Complex-scaling method for the complex plasmonic resonances of particles with corners

Singular Days, Nice 3rd November 2022

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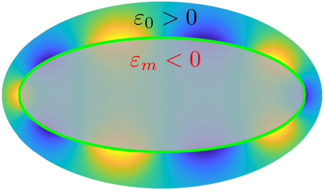
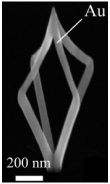
Motivation & objective

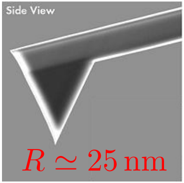
Motivation: Light concentration using “surface plasmons”.

Surface plasmon



Photonic devices





(Lalanne et al. 2018) (NanoWorld 2022)

Computational challenges

- **Interface geometry**
- Nonlinear materials

Motivation & objective

Motivation: Light concentration using “surface plasmons”.

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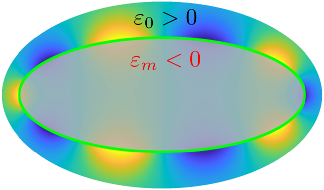

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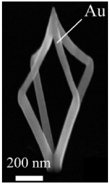

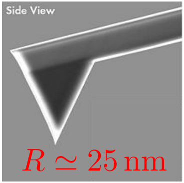

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Computational challenges

- **Interface geometry**
- Nonlinear materials

Objective: Evidence of complex resonances associated with a sign-changing corner.

1 – What are "complex resonances"? (Zworski 2017)

In scattering, complex resonances model **energy leaking at infinity**.

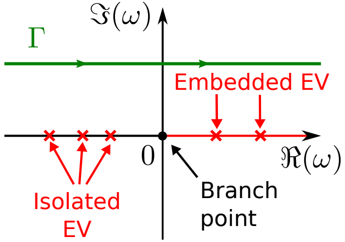
$$i\partial_t \psi(t,\boldsymbol{x}) = H\psi(t,\boldsymbol{x}) + f(\boldsymbol{x}),\ \psi(0,\boldsymbol{x}) = 0 \quad \left(x \in \mathbb{R}^3\right).$$

The wave function is formally given by

$$\psi(t,\boldsymbol{x}) = \frac{1}{2\pi}\int_{\Gamma} R(\omega) f(\boldsymbol{x}) e^{-i\omega t} \mathrm{d}\omega \quad (t > 0)\,,$$

where the outgoing resolvent is $R(\omega) = (H - \omega I)^{-1}$ for $\Im(\omega) > 0$.

$\sigma(H) \neq \sigma_p(H)$, bound states and quasi-normal modes



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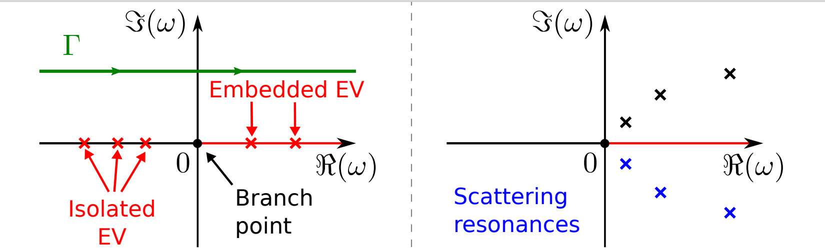


⇒ This work investigates a **plasmonic analogue** of scattering resonances.

2 – Corners as a source of essential spectrum (Bonnet-Ben Dhia et al. 2013)

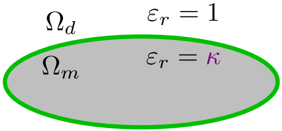
Plasmonic Eigenvalue Problem (PEP)

Find $(u, \kappa) \in H_0^1(\Omega) \times \mathbb{C}$ such that

$$\operatorname{div}\left[\varepsilon_r(\kappa)^{-1}\nabla u\right] = 0$$

with piecewise-constant permittivity:

$$\varepsilon_r(\kappa) = \kappa \mathbb{1}_{\Omega_m} + \mathbb{1}_{\Omega_d}$$



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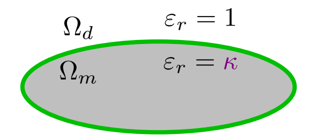

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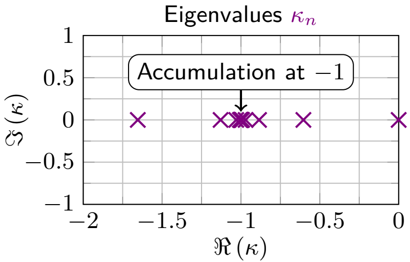
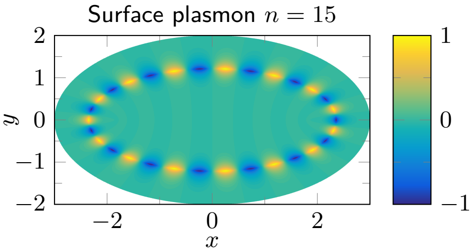
Point spectrum in H^1_{loc}: $\kappa_n < 0$, $\kappa_n \to -1$ (Grieser 2014, Thm. 1).





2 – Corners as a source of essential spectrum (Bonnet-Ben Dhia et al. 2013)

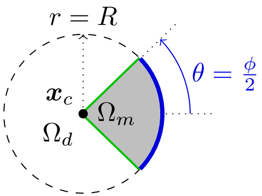
Local problem around corner $\boldsymbol{x_c}$:

$$\mathrm{div}\left[\varepsilon_r(\kappa)^{-1}\nabla u\right] = 0 \qquad (\star).$$

Countable family of solutions:

$$u_\eta(r,\theta) = r^{i\eta} \times \Phi_\eta(\theta) \quad (\eta \in \mathbb{H}(\kappa,\phi)),$$

where $\Phi_\eta \in H^1_{\text{per}}(-\pi,\pi)$.



