Fundamental Limitations on Absorption and Scattering of Electromagnetic Waves

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Gustafsson *etal*, "Upper bounds on absorption and scattering", 2020 New J. Phys. 22 073013
Schab *etal*, "Trade-offs in absorption and scattering by nanophotonic structures", 2000, arXiv:2009.08502

Outline

Absorption, scattering, and extinction

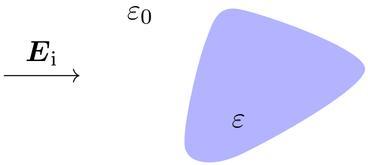
Absorption, scattering, and extinction can be calculated (and measured). Depend on

- wavelength, λ
- wavefront shape (often plane wave)

of the illuminating field, $\boldsymbol{E}_\mathrm{i}$, and

- material (complex permittivity ε)
- size
- shape

of the obstacle.



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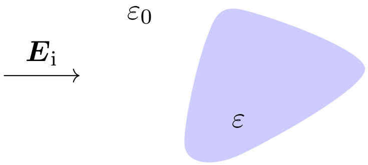

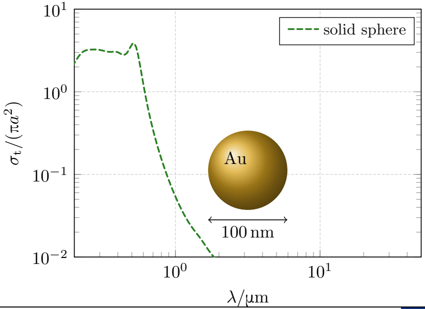

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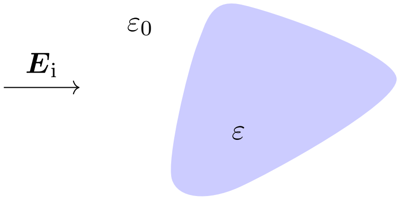

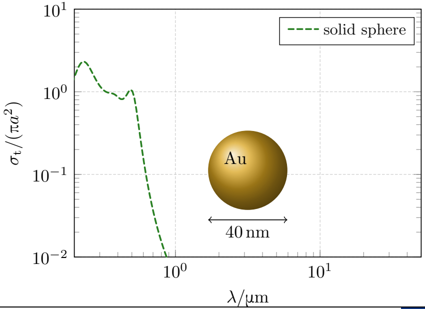

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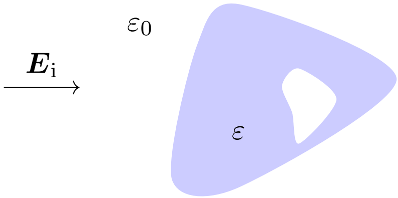

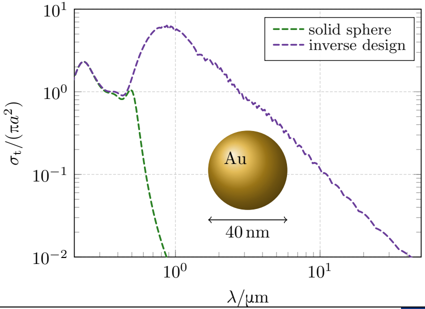

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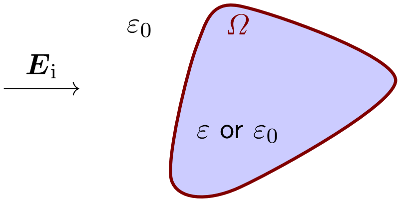
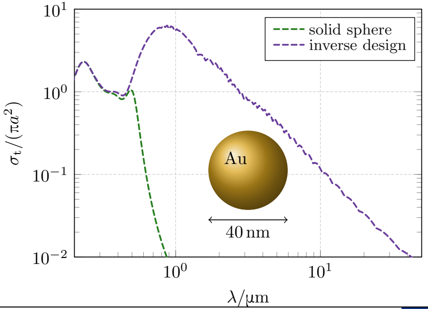


What can be said about the maximum absorption, scattering and extinction (here cross section σ_t) of all obstacles fitting inside a region Ω made of a material ε and fixed illumination?



