Permittivity eigenvalue problem of a single sphere

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1 Definition of the problem

Here, we follow Appendix A of [1] and its correction [2].

We would like to solve the permittivity eigenvalue problem for an isolated spherical inclusion of radius a whose permittivity $\epsilon_{nl}^{(F)}$ serves as the eigenvalue, namely,

$$\nabla \times \left(\nabla \times \vec{E}_{nlm}^{(F)}\right) - k_0^2 \epsilon_2 \vec{E}_{nlm}^{(F)} = \left(\epsilon_{nl}^{(F)} - \epsilon_2\right) \Theta(r) \vec{E}_{nlm}^{(F)}, \qquad \Theta(r) = \left\{ \begin{array}{ll} 1, & r < a \\ 0, & r > a \end{array} \right\}, \tag{1}$$

The corresponding eigenstates of the sphere are one of the two basic types of the vector spherical harmonic (VSHs) - the TE (or magnetic[1] ($F = M$) multipole) field and the TM (or electric ($F = E$) multipole) field as[2]

$$TE : \vec{E}_{nlm}^{(M)}(\vec{r}) = f_{nl}^{(M)}(r) \vec{X}_{lm}(\theta, \phi), \tag{2}$$

$$TM : \vec{E}_{nlm}^{(E)}(\vec{r}) = \frac{i}{k_0 \left[1 - u_{nl}^{(E)} \Theta(r)\right]} \left[\nabla \times \left(f_{nl}^{(E)}(r) \vec{X}_{lm}(\theta, \phi)\right)\right], \tag{3}$$

where $k_j = k_0 \sqrt{\epsilon_j}$ with $k_0 \equiv \omega / c$ and $u_{nl}^{(F)} \equiv (\epsilon_2 - \epsilon_{nl}^{(F)}) / \epsilon_2$. Note that in [1], Eq. (3) employed $1/k_2$ rather than $1/k_0$; I believe this is a mistake, because in the former case the scaling with the permittivity turns out to be wrong inside the sphere. The VSHs themselves are defined by [3]

$$\begin{aligned} \vec{X}_{lm}(r, \theta, \phi) &\equiv \frac{\vec{L} Y_{lm}(\theta, \phi)}{\sqrt{l(l+1)}} \equiv -\frac{ir}{\sqrt{l(l+1)}} \hat{e}_r \times (\nabla Y_{lm}) = -\frac{ir}{\sqrt{l(l+1)}} \hat{e}_r \times \left(\hat{e}_\theta \partial_\theta + \hat{e}_\phi \frac{1}{\sin\theta} \partial_\phi\right) Y_{lm} \\ &= -\frac{ir}{\sqrt{l(l+1)}} \left(\hat{e}_\phi \partial_\theta - \hat{e}_\theta \frac{im}{\sin\theta}\right) Y_{lm}, \end{aligned} \tag{4}$$

where (θ, ϕ) are the standard polar and azimuthal angles and Y_{lm} are the scalar spherical harmonics; Note that for convenience of the following analytical calculations, we assume an exponential dependence on the radial coordinate. For numerical calculations, the choice of trigonometric function is preferred, since it makes the V matrix below symmetric [4]. Thus,

[1] Note that the nomeclature was wrong in [1]!

[2] Phases the same as in [3]. Normalization differs but it affects only the coefficients $A_{nl}^{(F)}$ and $B_{nl}^{(F)}$ below.

in general, $\vec{X}_{lm}$ has two components - $\hat{e}_\theta$ and $\hat{e}_\phi$ so that it is perpendicular to the radial direction[3]. The VSHs are orthogonal to each other $\int \sin\theta d\theta d\phi \vec{X}^*_{l'm'} \cdot \vec{X}_{lm} = \delta_{l,l'}\delta_{m,m'}$.

The radial functions in Eqs. (2)-(3) have the following form for both cases:

$$f_{nl}^{(F)}(r) = \begin{cases} A_{nl}^{(F)} j_l \left(k_2 \left[1 - u_{nl}^{(F)} \right]^{1/2} r \right), & r < a, \\ B_{nl}^{(F)} h_l^{(1)}(k_2 r), & r > a, \end{cases} \tag{5}$$

where j_l and $h_l^{(1)}$ are the spherical Bessel functions [3] which ensure finiteness of the field inside the sphere and an outgoing wave in the far-field. Note that the TM VSH involves the $\Theta(r)$ function which vanishes out of the sphere and equals unity inside it; this ensures that the momentum is different in each media.