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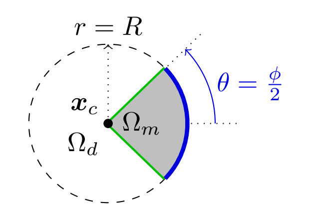
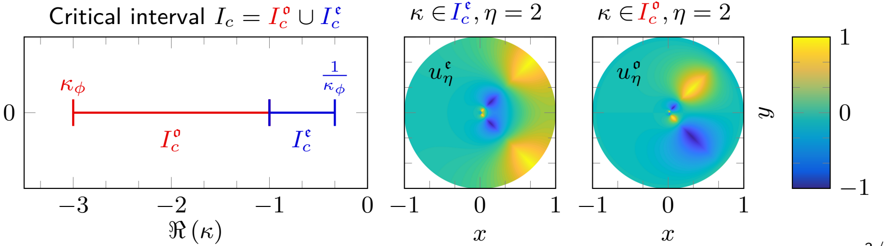


There is a **critical interval** I_c such that

$$\kappa \in I_c \iff \exists\, \eta_{\text{bh}} \in \mathbb{R} : \; u_{\eta_{\text{bh}}} \text{ solves } (\star).$$

⚠ $u_{\eta_{\text{bh}}} \in L^2_{\text{loc}} \backslash H^1_{\text{loc}}$ is a strongly-oscillating "black-hole" wave.

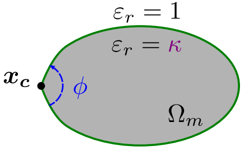


Objectives and outline

Plasmonic Eigenvalue Problem (PEP)

Find $(u, \kappa) \in U \times \mathbb{C}$ such that

$$\operatorname{div}\left[\varepsilon_r(\kappa)^{-1}\nabla u\right] = 0.$$



Objective: Numerical evidence of complex resonances for a piecewise-smooth negative particle.

Outline

2. Definition of complex plasmonic resonances
   What are they?
3. Applicability of corner complex scaling
   How to compute them?
4. Numerical results using corner perturbations
   Does this actually work?

Contents

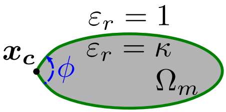
Definition of complex plasmonic resonances

Let $\Omega_m \Subset \Omega \Subset \mathbb{R}^2$, $\partial\Omega_m$ smooth except for one corner.

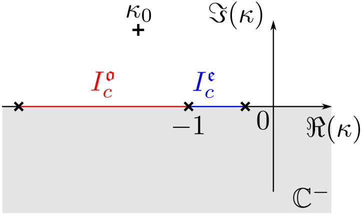
Operators:

$$\mathcal{A}(\kappa)u := \operatorname{div}\left[\varepsilon_r(\kappa)^{-1}\nabla u\right]$$

$$R(\kappa)f := \mathcal{A}(\kappa)^{-1}f$$



- When $\Im(\kappa) > 0$, $R(\kappa) : H^{-1}(\Omega) \to H^1_0(\Omega)$ is bounded.
- ⚠ When $\kappa \to I_c^{\mathfrak{o}} \cup I_c^{\mathfrak{e}}$, $\|R(\kappa)f\|_{H^1(\Omega)} \to \infty$ (Bonnet-Ben Dhia et al. 2013).



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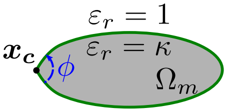

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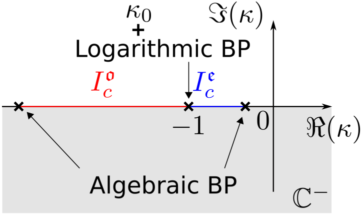
Crossing $\mathbb{R}$ once yields 3 continuations of $\kappa \mapsto R(\kappa)$:



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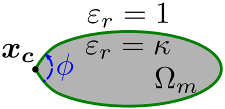

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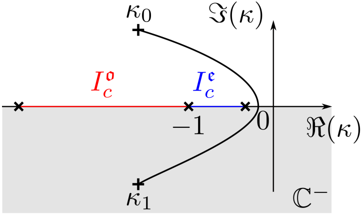

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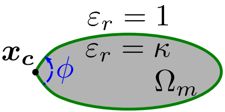

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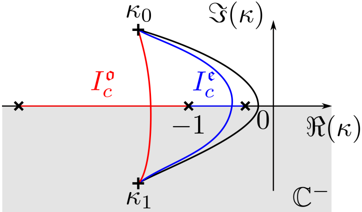

Definition. A *complex plasmonic (CP) resonance* is a pole of $\kappa \to R^{|\mathfrak{e}}(\kappa)$ or $\kappa \to R^{|\mathfrak{o}}(\kappa)$ in $\mathbb{C}^-$.

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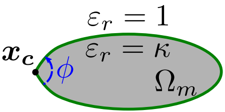

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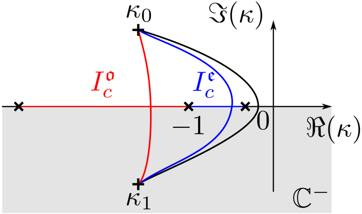

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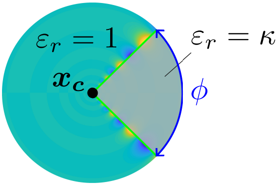
Next: characterization of resonance functions as $\boldsymbol{x} \to \boldsymbol{x_c}$.

Sketch of Mellin analysis (1) (Dauge and Texier 1997)

Local problem for $\kappa \in \mathbb{C}^+$:

$$\operatorname{div}\left[\varepsilon_r(\kappa)^{-1}\nabla u\right] = 0 \quad (\boldsymbol{x} \in D)\,.$$



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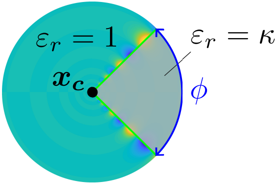

Local problem for $\kappa \in \mathbb{C}^+$:

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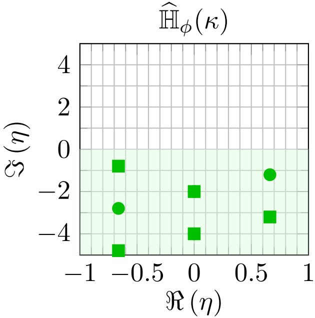
Expansion: If $u \in H^1(D)$ then $\forall \eta_\star < 0$,

$$u \underset{r\to 0}{=} c_0 + \sum_{\substack{\eta \in \widehat{\mathbb{H}}_\phi(\kappa) \\ \Im(\eta) > \eta_\star}} c_\eta\, r^{i\eta}\Phi_\eta(\theta) + \mathcal{O}\left(r^{-\eta_\star}\right)$$

with $\Phi_\eta \in H^1_{\text{per}}(-\pi,\pi)$ and

$$\widehat{\mathbb{H}}_\phi(\kappa) \coloneqq \{\eta \,|\, f_\phi(\eta,\kappa) = 0,\ \Im(\eta) < 0\}\,.$$



