Herglotz function and optimization-based bounds on electromagnetic systems

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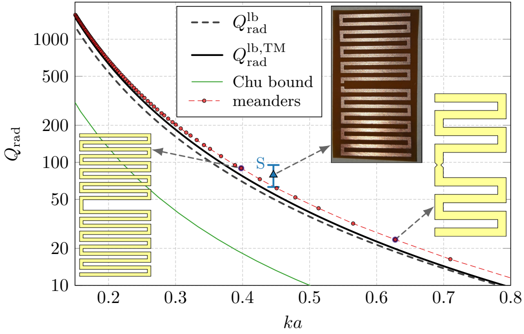
Physical bounds and optimal design

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.
  - Optimization based on parametrized structures.
  - Optimization based on pixeling.

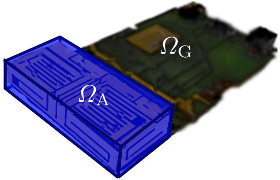


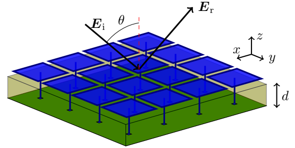
Optimal Planar Electric Dipole Antennas, IEEE-APM 2019 [Cap+19].

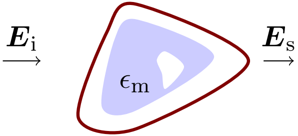
Physical bounds on EM devices

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

Optimization (power) bounds

- Physical modelling (integral equations (MoM))
- Optimization problems over sources
- Pointwise bounds from the solution (convex dual) of the optimization problem

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

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

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

- ☺ Pointwise bounds
- ☺ Easy to add (include) information
- ☹ Bandwidth (Q-factor for small ☺)
- ☹ Numerical solution (some explicit ☺)

Passive systems

Definition (Passivity)

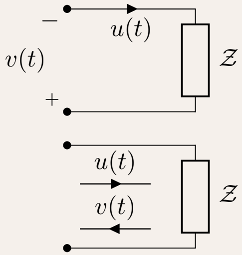
A system ($v = h * u$) is admittance-passive if

$$\mathcal{W}_{\mathrm{adm}}(T) = \operatorname{Re} \int_{-\infty}^{T} v^*(t)u(t)\,\mathrm{d}t \geq 0$$

and scatter-passive if

$$\mathcal{W}_{\mathrm{scat}}(T) = \int_{-\infty}^{T} |u(t)|^2 - |v(t)|^2\,\mathrm{d}t \geq 0,$$

for all $T \in \mathbb{R}$ and smooth functions of compact support u.

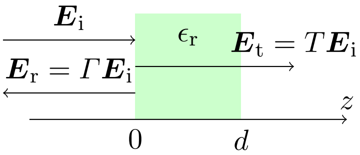


Passivity is a system concept. Not sufficient with passive materials (devices). Need less energy in the output signal than in the input signal for all times and signals.

The transfer function, $Z(s)$ is holomorphic (analytic) for $\operatorname{Re} s > 0$ and $\operatorname{Re}\{Z(s)\} \geq 0$, *i.e.*, a positive real (PR) (or Herglotz-Nevanlinna (HN)) function [WB65; YCC59; Zem63; Zem65].

Passive systems: examples

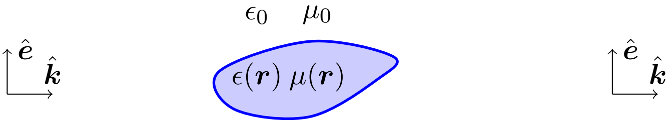
- Reflection and transmission of periodic slabs (scattering)



- Constitutive relations (admittance)

$$\boldsymbol{D}(t) = \epsilon_0\epsilon_\infty\boldsymbol{E}(t) + \epsilon_0\int_{\mathbb{R}}\chi_\mathrm{ee}(t-t')\boldsymbol{E}(t')\,\mathrm{d}t'$$

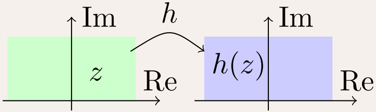
- Scattering (forward (admittance) and modes (scattering))



Definition (Herglotz-Nevanlinna functions (HN), $h(z)$)

A Herglotz-Nevanlinna (Pick, or R-) function $h(z)$ is holomorphic for $\operatorname{Im} z > 0$ and

$$\operatorname{Im} h(z) \geq 0 \quad \text{for} \quad \operatorname{Im} z > 0$$

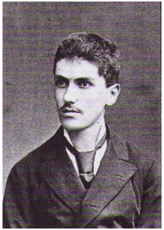


Representation for $\operatorname{Im} z > 0$, *cf.*, the Hilbert transform

$$h(z) = \alpha + \beta z + \int_{-\infty}^{\infty} \frac{1}{\xi - z} - \frac{\xi}{1 + \xi^2} \, \mathrm{d}\nu(\xi),$$

where $\alpha \in \mathbb{R}$, $\beta \geq 0$, and $\int_{\mathbb{R}} \frac{1}{1+\xi^2} \, \mathrm{d}\nu(\xi) < \infty$, see [Akh65; Cau32; GT00; Ned+19]

Gustav Herglotz
1881-1953[Her11]



Georg Alexander Pick
1859-1942

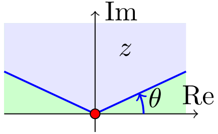
Rolf Nevanlinna
1895-1980 [Nev22]

