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]:

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

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]).

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

Since the electric LDOS ρ_e is the imaginary part of some function, say $\tilde{\rho_e}$:

$$\rho_e=\frac{\tilde{\rho_e}-\tilde{\rho_e}^*}{2i}=Im(\tilde{\rho_e})=Im[\frac{\varepsilon_0}{\pi\omega}\sum_j\hat{\mathbf{s}_j}\cdot\mathbf{E}_{s_j}(\mathbf{x}_0)] \tag{6}$$

For each direction j in Eq. (4), the source of the adjoint field is a electric dipole at $\mathbf{x}_0$ with the amplitude

$$\frac{\partial \rho_e}{\partial \mathbf{E}_{s_j}} = \frac{\partial \rho_e}{\partial \tilde{\rho_e}} \frac{\partial \tilde{\rho_e}}{\partial \mathbf{E}_{s_j}} = \frac{\varepsilon_0}{2i\pi\omega} \delta(\mathbf{x} - \mathbf{x}_0) \hat{\mathbf{s}_j} \tag{7}$$

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:

$$\mathbf{E}^{\mathbf{A}}_{s_j}(\mathbf{x}) = \frac{\varepsilon_0}{2i\pi\omega} \mathbf{E}_{sj} \tag{8}$$

Inserting Eq. (8) to Eq. (5), we then have the variation for the electric LDOS as

$$\delta\rho_e = \frac{\varepsilon_0}{\pi\omega} Im \sum_j \int \delta x_n(\mathbf{x}') \{(\varepsilon_2 - \varepsilon_1)[\mathbf{E}_{s_j\parallel}(\mathbf{x}')]^2 + (\frac{1}{\varepsilon_1} - \frac{1}{\varepsilon_2})[\mathbf{D}_{s_j\perp}(\mathbf{x}')]^2\} dA \tag{9}$$

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

$$\sigma = \mathbf{n} \cdot \mathbf{D} \tag{10a}$$
$$\mathbf{K} = \mathbf{n} \times \mathbf{H} \tag{10b}$$
$$\eta = \mathbf{n} \cdot \mathbf{B} \tag{10c}$$
$$\mathbf{N} = \mathbf{n} \times \mathbf{E} \tag{10d}$$

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

$$\mathbf{E}_\parallel = \mathbf{N} \tag{11a}$$
$$\mathbf{D}_\perp = \sigma \mathbf{n} \tag{11b}$$

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:

$$\varepsilon_m(E) H_l(k_m a)[k_d a J_l(k_d a)]' = \varepsilon_d J_l(k_d a)[k_m a H_l(k_m a)]' \tag{12}$$

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. (12), 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.

$$Y_l^m(\theta, \phi) = \begin{cases} \sqrt{\frac{2n+1}{4\pi} \frac{(n-m)!}{(n+m)!}} P_l^m(\cos\theta) \cos(m\phi), & m \leq 0 \\ \sqrt{\frac{2n+1}{4\pi} \frac{(n-m)!}{(n+m)!}} P_l^m(\cos\theta) \sin(m\phi), & m > 0 \end{cases} \tag{13}$$

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

$$x(\theta,\phi) = c_0 + |\sum_{n=1}^{N} c_n Y_n(\theta,\phi)|^2 \tag{14}$$

where $c_0 = d_{min}$ is the minimum distance and c_n is the expansion coefficients and the parameters that we need to optimize.

The normal direction is

$$\mathbf{n} = (1, -\frac{\partial x}{\partial \theta}, -\frac{\partial x}{\partial \phi}) \tag{15}$$

In numerical evaluation, we do the surface integral by summing up all panels with each panel $\delta A_p(\theta,\phi)$. Inserting Eq. (14) to Eq. (9) we get