Strategy: Characterize resonance functions by studying the continuation to $\mathbb{C}^-$ of the map

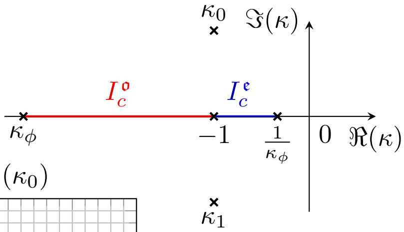
$$\mathbb{C}^+ \ni \kappa \mapsto \widehat{\mathbb{H}}_\phi(\kappa).$$

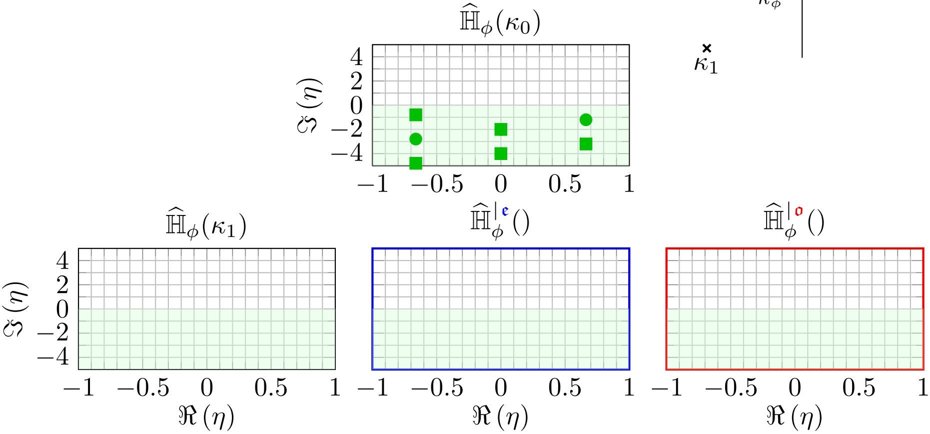
Sketch of Mellin analysis (2)

Let's compare three paths satisfying

$$\Gamma : (0,1) \to \mathbb{C},\ \Gamma(0) = \kappa_0,\ \Gamma(1) = \kappa_1$$

We track $\widehat{\mathbb{H}}_\phi(\kappa)$ as κ moves.





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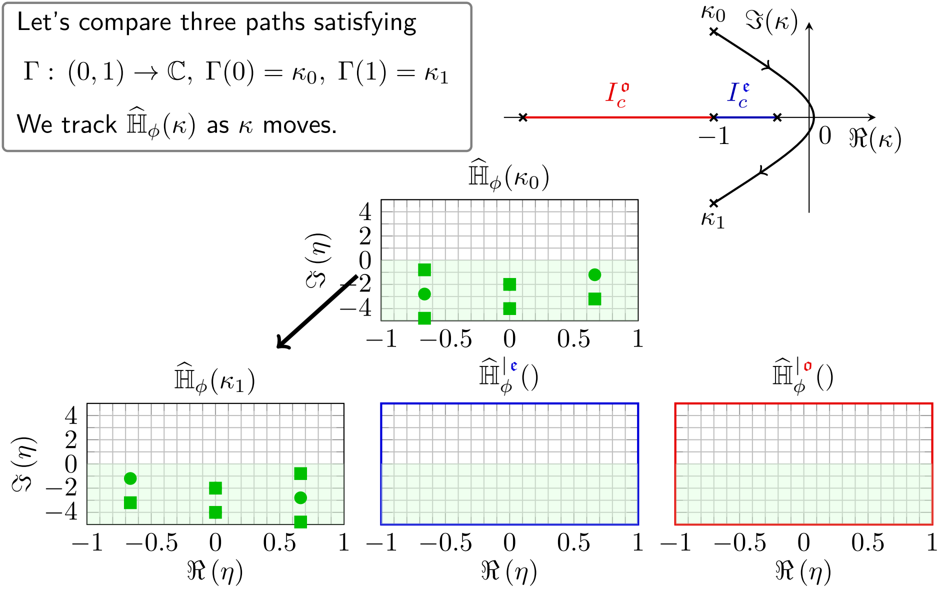

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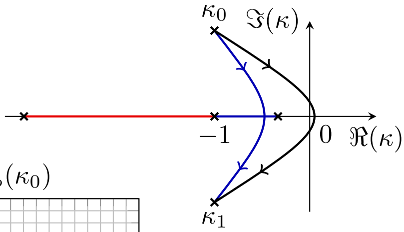