Wilhelm Cauer
1900-1945 [Cau32]

Integral identities for Herglotz functions

Herglotz functions with the symmetry $h(z) = -h^*(-z^*)$ (real-valued in the time domain) have asymptotic expansions ($N_0 \geq 0$ and $N_\infty \geq 0$)

$$\begin{cases} h(z) = \sum_{n=0}^{N_0} a_{2n-1} z^{2n-1} + o(z^{2N_0-1}) & \text{as } z \hat{\to} 0 \\ h(z) = \sum_{n=0}^{N_\infty} b_{1-2n} z^{1-2n} + o(z^{1-2N_\infty}) & \text{as } z \hat{\to} \infty \end{cases}$$



where $\hat{\to}$ denotes limits in the Stoltz domain $0 < \theta \leq \arg(z) \leq \pi - \theta$.They satisfy the identities ($1 - N_\infty \leq n \leq N_0$)

$$\lim_{\varepsilon \to 0^+} \lim_{y \to 0^+} \frac{2}{\pi} \int_{\varepsilon}^{\frac{1}{\varepsilon}} \frac{\operatorname{Im} h(x + \mathrm{i}y)}{x^{2n}} \, \mathrm{d}x = a_{2n-1} - b_{2n-1} = \begin{cases} -b_{2n-1} & n < 0 \\ a_{-1} - b_{-1} & n = 0 \\ a_1 - b_1 & n = 1 \\ a_{2n-1} & n > 1 \end{cases}$$

Bernland, Luger, Gustafsson, *Sum rules and constraints on passive systems*, J. Phys. A: Math. Theor., 2011.

Integral identities for Herglotz functions

Known low-frequency expansion ($a_1 \geq 0$):

$$h(z) \sim \begin{cases} a_1 z & \text{as } z \hat{\to} 0 \\ b_1 z & \text{as } z \hat{\to} \infty \end{cases}$$

which gives the $n = 1$ identity (we drop the limits for simplicity)

$$\lim_{\varepsilon \to 0^+} \lim_{y \to 0^+} \frac{2}{\pi} \int_{\varepsilon}^{1/\varepsilon} \frac{\mathrm{Im}\, h(x + \mathrm{i}y)}{x^2} \,\mathrm{d}x \overset{\text{def}}{=} \frac{2}{\pi} \int_0^{\infty} \frac{\mathrm{Im}\, h(x)}{x^2} \,\mathrm{d}x = a_1 - b_1 \leq a_1$$

Known high-frequency expansion (short times) ($b_{-1} \leq 0$):

$$h(z) \sim \begin{cases} a_{-1}/z & \text{as } z \hat{\to} 0 \\ b_{-1}/z & \text{as } z \hat{\to} \infty \end{cases}$$

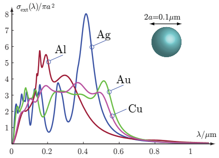
which gives the $n = 0$ identity

$$\frac{2}{\pi} \int_0^{\infty} \mathrm{Im}\, h(x) \,\mathrm{d}x = a_{-1} - b_{-1} \leq -b_{-1}.$$

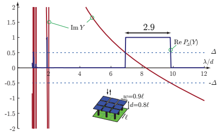
General simple approach to derive sum rules and physical bounds

1. Identify a linear and passive system.
2. Construct a Herglotz function $h(z)$ which models the parameter of interest.
3. Determine asymptotic expansions of $h(z)$ as $z \hat{\to} 0$ and $z \hat{\to} \infty$.
4. Use integral identities for Herglotz functions to relate the dynamic properties to the asymptotic expansions.
5. Bound the integral.

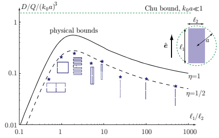
Some examples: Matching networks [Bod45; Fan50], Radar absorbers and Array antennas [DSV13; JKH13; Roz00], Antennas [GSK07; GSK09; Gus10a], Scattering [BGN11; SGK07], High-impedance surfaces [GS11], Metamaterials [GS10], Extraordinary transmission [Gus09; LO+19], Periodic structures [Gus+12], Superluminal [Gus12; WAJ14],...



Cross sections



High-impedance surface



Antennas

Bounds from optimization problem

Use integral equations (MoM) to model the device (antenna, scatterer,...) and the express physical quantities in operators (matrices), *e.g.*, the (time average) radiation intensity $U(\hat{\boldsymbol{r}})$ in a direction $\hat{\boldsymbol{r}}$ and dissipated power P_{d} are

$$U(\hat{\boldsymbol{r}}) = \frac{1}{2}\mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} = \frac{1}{2}|\mathbf{F}^{\mathsf{H}}\mathbf{I}|^2 \quad \text{and } P_{\mathrm{d}} = \frac{1}{2}\mathbf{I}^{\mathsf{H}}\mathbf{R}\mathbf{I},$$

respectively. With the corresponding gain

$$G(\hat{\boldsymbol{r}}) = 4\pi\frac{U(\hat{\boldsymbol{r}})}{P_{\mathrm{d}}} = 4\pi\frac{\mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I}}{\mathbf{I}^{\mathsf{H}}\mathbf{R}\mathbf{I}}$$

Optimize over $\mathbf{I}$ (eigenvalue problem) to determine the maximum gain for any structure which can be synthesized from the original structure [Har68].