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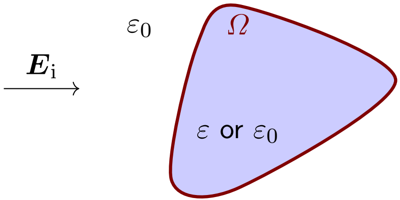

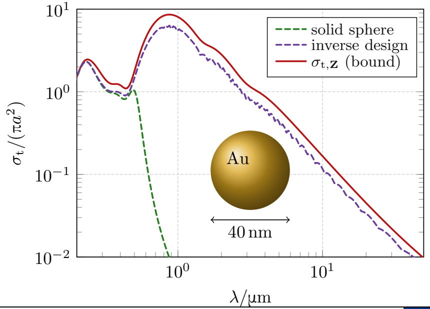

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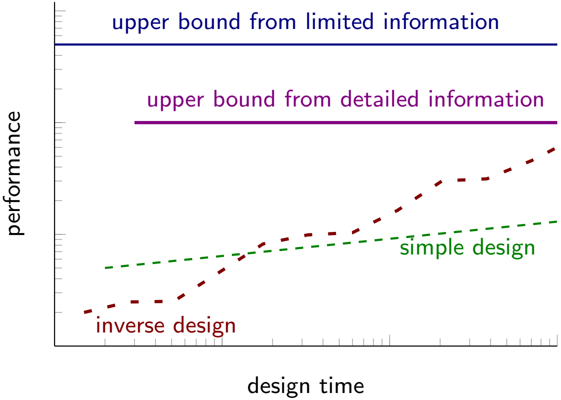
Physical bounds and optimal inverse design

We commonly desire to design devices as good as possible. What about designing the best?

- Need knowledge about optimality
  - Physical bounds (limitations).
  - Volume, shape, material, ...
- Need methodologies to design optimal structures
  - Classical design approaches.
  - Inverse design (topological optimization).



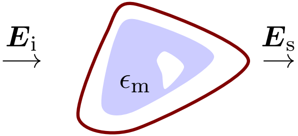
Physical bounds on EM devices

Bounds have been determined for, *e.g.*,

- Antennas (bandwidth, efficiency, gain, directivity, capacity, ...)
- Periodic structures (bandwidth for absorbers, high-impedance surfaces, transmission, extinction, ...)
- Scattering, absorption, and extinction cross sections
- Composite materials, homogenization, temporal dispersion

Many of the bounds are derived using

- Holomorphic properties originating from causality and passivity (*e.g.*, sum rules for Herglotz-Nevanlinna functions)
- Power/Energy relations and optimization techniques over induced sources



Passivity/Causality and Optimization (power) bounds

Passivity and Causality

- LTI system (Input and output signals)
- Analyticity from causality
- Definite sign from passivity (HN)
- Bounds from weighted integrals over all spectrum

$$\frac{2}{\pi}\int_{\mathbb{R}} \frac{\operatorname{Im} f(\omega)}{\omega^{2n}}\,\mathrm{d}\omega = a_{2n-1} - b_{2n-1}$$

- ☺ Simple closed form expressions
- ☺ Based on an identity
- ☹ Not pointwise (moments)
- ☹ Hard to add (include) information

Optimization (power) bounds

- Physical modelling (integral equations (MoM))
- Optimization problems over sources

$$f(\omega) \leq f_{\mathrm{opt}}(\omega)$$

- ☺ Pointwise bounds
- ☺ Easy to add (include) information

Outline

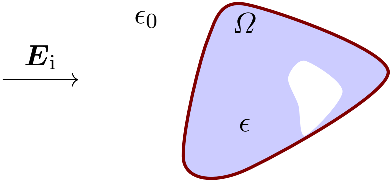
Relaxation of integral equation based models