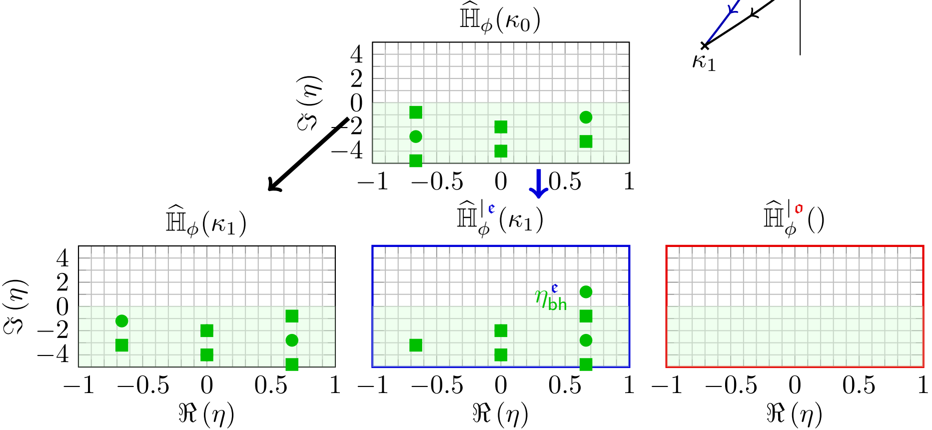

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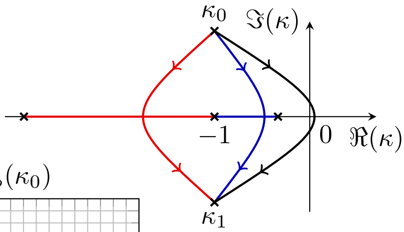
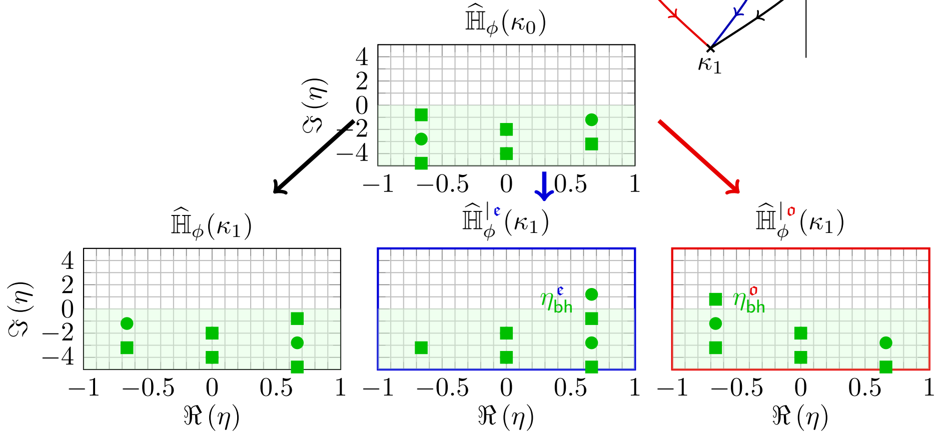
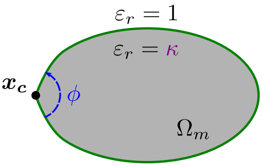


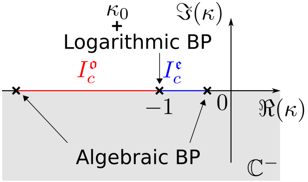


Characterization of resonance functions

Particle:



Spectrum:



Characterization. $\kappa \in \mathbb{C}^-$ is a resonance $\Leftrightarrow \exists u \notin H^1_{\text{loc}}(\Omega)$:

$$\operatorname{div}\left[\varepsilon_r(\kappa)^{-1}\nabla u\right](\boldsymbol{x}) = 0 \quad (\boldsymbol{x} \neq \boldsymbol{x_c}),\ u_{|\partial\Omega} = 0,$$
$$u(r,\theta) \underset{r\to 0}{\sim} c_1\, r^{i\eta_{\text{bh}}}\,\Phi(\theta) + c_0,$$

where $\eta_{\text{bh}} = \eta_{\text{bh}}(\kappa)$ and $\Im(\eta_{\text{bh}}) > 0$.

Next: applicability of corner complex scaling

Contents

Corner complex scaling: formulation

Principle. Let $\alpha \in \mathbb{C}$. Define a non self-adjoint "PEPα" such that:

κ complex resonance of PEP $\Longleftrightarrow$ κ eigenvalue of PEPα .

Intuitively, we would like

$$\text{(PEP)} \qquad u_{\text{res}} \underset{r \to 0}{\sim} e^{i\eta \ln r} \, \Phi_\eta(\theta) + c_0 \qquad (\Im(\eta) > 0)$$

$$\downarrow$$

$$\text{(PEP}\alpha\text{)} \qquad u_{\text{res},\alpha} \underset{r \to 0}{\sim} e^{i \frac{\eta}{\alpha} \ln r} \Phi_\eta(\theta) + c_0 \qquad \left(\Im\left(\frac{\eta}{\alpha}\right) < 0\right)$$

Corner complex scaling: formulation

Principle. Let $\alpha \in \mathbb{C}$. Define a non self-adjoint "PEPα" such that:

$$\kappa \text{ complex resonance of PEP} \iff \kappa \text{ eigenvalue of PEP}\alpha\ .$$

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$$\text{(PEP)} \qquad u_{\text{res}} \underset{r\to 0}{\sim} e^{i\eta \ln r}\, \Phi_\eta(\theta) + c_0 \qquad (\Im(\eta) > 0)$$

$$\downarrow$$

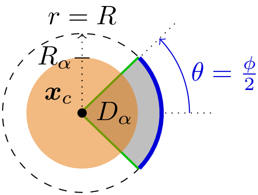
$$\text{(PEP}\alpha\text{)} \quad u_{\text{res},\alpha} \underset{r\to 0}{\sim} e^{i\frac{\eta}{\alpha}\ln r}\, \Phi_\eta(\theta) + c_0 \qquad \left(\Im\left(\frac{\eta}{\alpha}\right) < 0\right)$$

Definition of PEPα. Substitution

$$r\partial_r \to \alpha r \partial_r$$

around the corner.

(Bonnet-Ben Dhia, Carvalho, Chesnel, and Ciarlet 2016)



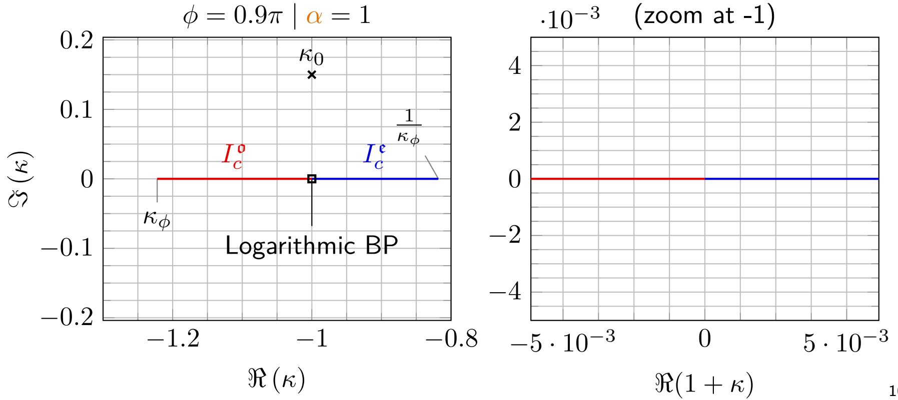
Next: Domain of validity?

