Non-selfadjoint operator functions and applications to plasmonics

Christian Engström

Umeå University, Sweden

christian.engstrom@math.umu.se

Joint work with Axel Torshage

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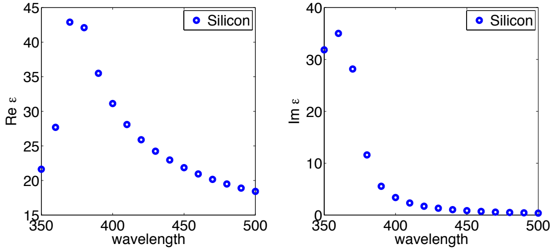
Outline

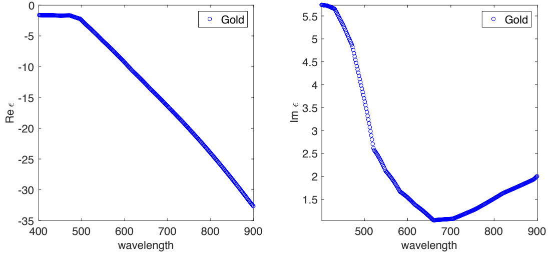
1. The Drude-Lorentz model
2. Operator functions whose values are a Maxwell operator
3. Enclosures for the spectrum and the numerical range
4. Properties of the first and second order formulations of the Maxwell operator function

Dielectric and metallic materials characterized by ϵ

Dielectric materials: Re $\epsilon \geqslant 1$



Metallic materials: Re $\epsilon < 0$



- $\omega = 2\pi v/s$, v- speed of light, s - wavelength [nm], ω frequency

Metal-dielectric structures

Define for $x \in \Omega := \Omega_1 \cup \Omega_2$ the Drude-Lorentz model

$$\epsilon(x,\omega) := \chi_{\Omega_1}(x) + \epsilon_2(\omega)\chi_{\Omega_2}(x), \quad \epsilon_2(\omega) := 1 + \frac{b}{c - \omega^2 - id\omega},$$

$\omega \in \mathcal{D} := \{\omega \in \mathbb{C} : \omega \neq -id/2 \pm \theta\}$, $\theta = \sqrt{c - \frac{d^2}{4}}$

Surface plasmons are waves that travel along a metal-dielectric interface

- Metall: $c = 0$ ($c < d^2/4$)
- Dielectric materials: $c > d^2/4$ (Air (vacuum): $\epsilon = 1$)

Related works:

- $\epsilon_2 = -1$, A.-S Bonnet-Ben Dhia/L. Chesnel/P. Ciarlet, Jr. ...
- $d = 0$, E./H. Langer/C. Tretter, M. Cassier, C. Hazard, P. Joly ...

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Operator functions whose values are a Maxwell operator

Define for $\omega \in \mathcal{D}$ the Maxwell operator $\mathcal{A}(\omega) : L^2(\Omega)^6 \to L^2(\Omega)^6$,

$$\mathcal{A}(\cdot) := \mathcal{M} - \mathcal{F}(\cdot, x),$$

$$\mathcal{M} := \begin{pmatrix} 0 & -i\text{curl} \\ i\text{curl} & 0 \end{pmatrix}, \quad \mathcal{F}(\omega, x) = \begin{pmatrix} \omega\epsilon(x,\omega) & 0 \\ 0 & \omega \end{pmatrix}.$$

The domain of $\mathcal{A}(\cdot)$ is chosen such that $\mathcal{M}$ is self-adjoint.