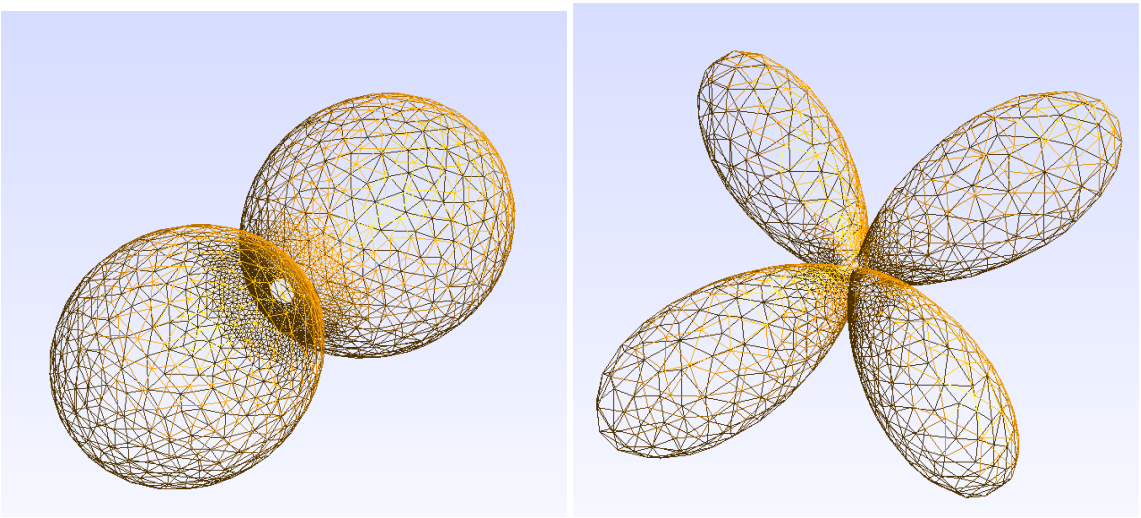
$$\delta\rho_e = \frac{2\varepsilon_0}{\pi\omega} Im \sum_{j,n,p} \delta c_n \sqrt{\frac{x'-c_0}{1+(\frac{\partial x'}{\partial\theta})^2+(\frac{\partial x'}{\partial\phi})^2}} Y_n(\theta,\phi)\{(\varepsilon_2-\varepsilon_1)[\mathbf{E}_{s_j\parallel}(\mathbf{x}')]^2 + (\frac{1}{\varepsilon_1}-\frac{1}{\varepsilon_2})[\mathbf{D}_{s_j\perp}(\mathbf{x}')]^2\}\delta A_p(\theta,\phi). \tag{16}$$

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

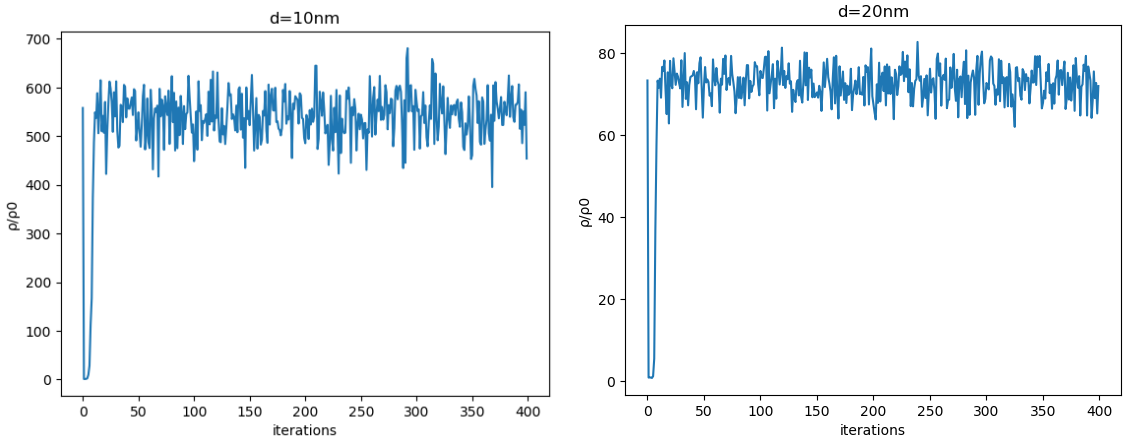
$$\frac{\partial\rho_e}{\partial c_n} = \frac{2\varepsilon_0}{\pi\omega} Im \sum_{j,p} \sqrt{\frac{x'-c_0}{1+(\frac{\partial x'}{\partial\theta})^2+(\frac{\partial x'}{\partial\phi})^2}} Y_n(\mathbf{x}')\{(\varepsilon_2-\varepsilon_1)[\mathbf{E}_{s_j\parallel}(\mathbf{x}')]^2 + (\frac{1}{\varepsilon_1}-\frac{1}{\varepsilon_2})[\mathbf{D}_{s_j\perp}(\mathbf{x}')]^2\}\delta A_p(\mathbf{x}'). \tag{17}$$

Regarding this gradient, there are several problems:

- We need to start with a good initial guess. If the initial guess lies far away from the peak, all gradients are very small, the iteration either stop or move only a little with the change of the LDOS is even smaller than the numerical errors. So far we only know the resonance of a metallic sphere void, the initial guess we implement should related to the sphere shape.
- We can't start with a sphere with minimum distance $c_0 = d_{min}$, this will cause all gradients equal to 0 since $x' = c_0$ at the first iteration. To resolve this problem, if we still want to start with a sphere, we need to set the initial radius of the sphere to be $r = c_0 + \frac{c_1^2}{4\pi}$ for some none zero c_1 (note that $Y_1^2 = \frac{1}{4\pi}$).
- When the initial guess is a sphere close to the resonance, we notice that the derivative $\partial\rho_e/\partial c_1$ is much larger than all other derivatives (approximately 10^5 times larger). This means the optimal structure near a sphere is just a sphere, and we can't find another structure since it will converge to the local maximum.
- To avoid the problem above, we need a initial guess other than the sphere. One possible shape is the combination of two resonant sphere, similar to the structure below.



