Shape optimization for LDOS inside a cativity

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Adjoint method for shape optimization

The local density of states (LDOS) is proportional to the imaginary party of the dyadic green's function [2]:

$$\rho(\mathbf{x}_0,\omega) = \frac{\omega}{\pi c^2} Im Tr[\overline{\overline{G^{EP}}}(\mathbf{x}_0,\mathbf{x}_0,\omega) + \overline{\overline{G^{HM}}}(\mathbf{x}_0,\mathbf{x}_0,\omega)] \tag{1}$$

We only consider the electric LDOS ρ_e which comes from the electric part of the green's function $\overline{\overline{G^{EP}}}(\mathbf{x}_0,\mathbf{x}_0,\omega)$. The electric field $\mathbf{E}(\mathbf{x}_0,\omega)$ is determined by the green's function by:

$$\mathbf{E}(\mathbf{x}_0,\omega) = i\mu_0\omega \int \overline{\overline{G^{EP}}}(\mathbf{x}_0,\mathbf{x},\omega)\cdot \mathbf{j}(\mathbf{x}) d^3\mathbf{x} \tag{2}$$

In the time harmonic case with only electric dipole at $\mathbf{x_0}$ as the source, we have $\mathbf{j}(\mathbf{x}_0) = \frac{\partial \mathbf{p}(\mathbf{x_0})}{\partial t} = -i\omega \mathbf{P}\delta^3(\mathbf{x}-\mathbf{x}_0)$, inserting this into Eq. (2) we hava

$$\mathbf{E}(\mathbf{x}_0,\omega) = \frac{\omega^2}{\varepsilon_0 c^2}\overline{\overline{G^{EP}}}(\mathbf{x}_0,\mathbf{x}_0,\omega)\cdot \mathbf{P} \tag{3}$$

Compare to the LDOS expression Eq. (1), we have

$$\rho_e(\mathbf{x_0}) = \frac{\varepsilon_0}{\pi\omega}\frac{1}{|\mathbf{P}_0|} Im \sum_j \hat{\mathbf{s}_j}\cdot \mathbf{E}_{s_j}(\mathbf{x}_0) \tag{4}$$

where $\mathbf{E}_{s_j}$ denotes the field from a dipole source at $\mathbf{x}_0$ polarized in the $\mathbf{s}_j$ direction, with an unit dipole moment $\mathbf{P}_0 = \mathbf{s}_j$ (thus $|\mathbf{P}_0| = 1$), and the sum over j accounts for all possible orientations. This is a small modification to Eq. (8) in Owen's paper [1], where we make the electric dipole to be unit dipole and the coefficient ε_0 to the front.

Therefore, we can get the LDOS of a specified by three scattering simulation.

In Owen's thesis, we have that for a shape deformation $\delta x_n(\mathbf{x}')$, the variation for the object function F is (Eq. (5.28) in Ref. [3]).

$$\delta F = 2Re\int \delta x_n(\mathbf{x}')[(\varepsilon_2-\varepsilon_1)\mathbf{E}_{\|}(\mathbf{x}')\cdot \mathbf{E}^{\mathbf{A}}_{\|}(\mathbf{x}') + (\frac{1}{\varepsilon_1}-\frac{1}{\varepsilon_2})\mathbf{D}_{\perp}(\mathbf{x}')\cdot \mathbf{D}^{\mathbf{A}}_{\perp}(\mathbf{x}')]dA \tag{5}$$

However, this equation is wrong because it assumed that $\partial F/\partial \mathbf{E}$ is the complex conjugate of $\partial F/\partial \bar{\mathbf{E}}$. In fact,

$$\overline{(\frac{F}{\partial \mathbf{E}})} = \frac{\partial \bar{F}}{\partial \bar{\mathbf{E}}} \neq \frac{\partial F}{\partial \bar{\mathbf{E}}} \tag{6}$$

Therefore, the right variation for the object function should be

$$\delta F = \int \delta x_n(\mathbf{x}')[(\varepsilon_2 - \varepsilon_1)\mathbf{E}_{\parallel}(\mathbf{x}') \cdot \mathbf{E}_{\parallel}^{\mathbf{A}}(\mathbf{x}') + (\frac{1}{\varepsilon_1} - \frac{1}{\varepsilon_2})\mathbf{D}_{\perp}(\mathbf{x}') \cdot \mathbf{D}_{\perp}^{\mathbf{A}}(\mathbf{x}')]dA + \text{Conjugate Adjoint.} \quad (7)$$

Since the electric LDOS ρ_e is the imaginary part of some function, say $\tilde{\rho}_e$. The optimum of $\tilde{\rho}_e$ must also be the optimum of ρ_e. So we can first take the object function to be $\tilde{\rho}_e$, for each direction j in Eq. (4), the source of the adjoint field is a electric dipole at $\mathbf{x}_0$ with the amplitude

$$\frac{\partial \tilde{\rho}_e}{\partial \mathbf{E}_{s_j}} = \frac{\varepsilon_0}{\pi\omega} \int dx^3 \delta(\mathbf{x} - \mathbf{x}_0)\hat{\mathbf{s}_j} \quad (8)$$

while the conjugate adjoint field part $\frac{\partial \tilde{\rho}_e}{\partial \bar{\mathbf{E}}_{s_j}} = 0$.