The eigenvalue $\epsilon_{nl}^{(F)}$ and the normalization coefficients of the eignefunctions $A_{nl}^{(F)}$ and $B_{nl}^{(F)}$ are determined by continuity conditions at $r = a$. By Eqs. (2)-(3) and Eq. (5), the dependence on the angular part on both sides of the interface is the same for multipoles with the same l and m and the same polarization. Thus, continuity has to be imposed only on the r-dependent parts $f_{nl}^{(M)}$ for each multipole so that the eigenvalues are independent of m[4], justifying the 2-index eigenvalue notation. Thus, in addition, eigenfunctions with the same values of l but different values of n differ only inside the sphere.

For a given "polar quantum number" l and polarization F, we get an infinite sequence of solutions which are enumerated by the "radial quantum number" n. Since the Hankel function is complex, the eigenvalues are, in general, complex too[5]. Ignoring the imaginary part, for $\epsilon_{nl}^{(F)} < 0$, it follows that $Re\left(u_{nl}^{(F)}\right)$ varies between 1 (non-metallic limit) and ∞ (PEC limit. In this case, $\sqrt{1 - u_{nl}^{(F)}}$ is purely imaginary, reflecting the gain that compensates for radiative losses, and the radial functions are essentially the modified Bessel functions (with a real argument). On the other hand, for $\epsilon_{nl}^{(F)} > 0$, it follows that $-\infty < u_{nl}^{(F)} < 1$ such that $1 - u_{nl}^{(F)} > 0$ and $\sqrt{1 - u_{nl}^{(F)}}$ is purely real. Accordingly, in this case, the radial functions are given essentially by the regular Bessels and the resulting modes are analogous to the whispering gallery modes.

For TE multipoles, $\vec{E} = \vec{E}_\parallel$ and by Eq. (2)

$$\begin{aligned} \vec{H}_{nlm}^{(M)} \sim \nabla \times \vec{E}_{nlm}^{(M)} &= \frac{1}{r\sin\theta}\left(\left[\partial_\theta \sin\theta E_\phi\right] - \partial_\phi E_\theta\right)\hat{e}_r - \frac{1}{r}\partial_r\left[rE_\phi\right]\hat{e}_\theta + \frac{1}{r}\partial_r\left[rE_\theta\right]\hat{e}_\phi \\ &= \frac{1}{r\sin\theta} f_{nl}^{(M)}(r)\left[...\right]\hat{e}_r - \frac{1}{r}\partial_r\left[rf_{nl}^{(M)}(r)\right]\left[...\right]\hat{e}_\theta + \frac{1}{r}\partial_r\left[rf_{nl}^{(M)}(r)\right]\left[...\right]\hat{e}_\phi, \end{aligned} \tag{6}$$

[3] $\vec{X}_{lm}$ consist of Y_{lm} of a fixed l and $m, m \pm 1$ [3, Eq. (9.104)], i.e., it is not an eigenvector of $\hat{L}^2$ nor of $\hat{L}_z \equiv -i\frac{\partial}{\partial\phi}$ (but Y_{lm} is..). As shown in [5, p. 83], it is constructed as the eigenfunction of $\hat{J}^2$ and $\hat{J}_z$, when the eigenvalues of the momentum operators are $S = 1$ and $J = l$ ($\hat{J} \equiv \hat{L} + \hat{S}$ where $\hat{L} \equiv ...$ and $\hat{S} \equiv i\hat{e}_r \times$). In fact, $\vec{X}_{lm} \equiv Y_{llm}$ are a special case of Y_{Jlm} [5] for which J may differ from l.

[4] This degeneracy is due to the fact that the total angular momentum operator of the EM field $\hat{J}$ commutes with the scattering operator $\hat{\Gamma}$.

[5] This reflects the non-Hermitian character of $\hat{\Gamma}$.

so that different vectorial components have a different radial dependence. Specifically, the continuity of $f_{nl}^{(M)}$ ensures continuity of $H_\perp = H_r$ and the continuity of $\frac{df_{nl}^{(M)}}{dr}$ ensures the continuity of $H_\parallel$.