Integral equations (MoM) to model interaction between EM fields and an obstacle

$$\mathbf{Z}\mathbf{I} = \mathbf{V}$$

with

- impedance matrix $\mathbf{Z}$ (Green's function)
- (contrast) current $\mathbf{I}$ $(\boldsymbol{J} = \mathrm{i}\omega(\varepsilon_0 - \varepsilon)\boldsymbol{E})$
- excitation $\mathbf{V}$ (illumination $\boldsymbol{E}_{\mathrm{i}}$)



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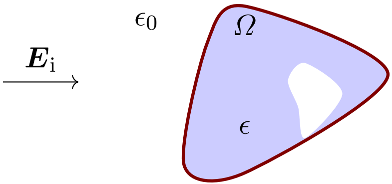
Solution $\mathbf{I} = \mathbf{Z}^{-1}\mathbf{V}$.



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Integral equations (MoM) to model interaction between EM fields and an obstacle

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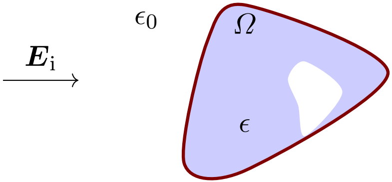

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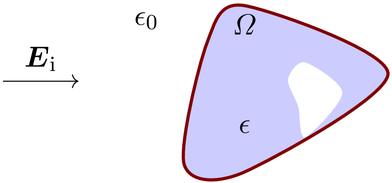
Relax the equation to [Gus+20]

$$\mathbf{I}^{\mathsf{H}}\mathbf{Z}\mathbf{I} = \mathbf{I}^{\mathsf{H}}\mathbf{V}$$

and use as a constraint in optimization.



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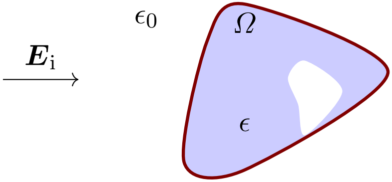

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Real part is the optical theorem (conservation of power) and imaginary part reactive power.

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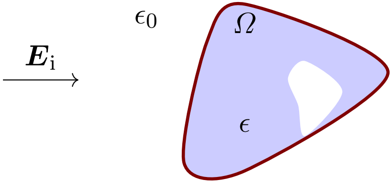

The impedance matrix can be divided as $\mathbf{Z} = \mathbf{R}_\rho + \mathbf{R}_0 + \mathrm{i}\mathbf{X}$ with

- absorbed power $\frac{1}{2}\mathbf{I}^{\mathsf{H}}\mathbf{R}_\rho\mathbf{I}$
- radiated power $\frac{1}{2}\mathbf{I}^{\mathsf{H}}\mathbf{R}_0\mathbf{I}$

Real part is the optical theorem (conservation of power) and imaginary part reactive power.

Maximum absorption cross sections

Absorbed power is a quadratic form

$$P_{\mathrm{a}} = \frac{1}{2}\mathbf{I}^{\mathsf{H}}\mathbf{R}_{\rho}\mathbf{I}$$

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to determine the maximum absorption of any object in the region Ω with permittivity

$$\begin{cases} \varepsilon & \text{parts made of the material} \\ \varepsilon_0 & \text{background material } (\boldsymbol{J}(\boldsymbol{r}) = \boldsymbol{0}) \end{cases}$$

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Similar for maximum scattering and extinction with

$$P_{\mathrm{s}} = \frac{1}{2}\mathbf{I}^{\mathsf{H}}\mathbf{R}_0\mathbf{I} \quad \text{and } P_{\mathrm{t}} = \frac{1}{2}\mathrm{Re}\{\mathbf{I}^{\mathsf{H}}\mathbf{V}\}$$

Maximum absorption cross sections

Absorbed power is a quadratic form

$$P_{\rm a} = \frac{1}{2}\mathbf{I}^{\sf H}\mathbf{R}_{\rho}\mathbf{I}$$

with current satisfying $\mathbf{Z}\mathbf{I} = \mathbf{V}$. Reformulate as an optimization problem

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- Quadratically constrained quadratic program (QCQP) with two constraints (Re,Im)
- Dual problem for a bound
- Dual problem is convex (easy)
- No dual gap

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Reduce to $\mathrm{Re}\{\mathbf{I}^{\mathsf{H}}\mathbf{Z}\mathbf{I}\} = \mathrm{Re}\{\mathbf{I}^{\mathsf{H}}\mathbf{V}\}$ for simpler bound solely dependent on losses.