Corner complex scaling: uncovered region

Definition of PEPα. Substitution $r\partial_r \to \alpha r\partial_r$ around the corner.
(Bonnet-Ben Dhia, Carvalho, Chesnel, and Ciarlet 2016)

Proposition. Let κ be an eigenvalue of PEPα with $\alpha \in \mathbb{C}\backslash\mathbb{R}$. Then,

$$\kappa \in U_\phi^\alpha \Rightarrow \kappa \text{ is a complex resonance.}$$



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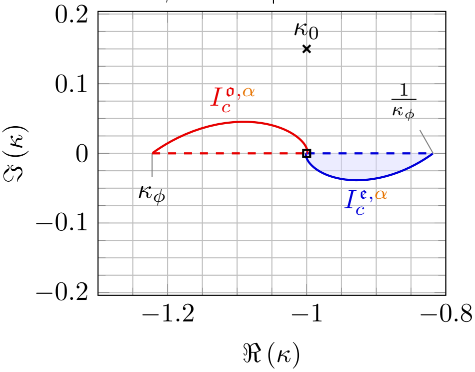
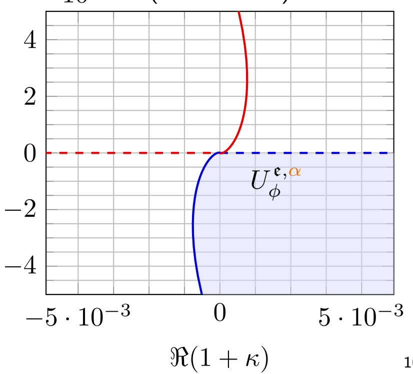
$\phi = 0.9\pi \mid \alpha = e^{i\frac{\pi}{10}}$



$\cdot 10^{-3}$ (zoom at -1)



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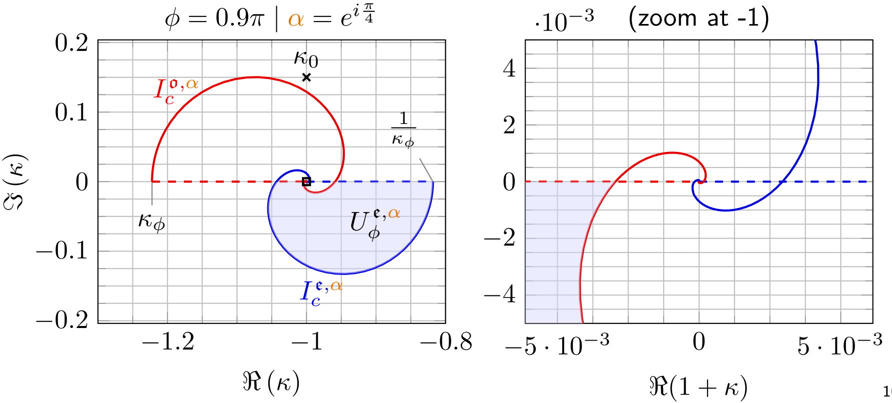
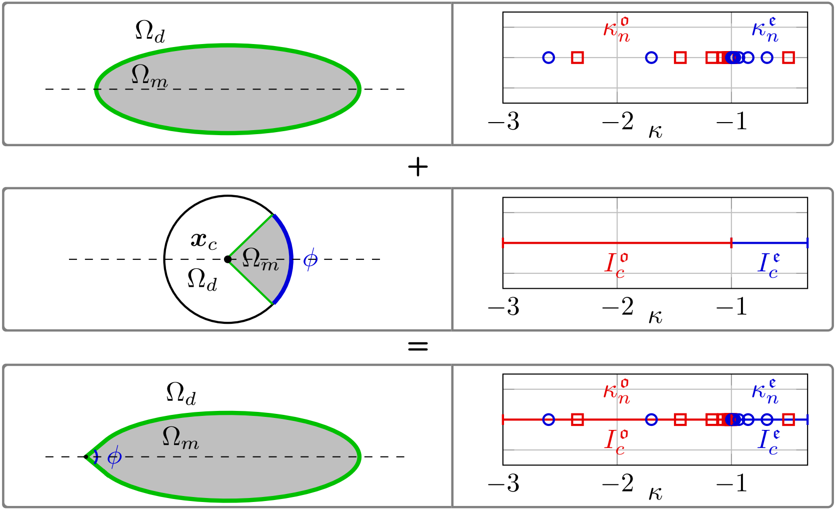


Contents

How to obtain complex resonances?

Perturbation of elliptical Ω_m by corner along major axis.

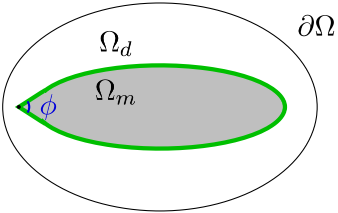
Embedded eigenvalues
→ Existence proof (Li and Shipman 2019, § 5.2)
→ Numerical evidence (Helsing, Kang, and Lim 2017)



Discretization without scaling

Geometry. Piecewise-smooth $\partial\Omega_m$.

- Ellipse perturbed by a straight corner of angle $\phi \in (0, \pi)$.
- $\mathcal{C}^1$ junction.



Weak Formulation: Find $(u, \kappa) \in H_0^1(\Omega) \times \mathbb{C}$ s.t.

$$\forall v \in H_0^1(\Omega), \int_{\Omega_m} \nabla u(\boldsymbol{x}) \cdot \nabla v(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} = -\kappa \int_{\Omega_d} \nabla u(\boldsymbol{x}) \cdot \nabla v(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}.$$

Discretization:

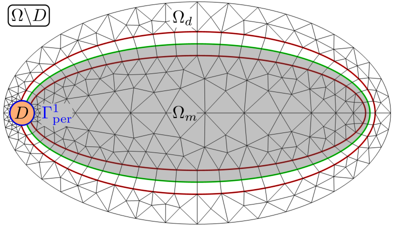
$$A_{\Omega_m} U = -\kappa\, A_{\Omega_d} U,$$

where A_{Ω_m}, A_{Ω_d} are real symmetric and positive (but not definite).

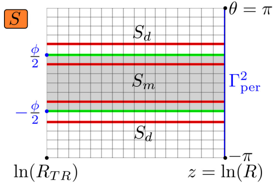
Next: addition of a complex scaling region around $\boldsymbol{x}_c$.