For TM multipoles, $\vec{H} = H_\parallel$ and by Eq. (3)

$$\vec{E} \sim \frac{1}{\epsilon}\nabla\times\vec{H} = \frac{1}{\epsilon}\left(\frac{1}{r\sin\theta}f_{nl}^{(E)}(r)\,[...]\,\hat{e}_r - \frac{1}{r}\partial_r\left[rf_{nl}^{(E)}(r)\right][...]\,\hat{e}_\theta + \frac{1}{r}\partial_r\left[rf_{nl}^{(E)}(r)\right][...]\,\hat{e}_\phi\right), \tag{7}$$

so that it follows from a similar procedure that the following radial functions must be continuous there: $f_{nl}^{(E)}$, $\frac{1}{1-u_{nl}^{(E)}\Theta(r)}\frac{d\left(rf_{nl}^{(E)}\right)}{dr} \equiv \frac{1}{\epsilon}\frac{d\left(rf_{nl}^{(E)}\right)}{dr}$.

Continuity of $f_{nl}^{(F)}$ dictates that

$$B_{nl}^{(F)} = A_{nl}^{(F)}\frac{j_l^{(1)}\left(x_{nl}^{(F)}\right)}{h_l^{(1)}(ka)}, \tag{8}$$

where

$$x_{nl}^{(F)} \equiv k_0\left(1-u_{nl}^{(F)}\right)^{1/2}a. \tag{9}$$

Now, demanding continuity of the derivative-associated terms (Eqs. (6)-(7)) and using Eqs. (5) and (9), we get the following equations for determining the eigenvalues, depending only on the radial functions:

$$\left.\frac{xj_l'(x)}{j_l(x)}\right|_{x=x_{nl}^{(M)}} = \left.\frac{xh_l^{(1)'}(x)}{h_l^{(1)}(x)}\right|_{x=k_2a}, \tag{10}$$

$$\left.\frac{1}{x^2}\left(1+\frac{xj_l'(x)}{j_l(x)}\right)\right|_{x=x_{nl}^{(E)}} = \left.\frac{1}{x^2}\left(1+\frac{xh_l^{(1)'}(x)}{h_l^{(1)}(x)}\right)\right|_{x=k_2a}. \tag{11}$$

Note that the index l sets the order of the Bessel function; then, there is an infinite number of solution, numbered through the (radial) index n.

By definition of the spherical Bessel functions,

$$z_l(x) = \sqrt{\frac{\pi}{2}}x^{-1/2}Z_{l+1/2}(x), \tag{12}$$

$$z_l'(x) = \sqrt{\frac{\pi}{2}}\left(-\frac{1}{2}x^{-3/2}Z_{l+1/2}(x) + x^{-1/2}Z_{l+1/2}'(x)\right), \tag{13}$$

where Z_l is any Bessel function. Thus,

$$\frac{xz_l'(x)}{z_l(x)} = \frac{x\sqrt{\frac{\pi}{2}}\left(-\frac{1}{2}x^{-3/2}Z_{l+1/2}(x)+x^{-1/2}Z_{l+1/2}'(x)\right)}{\sqrt{\frac{\pi}{2}}x^{-1/2}Z_{l+1/2}(x)} = \frac{xZ_{l+1/2}'(x)-\frac{1}{2}Z_{l+1/2}(x)}{Z_{l+1/2}(x)} = \frac{xZ_{l+1/2}'(x)}{Z_{l+1/2}(x)}-\frac{1}{2}. \tag{14}$$

We now substitute this in Eqs. (10)-(11) and get

$$\left.\frac{xJ'_{l+1/2}(x)}{J_{l+1/2}(x)}\right|_{x=x_{nl}^{(M)}} = \left.\frac{xH^{(1)'}_{l+1/2}(x)}{H^{(1)}_{l+1/2}(x)}\right|_{x=ka}, \tag{15}$$

$$\left.\frac{1}{x^2}\left(\frac{1}{2}+\frac{xJ'_l(x)}{J_l(x)}\right)\right|_{x=x_{nl}^{(E)}} = \left.\frac{1}{x^2}\left(\frac{1}{2}+\frac{xH^{(1)'}_l(x)}{H^{(1)}_l(x)}\right)\right|_{x=k_2a}. \tag{16}$$