1. Can we use a linearization to determine an enclosure of

$$\sigma(\mathcal{A}) := \{\omega \in \mathcal{D} \,:\, 0 \in \sigma(\mathcal{A}(\omega))\} \text{ ?}$$

2. Can we derive an enclosure of the numerical range of $\mathcal{A}$?

Metal-air structures

$$\epsilon(x,\omega) := \chi_{\Omega_1}(x) + \epsilon_2(\omega)\chi_{\Omega_2}(x), \quad \epsilon_2(\omega) := 1 + \frac{b}{-\omega^2 - id\omega},$$

Let $\hat{\mathcal{H}} := \operatorname{ran}\chi_{\Omega_2}$, where $\chi_{\Omega_2} : L^2(\Omega)^3 \to L^2(\Omega)^3$ and define

$$V^* : L^2(\Omega)^3 \to \hat{\mathcal{H}} \text{ such that } VV^* = \chi_{\Omega_2}, \; V^*V = I_{\hat{\mathcal{H}}}.$$

Then

$$-\omega\epsilon(x,\omega) = A(\omega) - BD^{-1}(\omega)B^* =: R$$

where

$$A(\omega) := -\omega, \quad B = \sqrt{b}V, \quad D(\omega) = -id - \omega$$

Equivalence and linearization

The following (well known) equivalence for $R = A - BD^{-1}C$ is called an equivalence after $D(\omega)$-extension:

$$\begin{bmatrix} R & 0 \\ 0 & D \end{bmatrix} = \begin{bmatrix} I & -BD^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} I & 0 \\ -D^{-1}C & I \end{bmatrix}$$

Let

$$\begin{bmatrix} R & X \\ Y & Z \end{bmatrix} = \mathcal{M} - \mathcal{F}(\cdot, x) = \begin{bmatrix} -\omega\epsilon(x,\omega) & -i\text{curl} \\ i\text{curl} & -\omega \end{bmatrix}$$

This operator is after $D(\cdot)$-extension equivalent to

$$\mathcal{T}(\omega) := \begin{bmatrix} A & B & X \\ B^* & D & 0 \\ Y & 0 & Z \end{bmatrix} = \begin{bmatrix} -\omega & B & -i\text{curl} \\ B^* & D(\omega) & 0 \\ i\text{curl} & 0 & -\omega \end{bmatrix}$$

See Theorem 3.4 in E./Torshage (2016), arXiv:1612.01373

Perturbations of self-adjoint operators

$$\mathcal{T}(\omega) = \begin{bmatrix} 0 & B & -i\,\mathrm{curl} \\ B^* & 0 & 0 \\ i\,\mathrm{curl} & 0 & 0 \end{bmatrix} - id - \omega = \mathcal{T}_0 + i\mathcal{T}_p - \omega$$

where $\mathcal{T}_0$ is self-adjoint and $\mathcal{T}_p$ is bounded.

Theorem (Kato 1980, Cuenin & Tretter 2016)

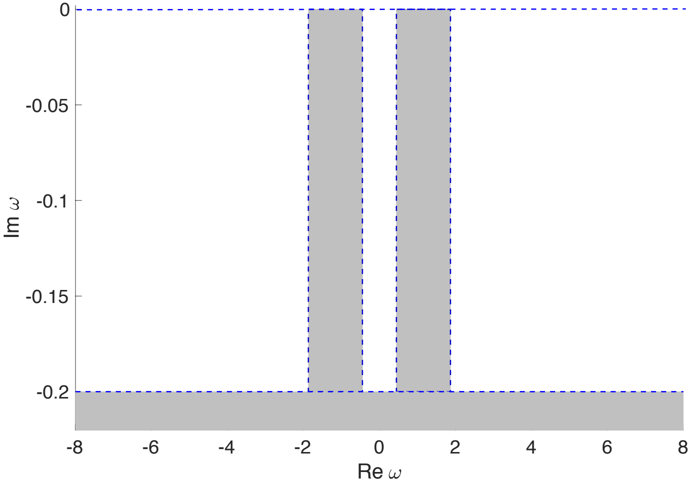
1. $\sigma(\mathcal{T}_0 + i\mathcal{T}_p) \subset \{z \in \mathbb{C} \,:\, -d \leqslant \operatorname{Im} z \leqslant 0\}$
2. *Assume*

$$\sigma(\mathcal{T}_0) \cap (0, \omega_1) = \varnothing, \quad 2d < \omega_1$$

$\Rightarrow$

$$\sigma(\mathcal{T}_0 + i\mathcal{T}_p) \cap \{z \in \mathbb{C} \,:\, d < \operatorname{Re} z < \omega_1 - d\} = \varnothing$$

Example: Perturbations of self-adjoint operators



- Enclosures under the condition $\sigma(\mathcal{T}_0) \cap (0, \omega_1) = \emptyset, \quad 2d < \omega_1$
- Can we improve these enclosures for our special structure?