Outline

Maximum absorption, scattering and extinction cross sections

Electrically small objects with minimum losses ρ_{r}: dipole fields

Absorption

$$\sigma_{\mathrm{a}} = \min_{\nu\geq 1}\frac{\nu^2}{4}\sum_n \frac{\tilde{a}_n^2\varrho_n}{(\nu-1)+\nu\varrho_n} \approx \frac{6\pi}{k^2}\frac{\varrho_1}{(1+\varrho_1)^2} \approx \frac{\eta_0 V}{\rho_{\mathrm{r}}\left(1+\frac{k^2\eta_0 V}{6\pi\rho_{\mathrm{r}}}\right)^2} \leq \begin{cases}\frac{\eta_0 V}{\rho_{\mathrm{r}}}\\ \frac{3\pi}{2k^2}\end{cases}$$

Scattering

$$\sigma_{\mathrm{s}} = \min_{\nu\geq \nu_1}\frac{\nu^2}{4}\sum_n \frac{\tilde{a}^2\varrho_n}{(\nu-1)\varrho_n+\nu} \approx \frac{6\pi}{k^2}\frac{\varrho_1^2}{(1+\varrho_1)^2} \approx \frac{k^2}{6\pi}\frac{\left(\frac{\eta_0 V}{\rho_{\mathrm{r}}}\right)^2}{\left(1+\frac{k^2\eta_0 V}{6\pi\rho_{\mathrm{r}}}\right)^2} \leq \begin{cases}\frac{k^2\eta_0^2 V^2}{6\pi\rho_{\mathrm{r}}^2}\\ \frac{\eta_0 V}{4\rho_{\mathrm{r}}}\\ \frac{6\pi}{k^2}\end{cases}$$

Extinction

$$\sigma_{\mathrm{t}} = \sum_n \frac{\tilde{a}_n^2\varrho_n}{\varrho_n+1} \approx \frac{6\pi}{k^2}\frac{\varrho_1}{1+\varrho_1} \approx \frac{V}{k^2 V/(6\pi)+\rho_{\mathrm{r}}/\eta_0} \leq \begin{cases}\frac{\eta_0 V}{\rho_{\mathrm{r}}}\\ \frac{6\pi}{k^2}\end{cases}$$

Radiation modes

Radiation modes ϱ_n are defined by the eigenvalue problem

$$\mathbf{R}_0\mathbf{I}_n = \varrho_n \mathbf{R}_\rho \mathbf{I}_n$$

- Electrically small limit $ka \to 0$ have three modes with

$$\varrho_n = \frac{k^2\eta_0}{6\pi}\int_\Omega \rho_\mathrm{r}^{-1}\,\mathrm{dV} = \frac{k^2\eta_0|\Omega|}{6\pi\rho_\mathrm{r}} \quad n = 1,2,3$$

- Homogeneous sphere (and similarly layered spheres)

$$\varrho_v = \frac{k^2\eta_0 a^3}{2\rho_\mathrm{r}}\left((\mathrm{R}_{1,l}^{(1)})^2 - \mathrm{R}_{1,l-1}^{(1)}\,\mathrm{R}_{1,l+1}^{(1)} + \frac{2}{ka}\,\mathrm{R}_{1,l}^{(1)}\,\mathrm{R}_{2,l}^{(1)}\,\delta_{\tau,2}\right)$$

$$\approx \frac{(ka)^{2l}}{\big((2l+1)!!\big)^2}\frac{\eta_0 a}{\rho_\mathrm{r}}\begin{cases}(ka)^2/(2l) & \tau = 1\\ (l+1) & \tau = 2\end{cases} \quad \text{as } ka \to 0,$$

Outline

Extinction cross section $\sigma_{\rm t}$ for Au in spherical region

QCLP (QCQP for $\sigma_{\rm a}, \sigma_{\rm s}$)