2 Linking the cylinder and sphere eigenvalue problems

We would like now to link the dispersion relations for the sphere to those for cylinders. We recall the dispersion relations for a wire [6]. The permittivity eigenvalue is denoted as $\epsilon_{nM}^{(F)}$ where n is the radial quantum number. For in plane propagation, $k_z = 0$, the TE and TM VCHs decouple, and the transverse momentum components equal the total momentum components, so that $\alpha_2 = k_2$ and $\alpha_1 a = x_{nM}^{(F)}$ where

$$x_{nM}^{(F)} \equiv k_0 a \left(1 - u_{nM}^{(F)}\right)^{1/2} \equiv ka\left(\epsilon_{nM}^{(F)}\right)^{1/2}. \tag{17}$$

For $\mu_1 = \mu_2 = 1$, the cylinder dispersion relations reduce to

$$\underbrace{\left(\frac{J'_M(k_1x)}{k_1J_M(k_1x)} - \frac{H^{(1)'}_M(k_2a)}{k_2aH^{(1)}_M(k_2a)}\right)}_{TE\ VCH}\underbrace{\left(\frac{\epsilon_1J'_M(k_1x)}{xJ_M(k_1x)} - \frac{\epsilon_2H^{(1)'}_M(k_2a)}{k_2aH^{(1)}_M(k_2a)}\right)}_{TM\ VCH} = 0. \tag{18}$$

Requiring that each of the expressions in parentheses vanish independently, we get

$$TE: \quad \frac{J'_M\left(x_{nM}^{(M)}\right)}{x_{nM}^{(M)}J_M\left(x_{nM}^{(M)}\right)} = \frac{H^{(1)'}_M(k_2a)}{k_2aH^{(1)}_M(k_2a)}, \tag{19}$$

$$TM: \quad \frac{x_{nM}^{(E)}J'_M\left(x_{nM}^{(E)}\right)}{J_M\left(x_{nM}^{(E)}\right)} = \frac{k_2aH^{(1)'}_M(k_2a)}{k_2aH^{(1)}_M(k_2a)}. \tag{20}$$

Therefore, one can use the codes developed for TM cylinder modes at $k_z = 0$ to solve the TE sphere problem (19) by setting $M = l + 1/2$ (maybe need to amend the contour choices?), but for the sphere TM problem (20) would require changing the existing wire codes of [6].

3 Normalization

Mode normalization can be performed numerically, but better computed analytically, to speed up this repeated calculation. This was done in [1] incorrectly, and then maybe corrected in [2]. Here, we repeat this calculation in order to verify the results.

As explained in [7, Appendix A], due to the choice of complex exponentials, instead of taking the complex conjugate of the entire isolated sphere right eigenfunction (ket), we only have to conjugate the radial part in order to get a left eigenfunction (bra). **but this means that the bra is conjugated..** [6]

This operation will be denoted by $\hat{C}$, so that

$$\begin{aligned}
\hat{C}\vec{E}^{(M)}_{nlm} &= f^{(M)^*}_{nl}(r)\vec{X}_{lm}(\theta,\phi), && (21)\\
\hat{C}\vec{E}^{(E)}_{nlm} &= \left(\frac{i}{k_0\left(1-u^{(E)}_{nl}\Theta(r)\right)}\right)^* f^{(E)^*}_{nl}(r)\vec{X}_{lm}(\theta,\phi), && (22)
\end{aligned}$$

Thus, the inner product involves the product f^2, rather than $|f|^2$.

The coefficients $A^{(F)}_{nl}$ are determined from the normalization condition on $\vec{E}^{(F)}_{nlm}$. For $F = M$,

$$\begin{aligned}
1 &= \langle C\vec{E}^{(M)}_{nlm}|\vec{E}^{(M)}_{nlm}\rangle = \int_{r<a} d^3r \left[A^{(M)}_{nl} j_l\left(k_0\left(1-u^{(M)}_{l,n}\right)^{1/2} r\right)\right]^2 \vec{X}^*_{lm}\cdot\vec{X}_{lm}\\
&= \left(A^{(M)}_{nl}\right)^2 \int_0^a r^2 dr \left[j_l\left(k_0\left(1-u^{(M)}_{l,n}\right)^{1/2} r\right)\right]^2 = \frac{\left(A^{(M)}_{nl}\right)^2 a^3}{\left(x^{(M)}_{nl}\right)^3}\int_0^{x^{(M)}_{nl}} dx x^2 \left[j_l(x)\right]^2\\
&= \frac{\left(A^{(M)}_{nl}\right)^2 a^3}{2}\left[j_{l+1}\left(x^{(M)}_{nl}\right)\right]^2, && (23)
\end{aligned}$$