Similar procedure can used for a many other cases by considering other matrices and more advanced optimization problems [CG14; CGS17; GC19; GCS19; GN13; Gus+16; JC17; Jon+17].

MoM matrix expressions for bounds

radiation intensity	$U(\hat{\boldsymbol{r}}) \approx \frac{1}{2}\mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I}$
radiated power	$P_{\mathrm{r}} \approx \frac{1}{2}\mathbf{I}^{\mathsf{H}}\mathbf{R}_{\mathrm{r}}\mathbf{I}$
ohmic losses	$P_{\Omega} \approx \frac{1}{2}\mathbf{I}^{\mathsf{H}}\mathbf{R}_{\Omega}\mathbf{I}$
reactance	$X \approx \frac{1}{2}\mathbf{I}^{\mathsf{H}}\mathbf{X}\mathbf{I}$
stored energy	$W_{\mathrm{s}} \approx \frac{1}{4\omega}\mathbf{I}^{\mathsf{H}}\mathbf{X}_{\mathrm{w}}\mathbf{I}$
capacity	$C \sim \log_2(\det(1 + \rho\mathbf{H}\mathbf{P}\mathbf{H}^{\mathsf{H}}))$
far field	$\boldsymbol{F}(\hat{\boldsymbol{r}}) = \mathbf{F}^{\mathsf{H}}\mathbf{I}$
incident field	$\boldsymbol{E}_{\mathrm{in}} = \mathbf{V}\mathbf{I}$
near field	$\boldsymbol{E}(\boldsymbol{r}) = \mathbf{N}^{\mathsf{H}}\mathbf{I}$
spherical modes	$\mathbf{S}\mathbf{I}$
subregion	$\mathbf{T}\mathbf{I}$

Matrices from standard MoM codes [Gus+16]

MoM matrix expressions for bounds

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Matrices from standard MoM codes [Gus+16]

Gain

$$G(\hat{\boldsymbol{r}}) = 4\pi\frac{U(\hat{\boldsymbol{r}})}{P_{\mathrm{r}} + P_{\Omega}} = 4\pi\frac{\mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I}}{\mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}} + \mathbf{R}_{\Omega})\mathbf{I}}$$

Reformulate as an optimization problem over the currents $\mathbf{I}$.

MoM matrix expressions for bounds

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Matrices from standard MoM codes [Gus+16]

Maximum gain

$$\begin{aligned} &\text{maximize} && \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ &\text{subject to} && \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}} + \mathbf{R}_{\Omega})\mathbf{I} = 1 \end{aligned}$$

MoM matrix expressions for bounds

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Matrices from standard MoM codes [Gus+16]

Maximum gain

$$\begin{aligned} &\mathrm{maximize} && \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ &\mathrm{subject\ to} && \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})\mathbf{I} = 1 \end{aligned}$$

add $\mathbf{I}^{\mathsf{H}}\mathbf{X}\mathbf{I} = \mathbf{0}$ for self resonance and $\mathbf{T}\mathbf{I} = \mathbf{0}$ for PEC subregions

$$\begin{aligned} &\mathrm{maximize} && \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ &\mathrm{subject\ to} && \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})\mathbf{I} = 1 \\ & && \mathbf{I}^{\mathsf{H}}\mathbf{X}\mathbf{I} = 0 \\ & && \mathbf{T}\mathbf{I} = \mathbf{0} \end{aligned}$$

Many (endless) possibilities to formulate bounds.

Optimization problem: maximum gain (II)

Maximum G for tuned and self-resonant antennas are analyzed by the QCQPs

$$\begin{aligned} &\text{maximize} && \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ &\text{subject to} && \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})\mathbf{I}=1 \end{aligned} \qquad \text{(T)}$$

$$\begin{aligned} &\text{maximize} && \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ &\text{subject to} && \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})\mathbf{I}=1 \\ & && \mathbf{I}^{\mathsf{H}}\mathbf{X}\mathbf{I}=0 \end{aligned} \qquad \text{(S)}$$

Optimizing over the current $\mathbf{I}$ ($N\times 1$-matrix) with given $N\times N$ matrices $\mathbf{U}=\mathbf{F}\mathbf{F}^{\mathsf{H}}\succeq\mathbf{0}$ (radiation intensity), $\mathbf{R}_{\mathrm{r}}\succeq\mathbf{0}$ (radiated power), $\mathbf{R}_{\Omega}\succeq\mathbf{0}$ (ohmic losses) and $\mathbf{X}$ (reactance) [GC19].

QCQP (T) is reformulated as a Rayleigh quotient and solved as an eigenvalue problem.
QCQP (S) is not convex/concave and needs to be reformulate in a solvable form.