This is a also a dipole at $\mathbf{x} = \mathbf{x}_0$ in the $\hat{\mathbf{s}_j}$ direction, so the adjoint field is the same as the original field up to a constant scalar:

$$\mathbf{E}_{s_j}^{\mathbf{A}}(\mathbf{x}) = \frac{\varepsilon_0}{\pi\omega}\mathbf{E}_{sj} \quad (9)$$

Therefore, we have the variation for the electric LDOS as

$$\delta\rho_e = \frac{\varepsilon_0}{\pi\omega} Im \sum_j \int \delta x_n(\mathbf{x}')\{(\varepsilon_2 - \varepsilon_1)[\mathbf{E}_{s_j\parallel}(\mathbf{x}')]^2 + (\frac{1}{\varepsilon_1} - \frac{1}{\varepsilon_2})[\mathbf{D}_{s_j\perp}(\mathbf{x}')]^2\}dA \quad (10)$$

In `scuff-scatter`, we can use `--EPFile` to get the electric field of specified points, however, it only applies to points away from the scattering surface. For points on the surface, the obtained data are just garbage. Instead, we can implement the option `--PSDFile` to obtain the effective electric and magnetic surface charge and current. In the `scuff` calculation, the effective electric and magnetic surface charge and current are defined as

$$\sigma = \mathbf{n} \cdot \mathbf{D} \quad (11a)$$
$$\mathbf{K} = \mathbf{n} \times \mathbf{H} \quad (11b)$$
$$\eta = \mathbf{n} \cdot \mathbf{B} \quad (11c)$$
$$\mathbf{N} = \mathbf{n} \times \mathbf{E} \quad (11d)$$

Therefore, the parallel electrical field and perpendicular displacement can be computed as

$$\mathbf{E}_{\parallel} = \mathbf{N} \quad (12a)$$
$$\mathbf{D}_{\perp} = \sigma\mathbf{n} \quad (12b)$$

After the surface fields are obtained, we can first verify this adjoint method on a void sphere case. For a void sphere, the electromagnetic surface modes satisfy:

$$\varepsilon_m(E)H_l(k_m a)[k_d a J_l(k_d a)]' = \varepsilon_d J_l(k_d a)[k_m a H_l(k_m a)]' \quad (13)$$

where a corresponds to the void radius, l is the (integer) index denoting the angular momentum, $k_m = \sqrt{\varepsilon_m}k_0$ and $k_d = \sqrt{\varepsilon_d}k_0$ are wave vectors in metal and void. J_l and H_l are spherical Bessel and Hankel functions of the first kind[4, 5].

By solving Eq. (13), we can quickly get some resonant parameters and use it as the initial guess for the general shape optimization purpose.

We use the boost library to create spherical harmonic basis functions.

$$Y_l^m(\theta,\phi) = \begin{cases} \sqrt{\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}}P_l^m(\cos\theta)\cos(m\phi), & m \leq 0 \\ \sqrt{\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}}P_l^m(\cos\theta)\sin(m\phi), & m > 0 \end{cases} \tag{14}$$

The basis function set contains various combinations of (l,m), we number them by $n = l(l+1)+m+1$, then an arbitrary shape function $x(\theta,\phi)$ can be expressed as

$$x(\theta,\phi) = \sum_{n=1}^{N} c_n Y_n(\theta,\phi) \tag{15}$$

where c_n is the expansion coefficients and the parameters that we need to optimize.

In numerical evaluation, we do the surface integral by summing up all panels with each panel $\delta A_p(\theta,\phi)$. Inserting Eq. (15) to Eq. (10) we get

$$\delta\rho_e = \frac{\varepsilon_0}{\pi\omega} Im \sum_{j,n,p} \delta c_n Y_n(\theta,\phi)\{(\varepsilon_2-\varepsilon_1)[\mathbf{E}_{s_j\|}(\mathbf{x}')]^2 + (\frac{1}{\varepsilon_1}-\frac{1}{\varepsilon_2})[\mathbf{D}_{s_j\perp}(\mathbf{x}')]^2\}\delta A_p(\theta,\phi). \tag{16}$$

Since (θ,ϕ) is determined by $\mathbf{x}'$, the derivate to one coefficient c_n is then

$$\frac{\partial\rho_e}{\partial c_n} = \frac{\varepsilon_0}{\pi\omega} Im \sum_{j,p} Y_n(\mathbf{x}')\{(\varepsilon_2-\varepsilon_1)[\mathbf{E}_{s_j\|}(\mathbf{x}')]^2 + (\frac{1}{\varepsilon_1}-\frac{1}{\varepsilon_2})[\mathbf{D}_{s_j\perp}(\mathbf{x}')]^2\}\delta A_p(\mathbf{x}'). \tag{17}$$

References

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