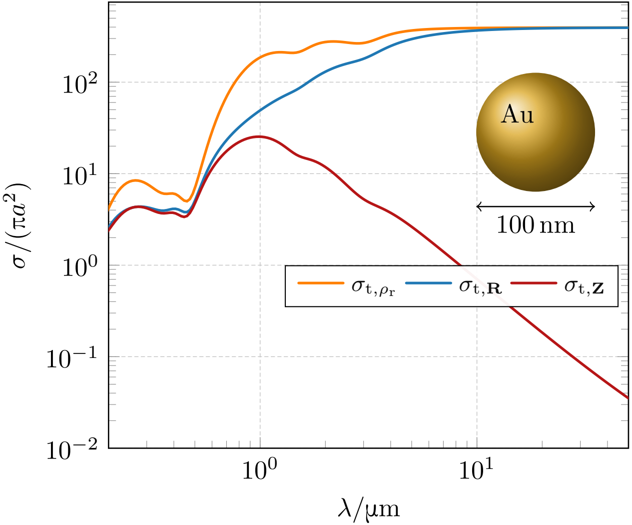
$$\begin{aligned} &\text{maximize} && \mathrm{Re}\{\mathbf{I}^{\mathsf{H}}\mathbf{V}\} \\ &\text{subject to} && \mathbf{I}^{\mathsf{H}}\mathbf{Z}\mathbf{I} = \mathbf{I}^{\mathsf{H}}\mathbf{V} \end{aligned}$$

Bounds based on

Red: $\sigma_{\rm t,\mathbf{Z}}$ shape, $\rho_{\rm r}$, and $\rho_{\rm i}$

Blue: $\sigma_{\rm t,\mathbf{R}}$ shape and $\rho_{\rm r}$

Orange: $\sigma_{\rm t,\rho_r}$ volume and $\rho_{\rm r}$



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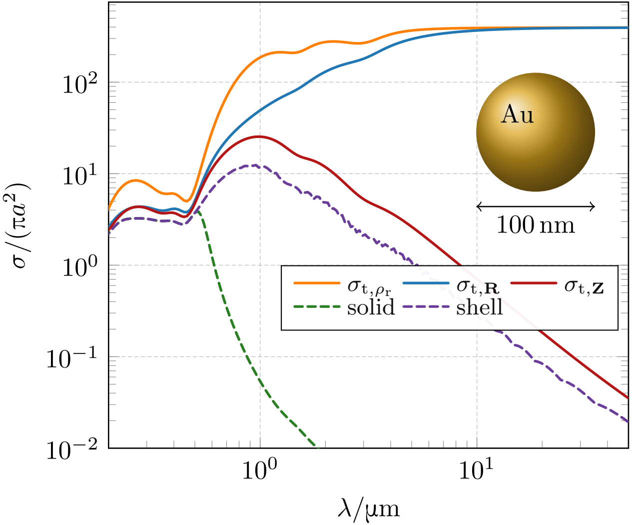
The bounds are compared with

Green: solid

Purple: optimized shell



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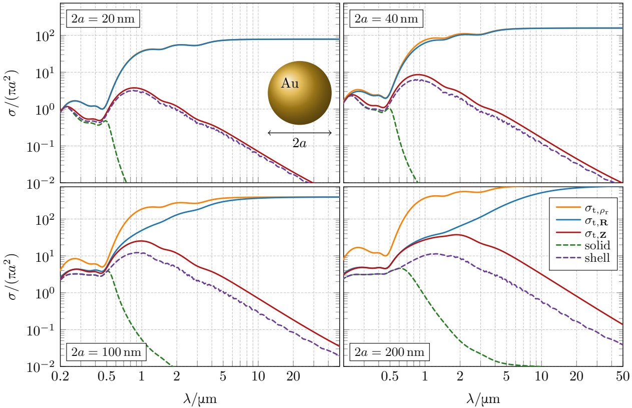