Optimization problem: maximum gain (III)

$$\begin{aligned} &\text{maximize} && \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ &\text{subject to} && \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})\mathbf{I}=1 \end{aligned} \qquad \text{(T)}$$

$$\begin{aligned} &\text{maximize} && \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ &\text{subject to} && \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})\mathbf{I}=1 \\ &&& \mathbf{I}^{\mathsf{H}}\mathbf{X}\mathbf{I}=0 \end{aligned} \qquad \text{(S)}$$

or as a Rayleigh quotient

$$G = 4\pi\frac{\mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I}}{\mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})\mathbf{I}}$$

with solution

$$G = 4\pi\max\operatorname{eig}(\mathbf{U},\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})$$

Optimization problem: maximum gain (III)

$$\begin{aligned} \text{maximize} \quad & \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ \text{subject to} \quad & \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}} + \mathbf{R}_{\Omega})\mathbf{I} = 1 \end{aligned} \qquad \text{(T)}$$

or as a Rayleigh quotient

$$G = 4\pi \frac{\mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I}}{\mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}} + \mathbf{R}_{\Omega})\mathbf{I}}$$

with solution

$$G = 4\pi \max \operatorname{eig}(\mathbf{U}, \mathbf{R}_{\mathrm{r}} + \mathbf{R}_{\Omega})$$

$$\begin{aligned} \text{maximize} \quad & \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ \text{subject to} \quad & \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}} + \mathbf{R}_{\Omega})\mathbf{I} = 1 \\ & \nu \mathbf{I}^{\mathsf{H}}\mathbf{X}\mathbf{I} = 0 \end{aligned} \qquad \text{(S)}$$

for all ν.

Optimization problem: maximum gain (III)

$$\begin{aligned} &\text{maximize} && \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ &\text{subject to} && \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})\mathbf{I}=1 \end{aligned} \qquad \text{(T)}$$

or as a Rayleigh quotient

$$G = 4\pi\frac{\mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I}}{\mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})\mathbf{I}}$$

with solution

$$G = 4\pi\max\operatorname{eig}(\mathbf{U},\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})$$

$$\begin{aligned} &\text{maximize} && \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ &\text{subject to} && \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega})\mathbf{I}=1 \\ &&& \nu\mathbf{I}^{\mathsf{H}}\mathbf{X}\mathbf{I}=0 \end{aligned} \qquad \text{(S)}$$

for all ν. Add the constraints

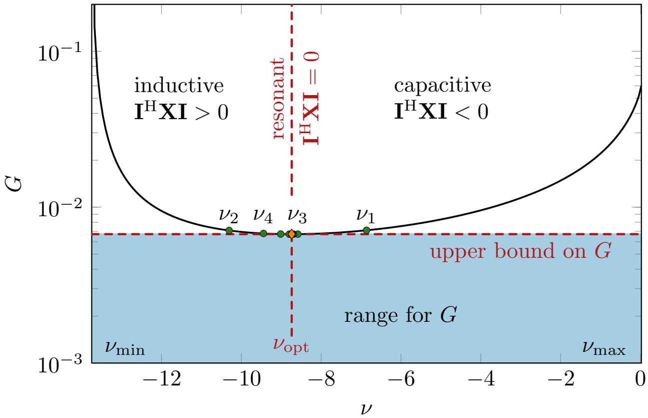
$$\begin{aligned} &\text{maximize} && \mathbf{I}^{\mathsf{H}}\mathbf{U}\mathbf{I} \\ &\text{subject to} && \mathbf{I}^{\mathsf{H}}(\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega}+\nu\mathbf{X})\mathbf{I}=1 \end{aligned} \qquad \text{(S')}$$

which has the same form as (T) and is hence solved by

$$G = 4\pi\text{minimize}_{\nu}\max\operatorname{eig}(\mathbf{U},\mathbf{R}_{\mathrm{r}}+\mathbf{R}_{\Omega}+\nu\mathbf{X})$$

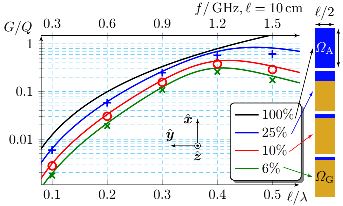
Computation of $\max G = \min_\nu \max \operatorname{eig}(\mathbf{R}_\mathrm{r} + \mathbf{R}_\Omega + \nu\mathbf{X}, \mathbf{U})$

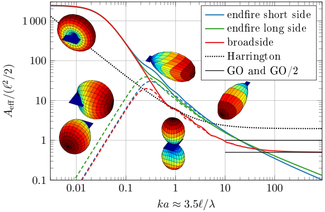
- $\nu\mathbf{X} + \mathbf{R}_\Omega + \mathbf{R}_\mathrm{r} \succeq \mathbf{0}$ is an eigenvalue problem to determine the range for $\nu_{\min} \leq \nu \leq \nu_{\max}$.
- Minimize over $[\nu_{\min}, \nu_{\max}]$ (Newton, bisection,..)
- Self resonant for $\nu = \nu_{\mathrm{opt}}$.
- ν_n valuation points using the bisection rule.
- Special treatment for degenerate cases.

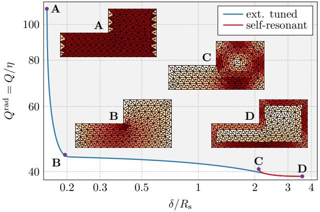


Constructs a self-resonant current with $G = G_{\mathrm{ub}}$ such that the duality gap is zero.