The numerical range W

The non-self-adjoint operator:

- The numerical range $W(\mathcal{T}_0 + i\mathcal{T}_p) = \{((\mathcal{T}_0 + i\mathcal{T}_p)u, u) : \, u \in \operatorname{dom} \mathcal{T}_0, \|u\| = 1\}$
- $\sigma(\mathcal{T}_0 + i\mathcal{T}_p) \subset \overline{W(\mathcal{T}_0 + i\mathcal{T}_p)}$ - convex and very large for our case

Non-self-adjoint operator functions:

- The numerical range: $W(T) = \{\omega \in \mathcal{D} : \, \exists u \in \operatorname{dom} T \backslash \{0\}, \|u\| = 1, \text{so that} \, (T(\omega)u, u) = 0\}$
- $\sigma(T) \subset \overline{W(T)}$ (under some conditions)
- $W(T)$ - not convex, not connected

Consider operator functions in the form

$$T(\omega) = f_0(\omega) + A_1 f_1(\omega) + A_2 f_2(\omega), \quad \omega \in \mathcal{D}$$

where f_ℓ are given complex functions and A_ℓ, $\ell = 1, 2$ are self-adjoint

Definition of the enclosure (E./Torshage (2017))

Consider the solutions of $f(\omega) := f_0(\omega) + \alpha_1 f_1(\omega) + \alpha_2 f_2(\omega) = 0$:

- Numerical range $W(T)$: Take

$$\alpha_\ell = (A_\ell u, u) \quad \text{for } u \in \mathrm{dom}\, T\backslash\{0\}, \|u\| = 1.$$

  Then $f(\omega) = (T(\omega)u, u)$.

- Enclosure for $W(T)$: Take **any**

$$(\alpha_1, \alpha_2) \in \Gamma := \overline{W(A_1)} \times \overline{W(A_2)}.$$

Define the enclosure for $\overline{W(T)}$ as

$$W_\Gamma(T) := \{\omega \in \mathcal{D} : f_0(\omega) + \alpha_1 f_1(\omega) + \alpha_2 f_2(\omega) = 0 \text{ for some } (\alpha_1, \alpha_2) \in \Gamma\}$$

The enclosure $W_\Gamma(\mathcal{A})$

$$\mathcal{A}(\omega) = \mathcal{M} - \omega - \frac{\omega b}{-\omega^2 - id\omega}\mathcal{G}$$

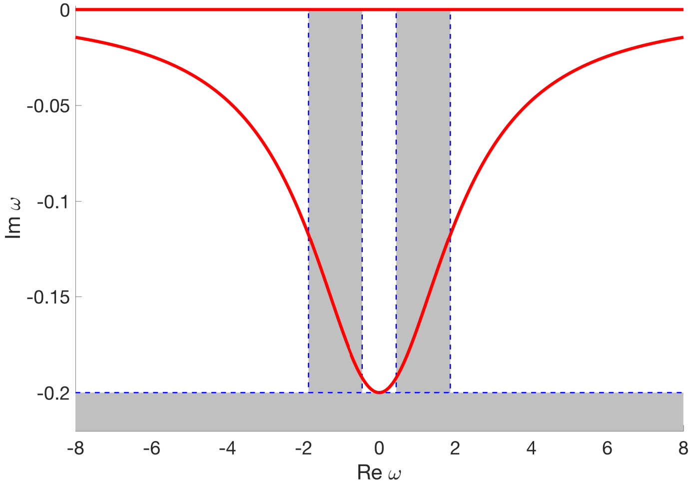
$$\mathcal{M} = \begin{pmatrix} 0 & -i\mathrm{curl} \\ i\mathrm{curl} & 0 \end{pmatrix}, \quad \mathcal{G} = \begin{pmatrix} \chi_{\Omega_2} & 0 \\ 0 & 0 \end{pmatrix}.$$