while for $F = E$,

$$\begin{aligned}
1 &= \langle C\vec{E}^{(E)}_{nlm}|\vec{E}^{(E)}_{nlm}\rangle\\
&= \left(\frac{iA^{(E)}_{l,n}}{k_0\left(\epsilon^{(E)}_{nl}\right)}\right)^2 \int_{r<a} d^3r \left[\nabla\times j_l\left(k_0\left(\epsilon^{(E)}_{nl}\right)^{1/2} r\right)\vec{X}^*_{lm}\right]\cdot\left[\nabla\times j_l\left(k_0\left(\epsilon^{(E)}_{nl}\right)^{1/2} r\right)\vec{X}_{lm}\right]\\
&= ????? - \frac{a^3}{x^{(E)^3}_{nl}\epsilon^{(E)}_{nl}}\left(A^{(E)}_{l,n}\right)^2\left(\int_0^{x^{(E)}_{nl}} dx x^2 j_l^2(x) + \left[x j_l(x^{(E)}_{nl}) j_l(x)\left(1+\frac{x j_l'(x)}{j_l(x)}\right)\right]_0^{x^{(E)}_{nl}}\right). && (24)
\end{aligned}$$

double check the above based on correcting the identity (27) below.. + compare to expressions in [2] which may already be corrected?

Thus,

$$1 = -\frac{a^3}{x^{(E)^3}_{nl}}\left(A^{(E)}_{l,n}\right)^2\left(\frac{x^{(E)^3}_{nl}}{2}\left[j_{l+1}(x^{(E)}_{nl})\right]^2 + x^{(E)}_{nl} j_l(x^{(E)}_{nl})^2\left(1+\frac{x j_l'(x)}{j_l(x)}\right)_0^{x^{(E)}_{nl}}\right). \quad (25)$$

[6] In [1], Bergman says the following - “Since $\vec{J}$ is a Hermitian operator, its eigenstates, namely the VSHs, satisfy the usual orthogonality relations when integrated over the angular variables. It is only the states with the same angular momentum and parity **how related??** but different radial quantum number n that satisfy instead the bi-orthogonality relations.”; we believe this approach to be awkward, if not incorrect in the general case, since the bi-orthogonality is inherent in the operator.

We note that the orthogonalization integrals extend to the sphere only. Since the argument of the Bessel function corresponds to the roots, these integrals coincide with the available formulae for integrals over the Bessel functions below. Specifically, in order to get Eq. (23) we had to use the integral formula [Wikipedia]

$$\int_0^{x_{nl}^{(F)}} y^2 dy j_l^2(y) = \frac{{x_{nl}^{(F)}}^3}{2} \delta_{nn'} \left[j_{l+1}(x_{nl}^{(F)}) \right]^2 , \tag{26}$$

where x_{nl} is the n'th zero of the spherical Bessel function.

In order to get Eq. (24) we had to use Eq. (16) and the integral formula **derived by David? double check - there is a unit problem..**

$$\int_{r<a} \left[\nabla \times z_l\left(\alpha r\right) \vec{X}_{lm}^* \right] \cdot \left[\nabla \times g_{l'}\left(\beta r\right) \vec{X}_{l'm'} \right] = \frac{\delta_{ll'}\delta_{mm'}}{\beta} \left[\int_0^{\beta a} dx x^2 z_l \left(\frac{\alpha}{\beta} x \right) g_l(x) + \left(x z_l(\alpha a) g_l(x) \left(1 + \frac{x g_l'(x)}{g_l(x)} \right) \right)_0^{\beta a} \right] \tag{27}$$

g_l' **more likely than** $g_{l'}$ **due to units???**

in order to fix it, one can replace the $\vec{X}$ **by Bessels, get rid of derivatives, and search for the relevant integral solution in Ryzhik.. alternatively, can go through the Wigner symbols calculations in [2]. or - use Parry's reduction of the 3D integral to a 2D integral?**

4 Work plan

- understand Parry's codes for cylinders
- implement the perturbation approach (overlap integrals of pairs of cylinder modes over difference geometry of embedding circle and scatterer; may not be as accurate as Parry's approach due to staircasing..). Implement for a cylinder inside a cylinder and compare to Parry's results.
- implement for a triangular wire.
- implement the second sphere polarization
- fix mode normalization (Section 3) and test vs. Mie theory/multiple scattering.

References

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