Physical bounds on antennas based on (convex) optimization







Gain, Q-factor, and efficiency problems are formulated as quadratically constrained quadratic programs (QCQP) and solved with the same (simple) algorithm, *e.g.*,

$$G: \ \min.\max\operatorname{eig}(\mathbf{F}^{\mathsf{H}}(\nu\mathbf{X} + \mathbf{R}_{\mathrm{r}} + \mathbf{R}_{\Omega})^{-1}\mathbf{F})$$

$$G/Q: \ \min.\max\operatorname{eig}(\mathbf{F}^{\mathsf{H}}(\nu\mathbf{X} + \mathbf{X}_{\mathrm{w}})^{-1}\mathbf{F})$$

$$Q^{\mathrm{rad}}: \ \min.\max\operatorname{eig}(\mathbf{S}(\nu\mathbf{X} + \mathbf{X}_{\mathrm{w}})^{-1}\mathbf{S}^{\mathsf{H}})$$

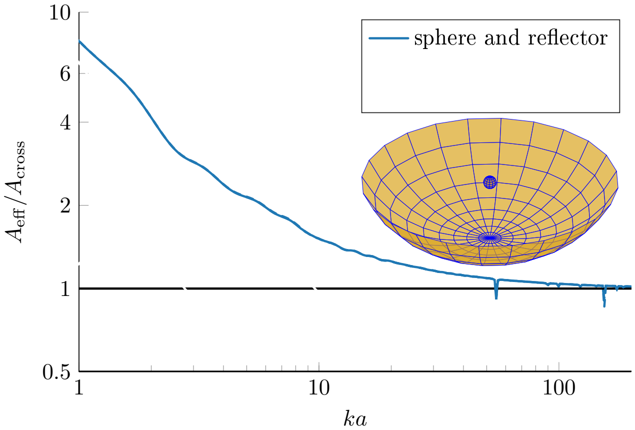
$$\delta = P_{\Omega}/P_{\mathrm{r}}: \ \min.\max\operatorname{eig}(\mathbf{S}(\nu\mathbf{X} + \mathbf{R}_{\Omega})^{-1}\mathbf{S}^{\mathsf{H}})$$

$$Q^{\mathrm{rad}} \text{ vs } \delta: \ \min.\max\operatorname{eig}(\mathbf{S}(\nu\mathbf{X} + \alpha\mathbf{X}_{\mathrm{w}} + \mathbf{R}_{\Omega})^{-1}\mathbf{S}^{\mathsf{H}})$$

$\mathbf{X}, \mathbf{X}_{\mathrm{w}}, \mathbf{R}_{\mathrm{r}}, \mathbf{R}_{\Omega}, \mathbf{F}$: MoM matrices determined for a design region Ω and used materials.

Maximum gain and effective area: parabola with sphere

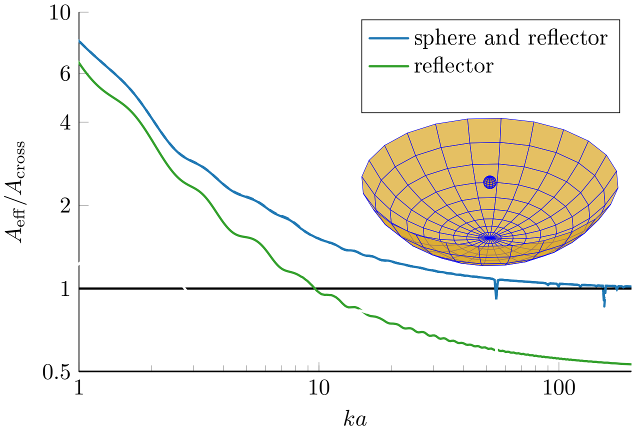
- Maximum effective area for a parabolic reflector (radius a, focal distance $a/2$, and depth $a/2$) with a sphere (radius $a/20$) having surface resistivity $R_s = 10^{-2}\,\Omega/\Box$
- Optimal currents on reflector and sphere
- Internal resonances of the sphere



From [GC19].

Maximum gain and effective area: parabola with sphere

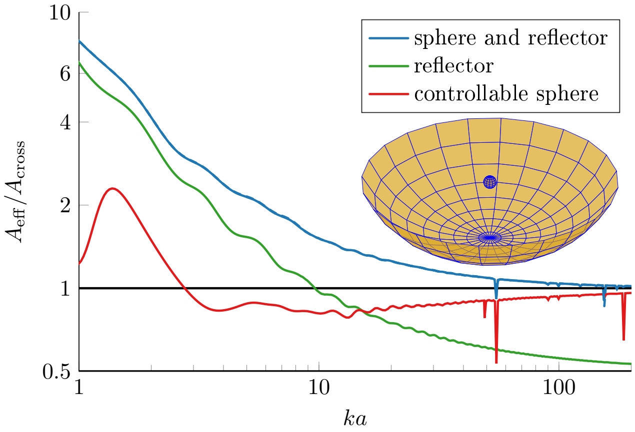
- Maximum effective area for a parabolic reflector (radius a, focal distance $a/2$, and depth $a/2$) with a sphere (radius $a/20$) having surface resistivity $R_s = 10^{-2}\,\Omega/\square$
- Optimal currents on reflector and sphere
- Internal resonances of the sphere
- Optimal currents on reflector



From [GC19].

Maximum gain and effective area: parabola with sphere

- Maximum effective area for a parabolic reflector (radius a, focal distance $a/2$, and depth $a/2$) with a sphere (radius $a/20$) having surface resistivity $R_s = 10^{-2}\,\Omega/\Box$
- Optimal currents on reflector and sphere
- Internal resonances of the sphere
- Optimal currents on reflector
- Optimal currents on sphere and induced currents on reflector



From [GC19].

