbf{r}' = \mathbf{r} + \mathbf{d}$, and expand $e^{i\mathbf{k}\cdot\mathbf{r}'}$ in terms of \mathbf{r} ,

$$\begin{aligned} e^{i\mathbf{k}\cdot\mathbf{r}} &= \sum_{lm} 4\pi i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}), \\ e^{i\mathbf{k}\cdot\mathbf{r}'} &= \sum_{lm} 4\pi i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}'), \\ &= \sum_{lm} 4\pi i^l u_l(k\mathbf{r}) Y_{lm}^*(\hat{\mathbf{k}}), \end{aligned}$$

where $v_l(k\mathbf{r})$ are to be determined. To compute these, we can write

$$\begin{aligned} e^{i\mathbf{k}\cdot\mathbf{r}'} &= e^{i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{d}} \\ &= \sum_{lm} \sum_{l'm'} 4\pi i^l 4\pi i^{l'} u_{lm}(k\mathbf{r}) u_{l'm'}(k\mathbf{d}) Y_{l'm'}^*(\hat{\mathbf{k}}) Y_{lm}^*(\hat{\mathbf{k}}). \end{aligned}$$

Thus

$$\begin{aligned} & \sum_{pq} 4\pi i^p u_{pq}(k\mathbf{r}) Y_{pq}^*(\hat{\mathbf{k}}) \\ &= \sum_{lm} \sum_{l'm'} 4\pi i^l 4\pi i^{l'} u_{lm}(k\mathbf{r}) u_{l'm'}(k\mathbf{d}) Y_{l'm'}^*(\hat{\mathbf{k}}) Y_{lm}^*(\hat{\mathbf{k}}). \end{aligned}$$

Multiply by $Y_{pq}(\hat{\mathbf{k}})$ and integrate over the unit sphere:

$$\begin{aligned} i^p u_{pq}(k\mathbf{r}) &= \sum_{lm} \sum_{l'm'} i^{l+l'} u_l(k\mathbf{r}) u_{l'}(k\mathbf{d}) \int d\hat{\mathbf{k}} Y_{pq}(\hat{\mathbf{k}}) Y_{l'm'}^*(\hat{\mathbf{k}}) Y_{lm}^*(\hat{\mathbf{k}}) \\ &= \sum_{lm} S_{pq;lm}(k\mathbf{d}) u_{lm}(k\mathbf{r}). \end{aligned}$$

I defined

$$\begin{aligned} S_{pq;lm} &= 4\pi \sum_{l'm'} i^{l+l'} u_{l'm'}(k\mathbf{d}) W_{pq;lm;l'm'}, \\ W_{pq;lm;l'm'} &= \int d\hat{\mathbf{k}} Y_{pq}(\hat{\mathbf{k}}) Y_{lm}^*(\hat{\mathbf{k}}) Y_{l'm'}^*(\hat{\mathbf{k}}), \\ &= \sum_{p'q'} Y_{p'q'}(\hat{\mathbf{k}}) \left[\int d\hat{\mathbf{k}} Y_{p'q'}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}) \right]^*. \end{aligned}$$

We may also write

$$W_{pq;lm;l'm'} = (-1)^{m+m'} \int d\hat{\mathbf{k}} Y_{pq}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}).$$

Both the expressions depend on the integral of 3 spherical harmonics, which is given by the expression,

$$\int d\hat{\mathbf{k}} Y_{pq}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}) = \sqrt{\frac{(2p+1)(2l+1)(2l'+1)}{4\pi}} \begin{pmatrix} p & l & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} p' & l & l' \\ q & m & m' \end{pmatrix},$$

where $\begin{pmatrix} p' & l & l' \\ q & m & m' \end{pmatrix}$ is the Wigner 3j symbol. Thus

$$\begin{aligned} S_{pq;lm} &= 4\pi \sum_{l'm'} i^{l+l'} u_{l'm'}(k\mathbf{d}) W_{pq;lm;l'm'}, \\ W_{pq;lm;l'm'} &= (-1)^{m+m'} \sqrt{\frac{(2p+1)(2l+1)(2l'+1)}{4\pi}} \begin{pmatrix} p & l & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} p' & l & l' \\ q & m & m' \end{pmatrix}. \end{aligned}$$

E Planar Fourier Transform of Scalar Green Function

Defin

$$\rho(x, y, z) = \sqrt{x^2 + y^2 + z^2}.$$

Sommerfeld identity

$$\begin{aligned}
\frac{e^{ik\rho}}{\rho} &= \frac{i}{2\pi k_z} \int dk_x dk_y e^{ik_x x + ik_y y + ik_z z} . \\
&\int dx' dy' e^{-ik_x x'} e^{-ik_y y'} \frac{\exp[ik\rho(x' - x, y' - y, z)]}{\rho(x' - x, y' - y, z)} \\
&= \frac{i}{2\pi k_z} \int dk'_x dk'_y \int dx' dy' e^{-ik_x x'} e^{-ik_y y'} e^{ik'_x(x' - x)} e^{ik'_y(y' - y)} e^{ik'_z z} \\
&= \frac{i}{2\pi k_z} \int dk'_x dk'_y \delta(k_x - k'_x) \delta(k_y - k'_y) e^{ik'_z z} \\
&= \frac{i}{2\pi k_z} e^{-i\mathbf{k}_\perp \cdot \mathbf{r}_\perp} e^{ik_z z} .
\end{aligned}$$