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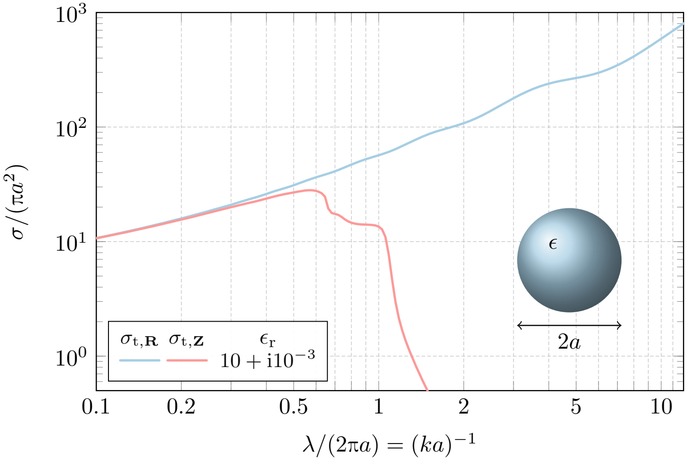

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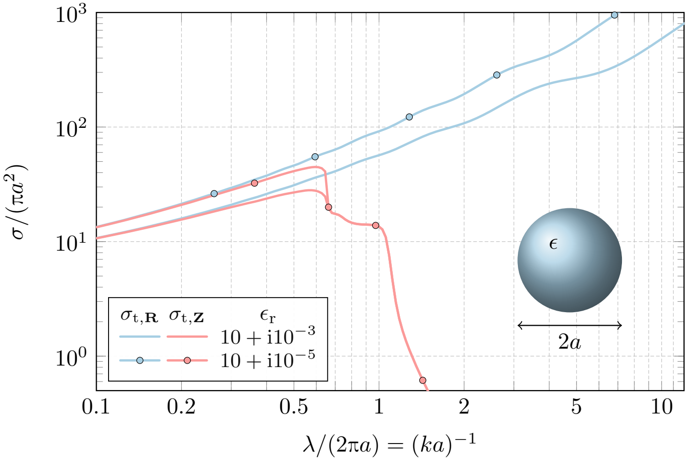

Extinction cross section σ_t for dielectric in spherical regions

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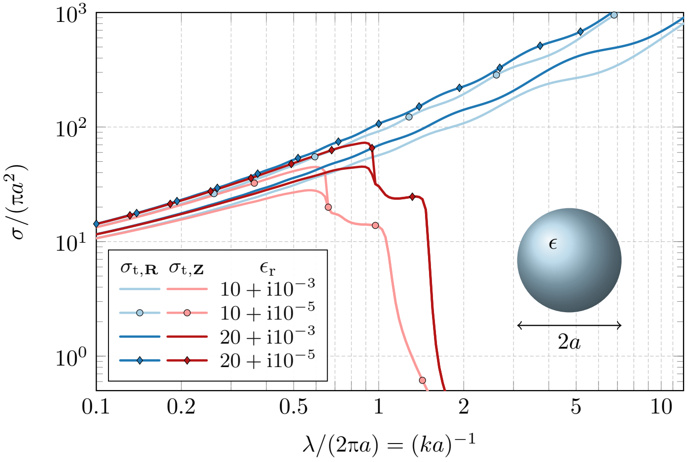
$$\begin{aligned} &\text{maximize} && \mathrm{Re}\{\mathbf{I}^\mathsf{H}\mathbf{V}\} \\ &\text{subject to} && \mathbf{I}^\mathsf{H}\mathbf{Z}\mathbf{I} = \mathbf{I}^\mathsf{H}\mathbf{V} \end{aligned}$$

Bounds based on

Red: $\sigma_{\mathrm{t},\mathbf{Z}}$ shape, ρ_r, and ρ_i

Blue: $\sigma_{\mathrm{t},\mathbf{R}}$ shape and ρ_r



Extinction cross section σ_t for dielectric in spherical regions

QCLP (QCQP for $\sigma_\mathrm{a}, \sigma_\mathrm{s}$)

$$\begin{aligned} &\text{maximize} && \mathrm{Re}\{\mathbf{I}^\mathsf{H}\mathbf{V}\} \\ &\text{subject to} && \mathbf{I}^\mathsf{H}\mathbf{Z}\mathbf{I} = \mathbf{I}^\mathsf{H}\mathbf{V} \end{aligned}$$