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

Optimization (power) bounds

- Physical modelling (integral equations (MoM))
- Optimization problems over sources
- Pointwise bounds from the solution (convex dual) of the optimization problem

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

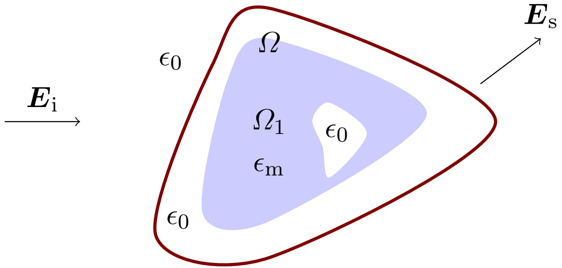
- ☺ Simple closed form expressions
- ☺ Based on an identity
- ☹ Not pointwise (moments)
- ☹ Hard to add (include) information

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

- ☺ Pointwise bounds
- ☺ Easy to add (include) information
- ☹ Bandwidth (Q-factor for small ☺)
- ☹ Numerical solution (some explicit ☺)

Sum rule (Herglotz) and current optimization for σ_t

Bounds on the extinctions cross section $\sigma_\mathrm{t} = \sigma_\mathrm{a} + \sigma_\mathrm{s}$ for linear, passive, time-invariant, non-magnetic object with support in the region $\Omega_1 \subset \Omega$.

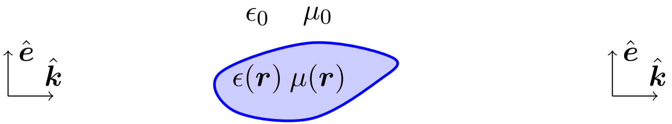


Can consider different amount of information

1. region Ω
2. region Ω and losses $\rho_\mathrm{r} = \frac{-\eta_0 \operatorname{Im} \chi}{k|\chi|^2}$ in Ω_1
3. region Ω and permittivity $\epsilon = \epsilon_0(1+\chi)$ in Ω_1

Note can easy generalize to $\epsilon(\boldsymbol{r})$, anisotropic, and magnetic cases.

Forward scattering sum rule: assumptions



Assumptions:

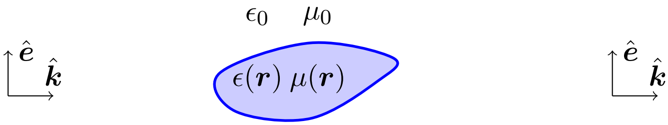
- Finite scattering object composed of a linear, passive, and time translational invariant materials.
- Incident linearly polarized plane wave.

From physics:

- The propagation speed is limited by the speed of light.
- Optical theorem (energy conservation).
- Induced dipole moment in the static limit.

Passive system with $h(k) \sim \gamma k$ as $k\to 0$ and $\sigma_{\text{ext}} = \operatorname{Im} h$.

Forward scattering sum rule



Use the $n = 1$ identity with $a_1 = \gamma = \hat{\boldsymbol{e}} \cdot \boldsymbol{\gamma}_{\mathrm{e}} \cdot \hat{\boldsymbol{e}} + (\hat{\boldsymbol{k}} \times \hat{\boldsymbol{e}}) \cdot \boldsymbol{\gamma}_{\mathrm{m}} \cdot (\hat{\boldsymbol{k}} \times \hat{\boldsymbol{e}})$ and $b_1 = 0$, *i.e.*,

$$\frac{2}{\pi} \int_0^\infty \frac{\sigma_{\mathrm{ext}}(k)}{k^2} \,\mathrm{d}k = \hat{\boldsymbol{e}} \cdot \boldsymbol{\gamma}_{\mathrm{e}} \cdot \hat{\boldsymbol{e}} + (\hat{\boldsymbol{k}} \times \hat{\boldsymbol{e}}) \cdot \boldsymbol{\gamma}_{\mathrm{m}} \cdot (\hat{\boldsymbol{k}} \times \hat{\boldsymbol{e}})$$

or written in the free-space wavelength $\lambda = 2\pi/k$

$$\frac{1}{\pi^2} \int_0^\infty \sigma_{\mathrm{ext}}(\lambda) \,\mathrm{d}\lambda = \hat{\boldsymbol{e}} \cdot \boldsymbol{\gamma}_{\mathrm{e}} \cdot \hat{\boldsymbol{e}} + (\hat{\boldsymbol{k}} \times \hat{\boldsymbol{e}}) \cdot \boldsymbol{\gamma}_{\mathrm{m}} \cdot (\hat{\boldsymbol{k}} \times \hat{\boldsymbol{e}})$$

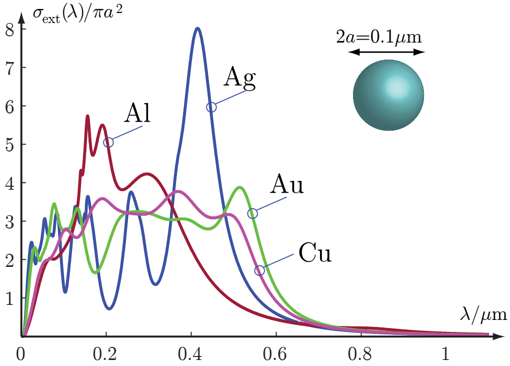
Bounds on $\sigma_{\mathrm{t}} = \sigma_{\mathrm{ext}}$ (solely) based on Ω

Forward scattering forms a passive system with the sum rule [SGK07]

$$\frac{1}{\pi^2}\int_0^{\infty} \sigma_{\mathrm{t}}(\lambda)\,\mathrm{d}\lambda = \hat{\boldsymbol{e}}\cdot\boldsymbol{\gamma}_{\mathrm{e}}\cdot\hat{\boldsymbol{e}} \leq \hat{\boldsymbol{e}}\cdot\boldsymbol{\gamma}_{\infty}\cdot\hat{\boldsymbol{e}}$$

where γ_{e} and γ_{∞} are the (static) polarizability dyadic of the object and high contrast polarizability dyadic of the region Ω, respectively.