Disretization with scaling

$\partial\Omega_m$ = ellipse perturbed by a corner of angle $\phi \in (0,\pi)$, $\mathcal{C}^1$ junction.



$$H_e := \left\{u \in H^1(\Omega\backslash\overline{D}) \;\middle|\; u_{|\partial\Omega} = 0\right\}$$



Euler coordinates $(z = \ln(r), \theta)$.

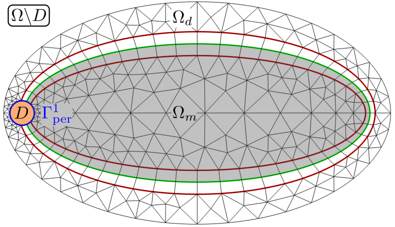
$$H_c := \left\{\breve{u} \in H^1(S) \;|\; \breve{u}(\cdot,\pi) = \breve{u}(\cdot,-\pi)\right\}$$

Solution space:

$$V = \left\{(u,\breve{u}) \in H_e \times H_c \;\middle|\; u_{|\Gamma^1_{\text{per}}} = \breve{u}_{|\Gamma^2_{\text{per}}}\right\}.$$

Disretization with scaling

$\partial\Omega_m$ = ellipse perturbed by a corner of angle $\phi \in (0,\pi)$, $\mathcal{C}^1$ junction.



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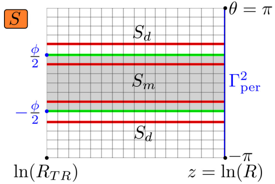

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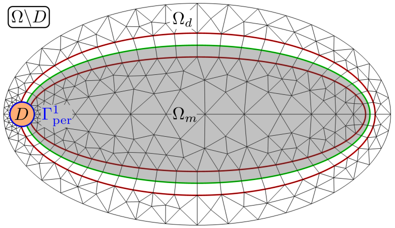
Discretization with H^1-conforming elements (isoparametric P^2/Q^2).
Find $(\kappa, U) \in \mathbb{C} \times \mathbb{C}^N$:

$$\left[A^{(x,y)}_{\Omega_m\backslash D} + \alpha\, A^{(z)}_{S_m} + \frac{1}{\alpha}\, A^{(\theta)}_{S_m} \right] U = -\kappa \left[A^{(x,y)}_{\Omega_d\backslash D} + \alpha\, A^{(z)}_{S_d} + \frac{1}{\alpha}\, A^{(\theta)}_{S_d} \right] U,$$

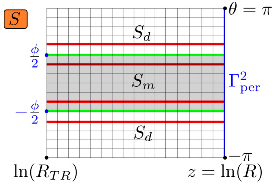
where all matrices are real.

Disretization with scaling

$\partial\Omega_m$ = ellipse perturbed by a corner of angle $\phi \in (0, \pi)$, $\mathcal{C}^1$ junction.



$$H_e := \left\{ u \in H^1(\Omega\backslash\overline{D}) \,\middle|\, u_{|\partial\Omega} = 0 \right\}$$



Euler coordinates $(z = \ln(r), \theta)$.

$$H_c := \left\{ \breve{u} \in H^1(S) \mid \breve{u}(\cdot, \pi) = \breve{u}(\cdot, -\pi) \right\}$$

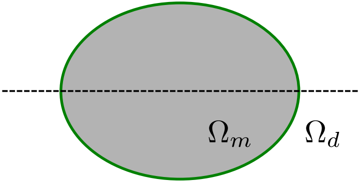
⚠ Mesh symmetry at $\partial\Omega_m$ to avoid spurious plasmons.
Proof for polygonal interfaces: (Bonnet-Ben Dhia, Carvalho, and Ciarlet 2018).

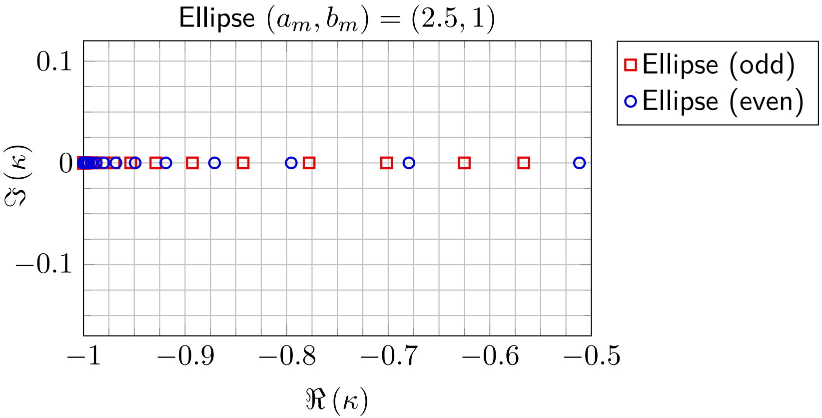
Methodology to deal with curvilinear $\partial\Omega_m$:

- One-cell thick structured layer.
- Symmetry w.r.t. elliptic coordinates (μ, θ) using isoparametric Q^2.

Implementations COMSOL 5.4 and `gmsh/dolfinx/PETSc/SLEPc`.

Results: corner perturbation along major axis (1)





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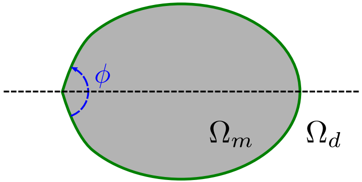
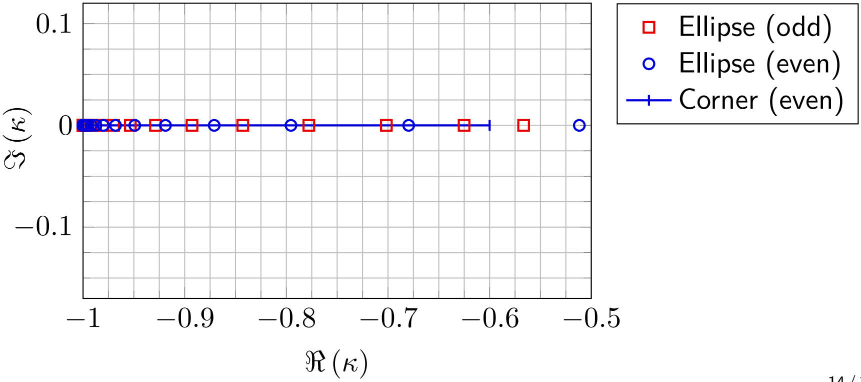