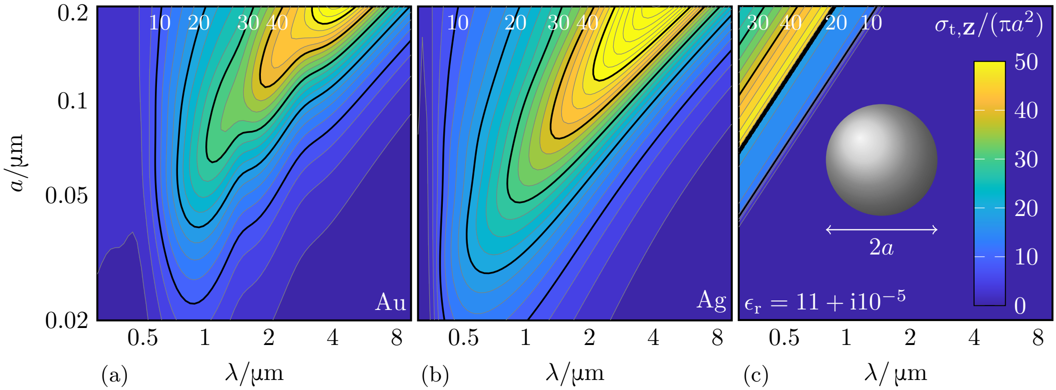
Bounds based on

Red: $\sigma_{\mathrm{t},\mathbf{Z}}$ shape, ρ_r, and ρ_i

Blue: $\sigma_{\mathrm{t},\mathbf{R}}$ shape and ρ_r

- Small difference for $ka \gg 1$ but large difference for $ka \ll 1$
- Reactance constraint can be neglected for $ka \gg 1$ which simplifies solution.

Comparison: Gold (Au), Silver (Ag), and dielectric (Si)



- Normalized extinction cross section $\sigma_t/(\pi a^3)$ for spherical regions.
- Similar results for absorption, scattering, and near-field illumination.
- Is the extinction dominated by scattering or absorption?

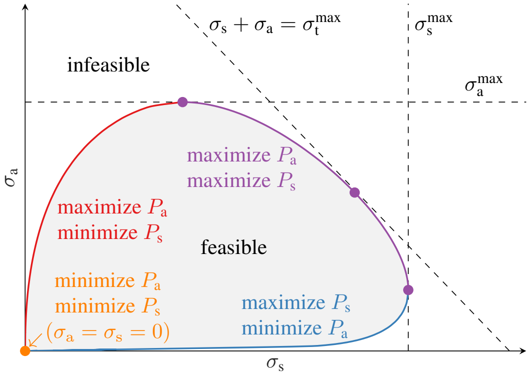
Outline

Trade-off between scattering and absorption

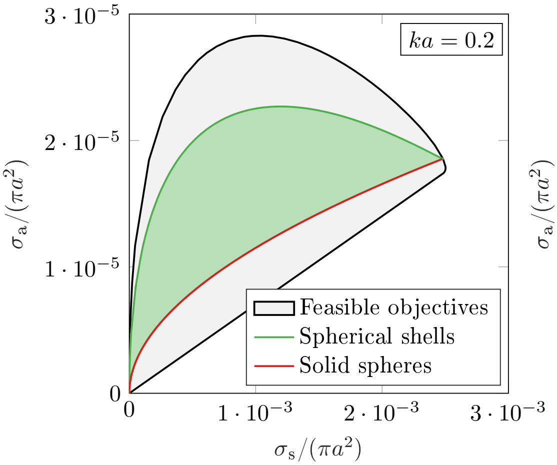
- How is scattering and absorption related for an obstacle?
- Use Pareto optimization to determine the trade-off between absorption and scattering
- Feasible region in the $\{\sigma_\mathrm{s}, \sigma_\mathrm{a}\}$-plane