An identity showing that the area under the curve $\sigma_{\mathrm{t}}(\lambda)$ is given by the polarizability (many good properties, analytic expressions, and easily computable), here $4\pi a^3$.



Same area but different peak values [Gus10b]. No sum rule bound on the peak value. Theoretical constructions have $\sigma_{\mathrm{t}} \to \infty$, *cf.*, superdirectivity.

Bounds on $\sigma_t = \sigma_{ext}$ (solely) based on Ω

Forward scattering forms a passive system with the sum rule [SGK07]

$$\frac{1}{\pi^2}\int_0^{\infty} \sigma_t(\lambda)\,d\lambda = \hat{\boldsymbol{e}}\cdot\boldsymbol{\gamma}_e\cdot\hat{\boldsymbol{e}} \leq \hat{\boldsymbol{e}}\cdot\boldsymbol{\gamma}_\infty\cdot\hat{\boldsymbol{e}}$$

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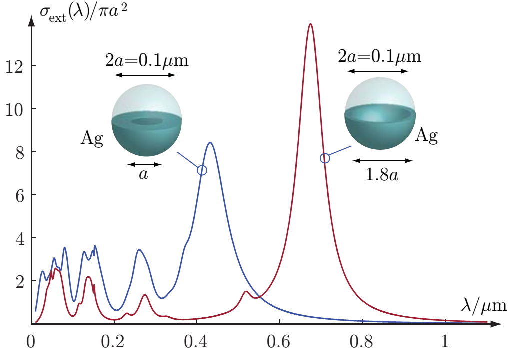


Same area but different peak values [Gus10b]. No sum rule bound on the peak value. Theoretical constructions have $\sigma_t \to \infty$, *cf.*, superdirectivity.

Extinction cross section σ_t for Au (circumscribing) spheres

Use dual form of the QCLP (QCQP for $\sigma_\mathrm{a}, \sigma_\mathrm{s}$)

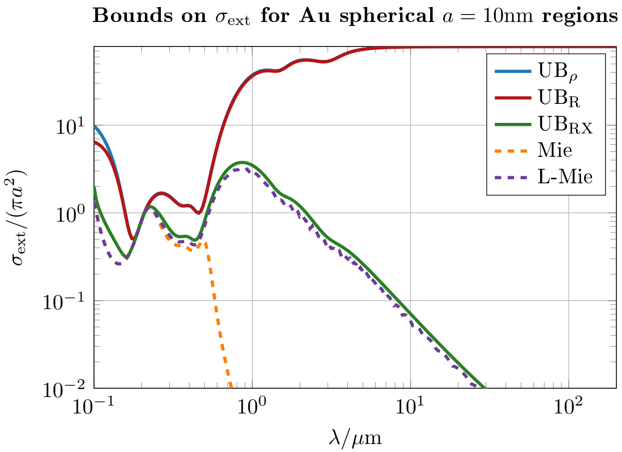
$$\begin{aligned} \text{maximize} \quad & \mathrm{Re}\{\mathbf{V}^\mathsf{H}\mathbf{I}\} \\ \text{subject to} \quad & \mathrm{Re}\{\mathbf{V}^\mathsf{H}\mathbf{I}\} - \mathbf{I}^\mathsf{H}\mathbf{R}\mathbf{I} = 0 \\ & \mathrm{Im}\{\mathbf{V}^\mathsf{H}\mathbf{I}\} - \mathbf{I}^\mathsf{H}\mathbf{X}\mathbf{I} = 0 \end{aligned}$$

Bounds based on

- Blue: Volume and ρ_r
- Red: Shape and ρ_r
- Green: Shape, ρ_r, and ρ_i

The bounds are compared with

- Yellow: Solid sphere
- Purple: Optimized layered sphere



Extinction cross section σ_t for Au (circumscribing) spheres

Use dual form of the QCLP (QCQP for σ_a, σ_s)

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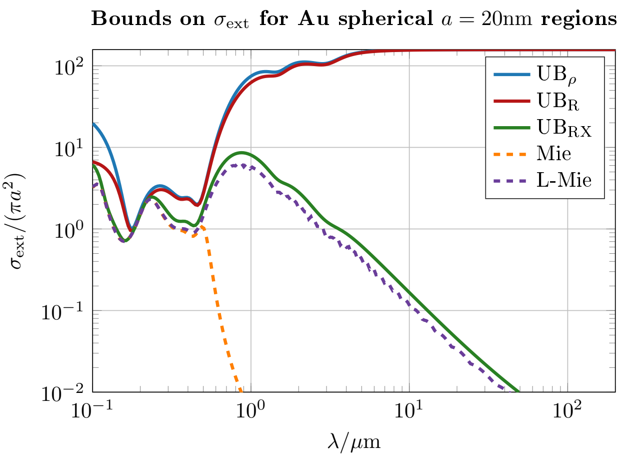