However, it's very hard to get convergence and the LDOS falls far short from the limit. For the 10nm case the limit is around 9000 and the limit is 1000 for 20nm.



Limits to LDOS

In Owen's paper [1], the limits to the LDOS is

$$\frac{\rho_{tot}}{\rho_0} \leq \frac{2\pi}{k^3} \sum_j \int_V \tilde{F}_{inc,s_j} \cdot \overline{\overline{\chi}}^{\dagger} (\mathrm{Im}\overline{\overline{\chi}})^{-1} \overline{\overline{\chi}} \tilde{F}^*_{inc,s_j} d^3x \tag{18}$$

For metals, the limits can be simplified with the optimal incident field $F_{inc,s_j} = \overline{\overline{\overline{G^{EP}}}} \hat{\mathbf{s}}_j$:

$$\frac{\rho_{tot}}{\rho_0} \leq \frac{2\pi}{k^3} \frac{|\chi(\omega)|^2}{\mathrm{Im}\chi(\omega)} \int_V ||\overline{\overline{\overline{G^{EP}}}}||_F^2 d^3x \tag{19}$$

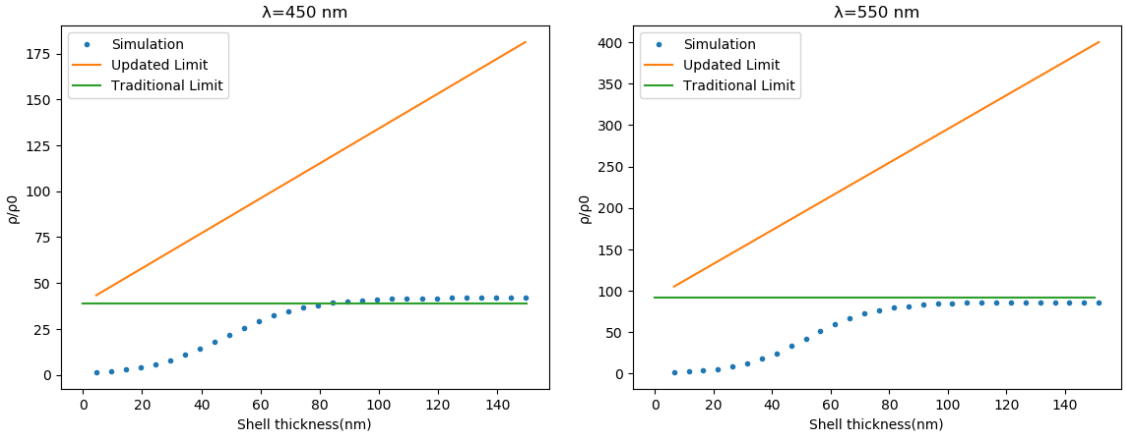
$$= \frac{k^3}{4\pi} \frac{|\chi(\omega)|^2}{\mathrm{Im}\chi(\omega)} \int_V [\frac{3}{(kr)^6} + \frac{1}{(kr)^4} + \frac{1}{(kr)^2}] d^3x \tag{20}$$

For a enclosure of minimum separation distance d, we have

$$\frac{\rho_{tot}}{\rho_0} \leq \frac{|\chi(\omega)|^2}{\mathrm{Im}\chi(\omega)}[\frac{1}{(kd)^3} + \frac{1}{kd} + O(kL)] \tag{21}$$

As discussed in Owen's paper, the $O(kL)$ term represents the largest interaction distances over which polarization currents contribute to the LDOS. For small d, we can neglect this term since $\frac{1}{(kd)^3}$ is the dominant term and is much larger than other terms. However, for $kd \leq 1$ (for example, $d = 200$ nm), the first two terms are smaller than 1, now the problem is what is the approximate value for $O(kL)$? If it is in the order of 1, then the bound should approximately double, which is not really we want to see. Therefore we might need to stick with the small d case?

If we add the $O(kL)$ term as kt where t is the thickness of the sphere shell, we have



References

[1] O. D. Miller, A. G. Polimeridis, M. T. H.Reid, C. W.Hsu, B. G. DeLacy, J. D. Joannopoulos, M. Soljacic, and S. G. Johnson, "Fundamental limits to optical response in absorptive systems," Opt. Express **24**, 3329-3364 (2016).

[2] K. Joulain, R. Carminati, J.-P. Mulet, and J.-J. Greffet, "Definition and measurement of the local density of electromagnetic states close to an interface," Phys. Rev. B **68**, 245405 (2003).

[3] O. D. Miller, "Photonic Design: From Fundamental Solar Cell Physics to Computational Inverse Design," PhD Thesis in University of California, Berkeley (2012).

[4] M. E. Abdelsalam S. Cintra, S. Mahajan, A. E. Russell, and P. N. Bartlett, "Localized and delocalized plasmons in metallic nanovoids" Phys. Rev. B **74**, 245415 (2006).

[5] A. D. Boardman, *Electromagnetic Surface Modes*, Wiley-Interscience, 1982