Perturbed ellipse: $(a_m, b_m) = (2.5, 1)$, $\phi = 0.75\pi$



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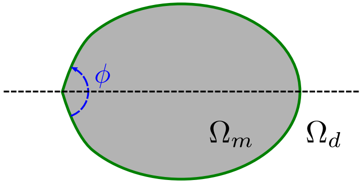

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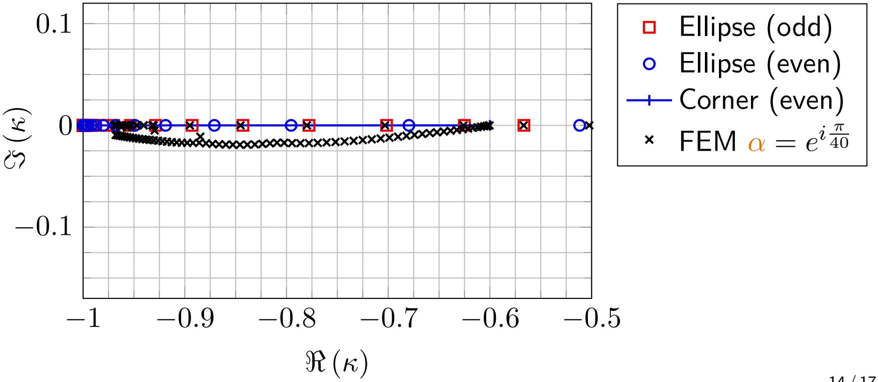

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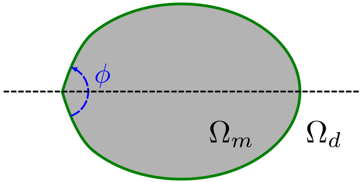

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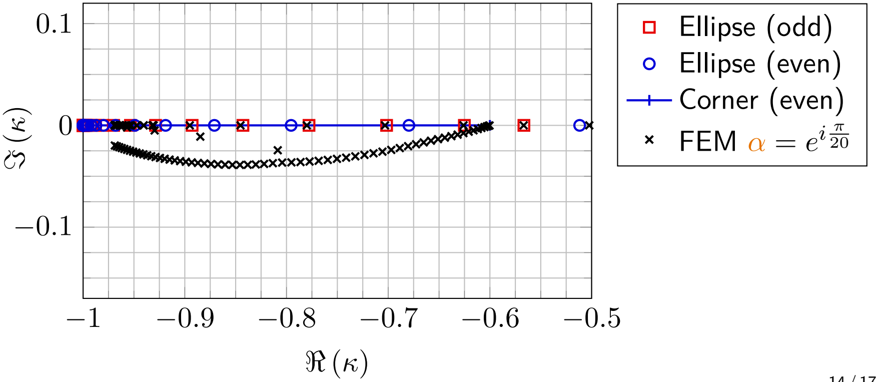

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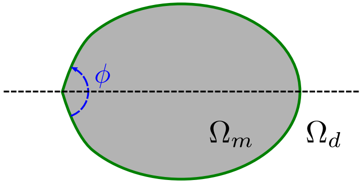

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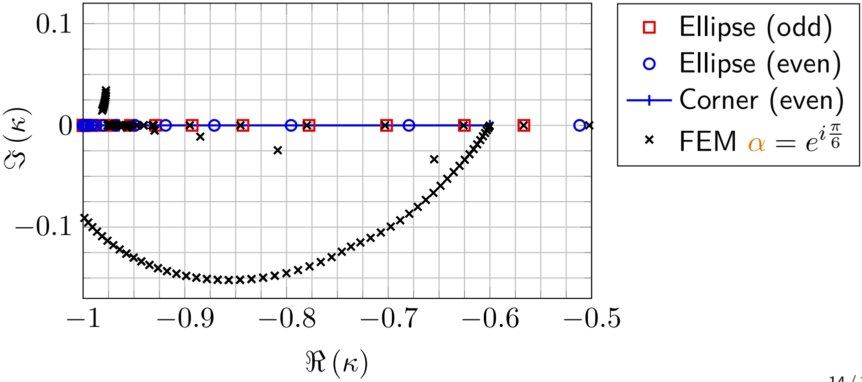

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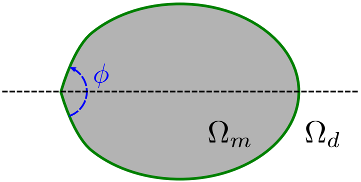

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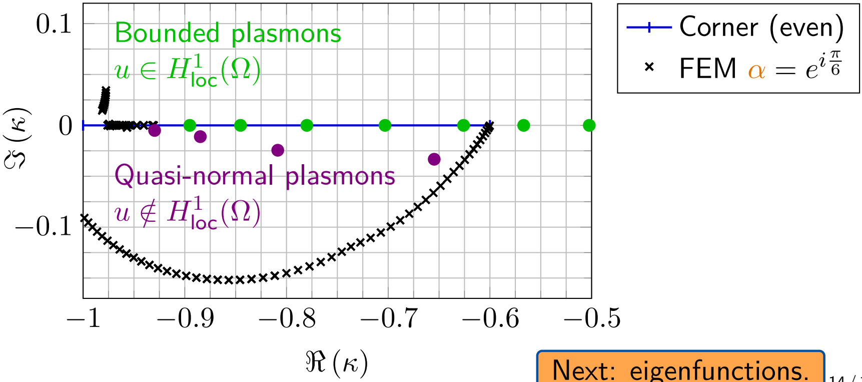


Next: eigenfunctions.