Take

- $\Gamma = \overline{W(\mathcal{M})} \times \overline{W(\mathcal{G})}$
- $W(\mathcal{M}) = (-\infty, \infty)$, $W(\mathcal{G}) = [0, 1]$

- The enclosure is minimal given only $W(\mathcal{M})$, $W(\mathcal{G})$
- See E./Torshage (2017)

Linearization vs the enclosure $W_\Gamma(\mathcal{A})$



- Can we improve these enclosures using a different formulation?

Second order formulation

The operator function $\mathcal{A}(\cdot)$ is applied to $(E, H)^t \in \operatorname{dom} \mathcal{M} \subset L^2(\Omega)^6$, where

- E is the electric field
- H is the magnetic field

The spectral problem can also be written in terms of the electric field. Let $\hat{\mathcal{A}}(\omega) : L^2(\Omega)^3 \to L^2(\Omega)^3$,

$$\hat{\mathcal{A}}(\omega) := \hat{\mathcal{M}} - \omega^2 \epsilon(x, \omega), \quad \hat{\mathcal{M}} := \operatorname{curl} \operatorname{curl}$$

- Assume $\hat{\mathcal{M}}$ self-adjoint and $\hat{\mathcal{M}} \geqslant \alpha$

Self-adjointness and spectral gaps

$$\epsilon(x,\omega) := \chi_{\Omega_1}(x) + \epsilon_2(\omega)\chi_{\Omega_2}(x), \quad \epsilon_2(\omega) := 1 + \frac{b}{c - \omega^2 - id\omega},$$

Case $c = 0$:

✓ $\hat{\mathcal{M}} \geqslant \alpha > 0 \Rightarrow \sigma(\mathcal{T}_0) \cap (0, \omega_1) = \emptyset$

Case $c \geqslant 0$:

- Linearization of $\hat{\mathcal{A}}$ gives an operator that is a bounded perturbation of an operator that is self-adjoint in a Krein space
- We will under some conditions have $\sigma(\mathcal{T}_0) \cap (\omega_0, \omega_1) = \emptyset$ (Adamjan/Langer/Mennicken/Saurer (1996))
- See E./Langer/Tretter (2017) for more on spectral gaps for the case $d = 0$

First order $\mathcal{A}(\cdot)$ vs second order $\hat{\mathcal{A}}(\cdot)$ formulation

Define for

$$\epsilon(x,\omega) := \chi_{\Omega_1}(x) + \epsilon_2(\omega)\chi_{\Omega_2}(x), \quad \epsilon_2(\omega) := 1 + \frac{b}{c - \omega^2 - id\omega}.$$

the operator functions

$$\mathcal{A}(\omega) = \mathcal{M} - \omega - \frac{\omega b}{c - \omega^2 - id\omega}\mathcal{G},\ \hat{\mathcal{A}}(\omega) = \hat{\mathcal{M}} - \omega^2 - \frac{\omega^2 b}{c - \omega^2 - id\omega}\hat{\mathcal{G}}$$

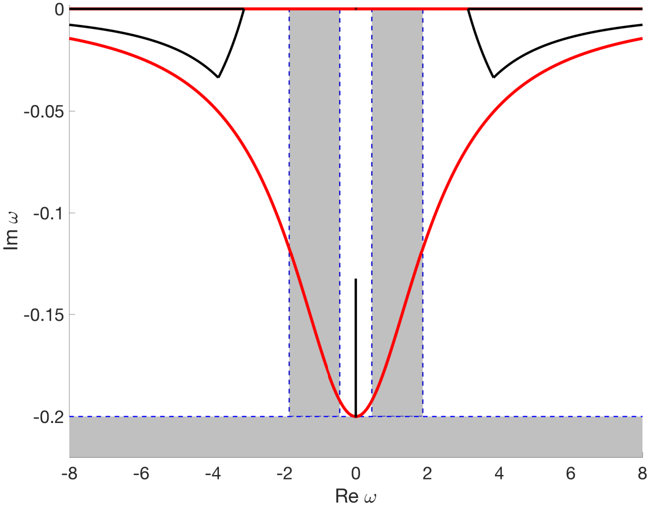
where $W(\mathcal{M}) = (-\infty,\infty)$, $W(\hat{\mathcal{M}}) = [0,\infty)$ and $W(\mathcal{G}) = W(\hat{\mathcal{G}}) = [0,1]$.