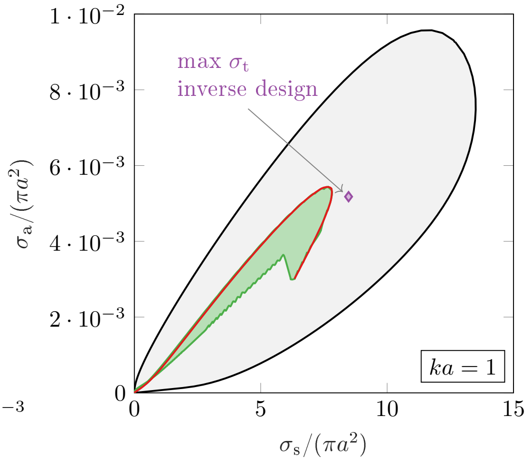
$$\begin{aligned} &\text{maximize} && \mathbf{I}^\mathsf{H}(w_\mathrm{a}\mathbf{R}_\rho + w_\mathrm{s}\mathbf{R}_0)\mathbf{I} \\ &\text{subject to} && \mathbf{I}^\mathsf{H}\mathbf{Z}\mathbf{I} = \mathbf{I}^\mathsf{H}\mathbf{V} \end{aligned}$$

with weights $w_\mathrm{a}, w_\mathrm{s}$. See [Sch+20] for details and alternative formulations.

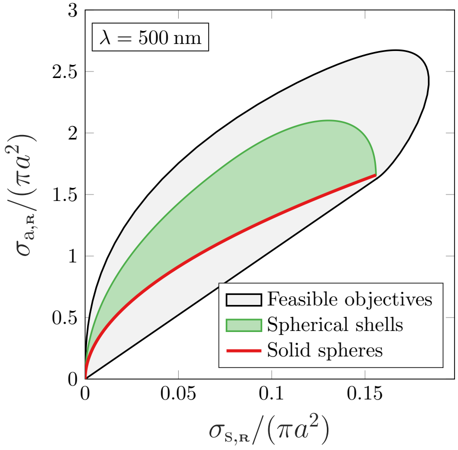


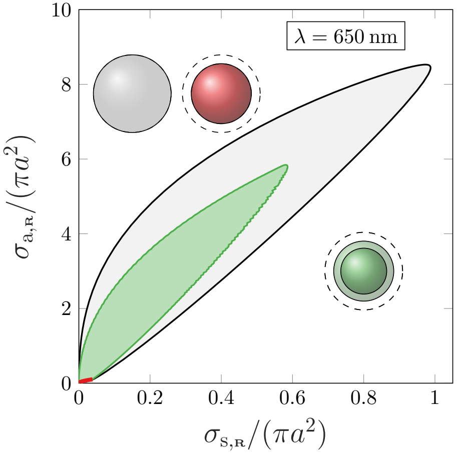
Feasible region and realized cross-sections in a sphere with $\varepsilon_r = 10 + i10^{-3}$





Feasible region for Au obstacles fitting within a $a = 30\,\mathrm{nm}$ sphere

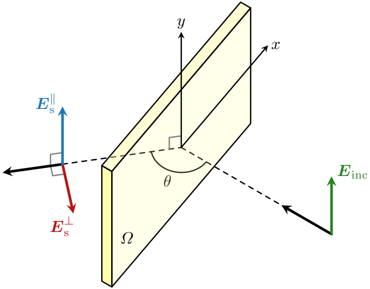


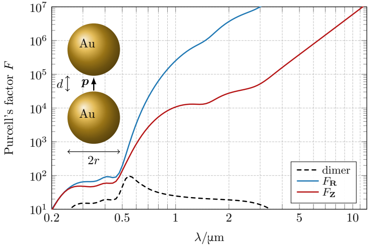


Outline

Conclusions

- General method to compute bounds on systems of the form $\mathbf{ZI} = \mathbf{V}$ by relaxation to $\mathbf{I}^{\mathsf{H}}\mathbf{ZI} = \mathbf{I}^{\mathsf{H}}\mathbf{V}$
- QCQP with computationally efficient solution of the dual
- Here, scattering, absorption, and extinction
- Directional scattering, Purcell factor, …





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