Results: corner perturbations along major axis (2)

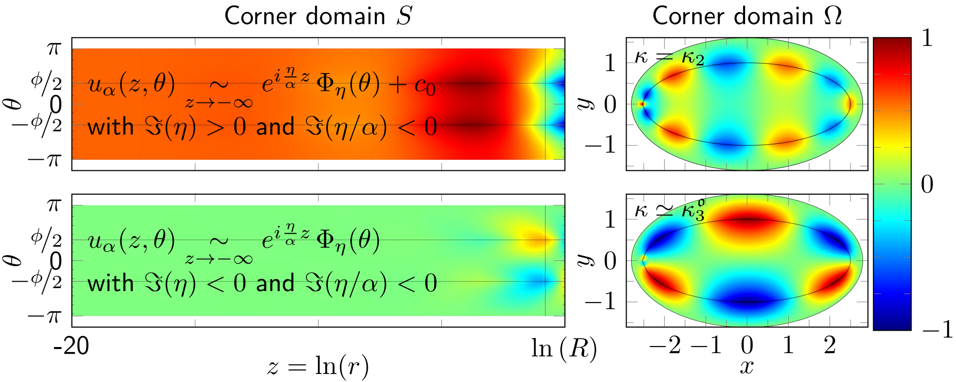
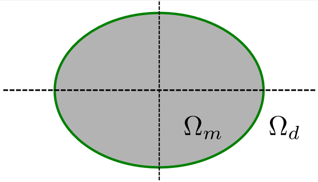
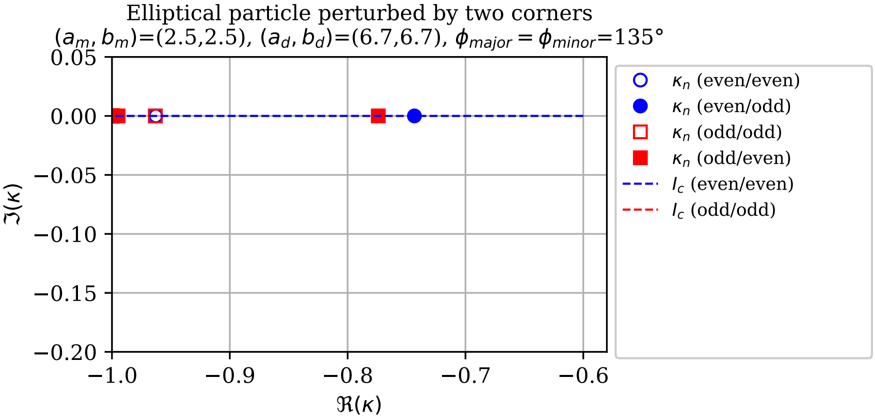


Fig. Eigenfunctions $\Re(u_\alpha)/\|u_\alpha\|_\infty$ of PEP-α with $\alpha = e^{i\frac{\pi}{6}}$.
(Top row) $\kappa = \kappa_2 \simeq 0.8086 - 0.02445i$, complex plasmonic resonance,
(Bottom row) $\kappa \simeq 0.70313 - 8.0357 \cdot 10^{-8} i \simeq \kappa_3^{\mathfrak{o}}$, embedded eigenvalue.

Results: corner perturbations along both major / minor axes





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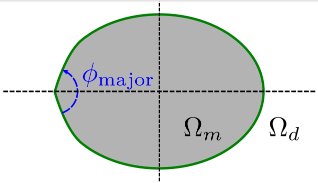

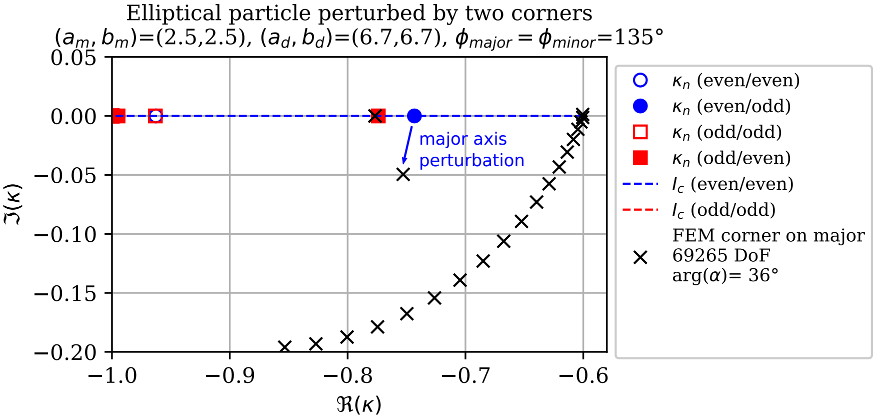

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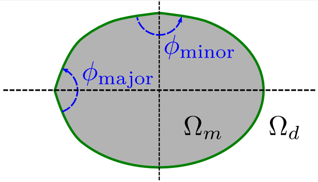

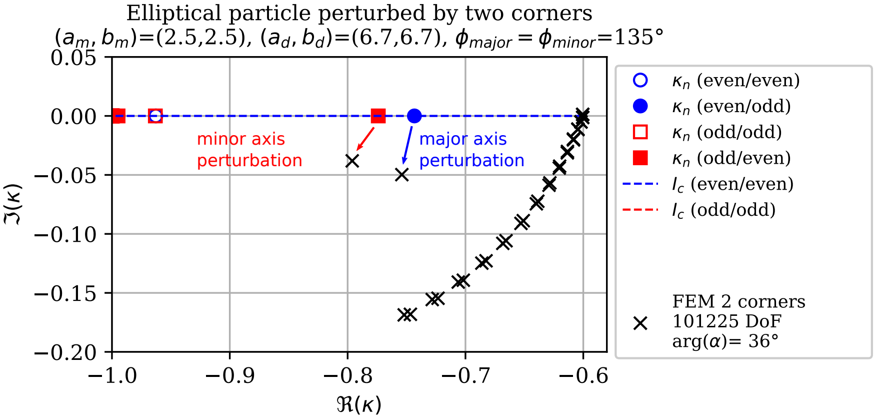

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Conclusions & outlook

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Takeaways

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  - trap energy at corners,
  - are associated with complex resonances $\kappa = \frac{\varepsilon}{\varepsilon_0} \notin \mathbb{R}$,
  - are analogous to quasi-normal modes ("infinity $\Leftrightarrow$ corner")
- FE with corner complex scaling $\Rightarrow$ linear eigenvalue problem (Bonnet-Ben Dhia, Carvalho, Chesnel, and Ciarlet 2016)
- Agreement with (Li and Shipman 2019)

Outlook

- Interest of working with $\alpha(\kappa)$. (Nannen and Wess 2018)
- Properties and application of QNSP expansions. (Truong et al. 2020)
- Extension to e.g. $\Omega_m \subset \mathbb{R}^3$, Maxwell. (Helsing and Perfekt 2018) (Li, Perfekt, and Shipman 2020) (Bonnet-Ben Dhia, Chesnel, and Rihani 2022)

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Thanks for your attention.

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