Define the sets $\Gamma_1 = \overline{W(\mathcal{M})} \times \overline{W(G)}$ and $\Gamma_2 = \overline{W(\hat{\mathcal{M}})} \times \overline{W(\hat{G})}$ then

$$W_{\Gamma_1}(\mathcal{A}) \supset W_{\Gamma_2}(\hat{\mathcal{A}}).$$

Proof: Based on conditions for $\omega \in W_{\Gamma_2}(\hat{\mathcal{A}})$ in E./Torshage (2017)

Linearization vs first order vs second order formulation



Examples for dielectric materials: $c > d^2/4$

- I will approximate the spectrum of $\mathcal{T}_0$ with FEM for the TM case: $(E, H) = (0, 0, E_3, H_1, H_2, 0)$

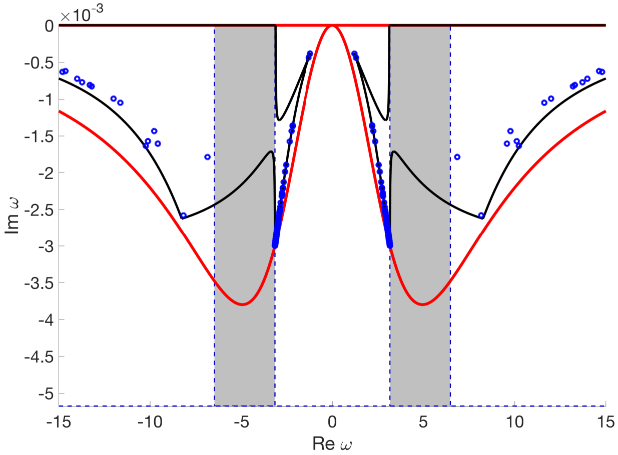
$$\Rightarrow \sigma(\mathcal{T}_0) \cap (\omega_0, \omega_1) = \emptyset \text{ (finite dimensional case)}$$

- We can then use the bounds on $\mathcal{T}_0 + i\mathcal{T}_p$ from Cuenin & Tretter (2016) for the TM case

- I will show the exact enclosures $W_{\Gamma_1}(\mathcal{A})$ and $W_{\Gamma_2}(\hat{\mathcal{A}})$

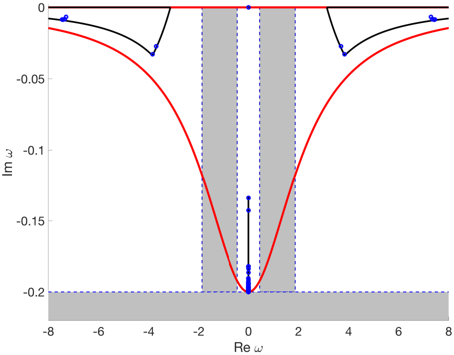
- I will approximate the spectrum of $\mathcal{T}_0 + i\mathcal{T}_p$ with FEM for the TM case

Enclosures for the case $b = 50$, $c = 10$, $d = 0.006$



- FEM eigenvalues for a photonic crystal application

Accumulation of eigenvalues to the poles?



- Linearization: $i\mathcal{T}_p$ is not a relatively compact perturbation of $\mathcal{T}_0$
- Approach based on theory for bounded operator polynomials gives interesting results!

Talk on accumulation: Thursday at 09:45 by Axel Torshage

References

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