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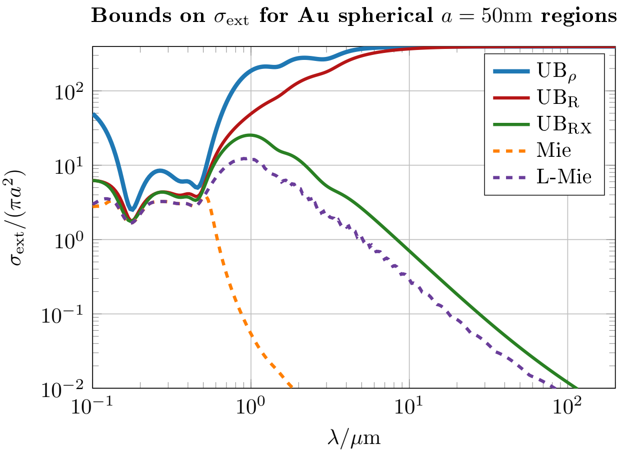

Extinction cross section σ_t for Au (circumscribing) spheres

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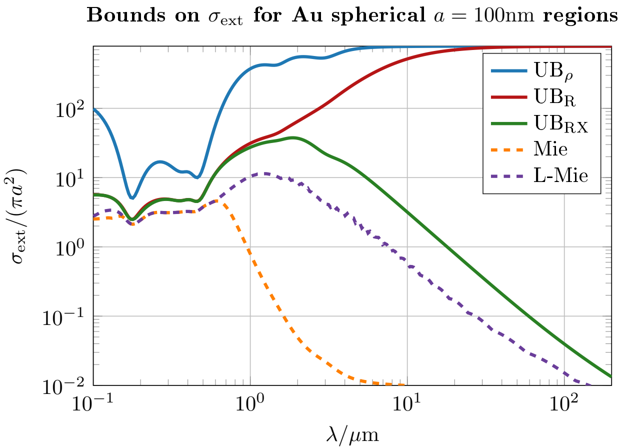
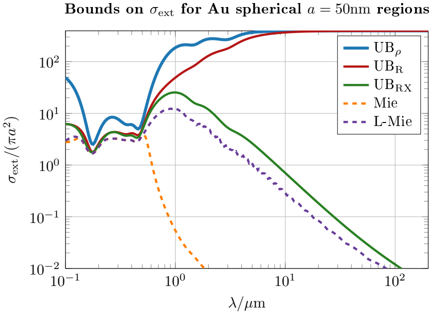
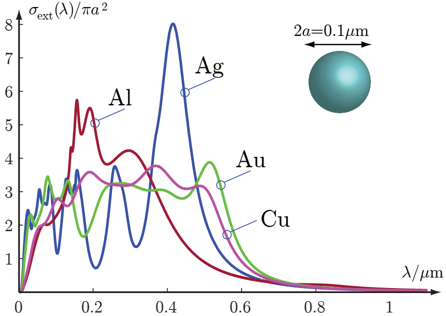


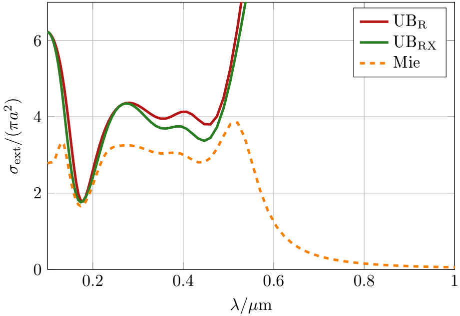
Can we combine them?

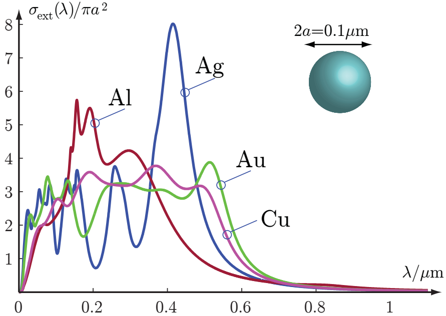




- Area from sum rule and maximum value from optimization.
- Single resonance model (Lorentzian) for bandwidth.
- Sum rule for a product gh, where g is real valued at the frequency axis and has simple poles in the upper complex half plane, *cf.*, [Shi+19].
- Optimization approaches.

Can we combine them?

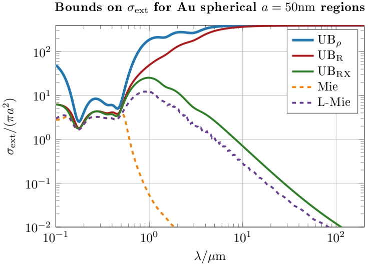


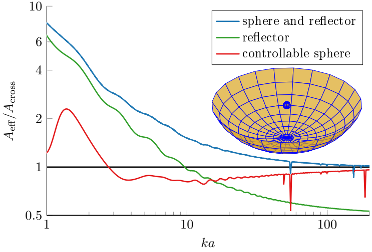


- Area from sum rule and maximum value from optimization.
- Single resonance model (Lorentzian) for bandwidth.
- Sum rule for a product gh, where g is real valued at the frequency axis and has simple poles in the upper complex half plane, *cf.*, [Shi+19].
- Optimization approaches.

Conclusions

- Passive systems and HN functions
  - Sum rules
  - Bounds for weighted averages
  - Closed for expressions
  - Hard to add information
- Optimization problems
  - Very general and easy to add information
  - Solution from dual form
  - Pointwise bounds





Work in progress

- Combinations between the two approaches
- Generalization from passive to causal and active

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