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

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Anne-Sophie Bonnet-Ben Dhia[2], Christophe Hazard[2], Florian Monteghetti[1]

[1]DISC, ISAE-SUPAERO, Université de Toulouse, France
[2]POEMS (CNRS-INRIA-ENSTA Paris), Palaiseau, France

Contact: florian.monteghetti@isae-supaero.fr, f.monteghetti@gmail.com

What are "complex resonances"? (Zworski 2017)

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

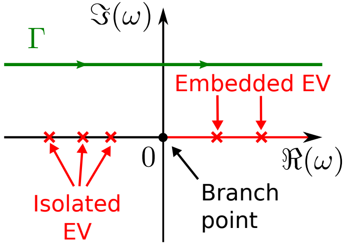
$$i\partial_t \psi(t,\boldsymbol{x}) = H\psi(t,\boldsymbol{x}) + f(\boldsymbol{x}),\ \psi(0,\boldsymbol{x}) = 0 \quad \left(x \in \mathbb{R}^3\right).$$

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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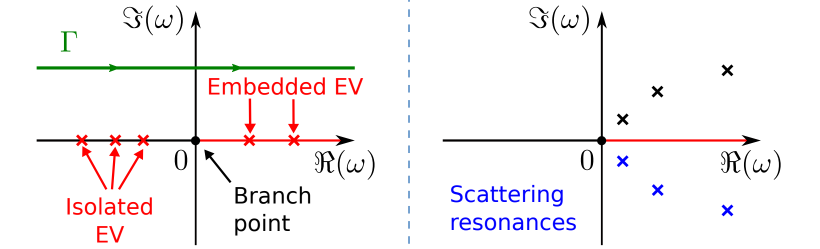


⇒ This work investigates a **plasmonic analogue** of scattering resonances.

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

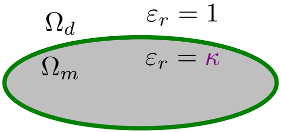
Plasmonic Eigenvalue Problem (PEP)

Find $(u, \kappa) \in H^1_0(\Omega) \times \mathbb{C}$ such that

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

with piecewise-constant permittivity:

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



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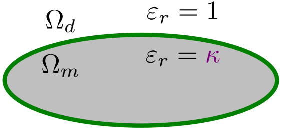

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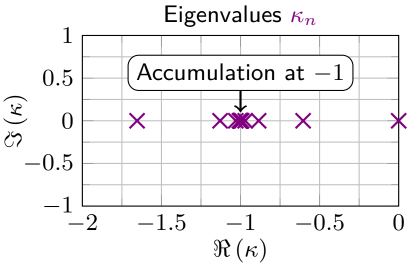
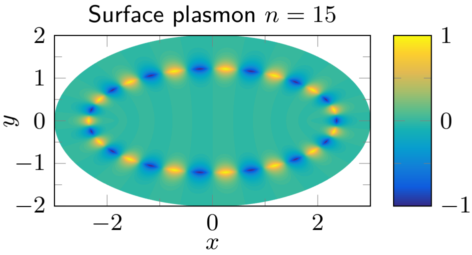
Smooth $\partial\Omega_m$ Point spectrum in H^1_{loc}: $\kappa_n < 0$, $\kappa_n \to -1$ (Grieser 2014, Thm. 1).





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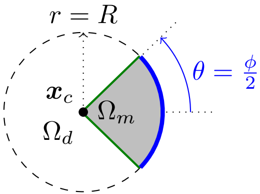

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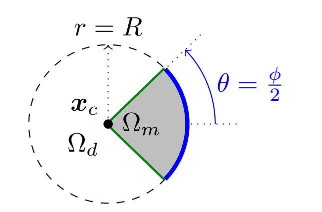
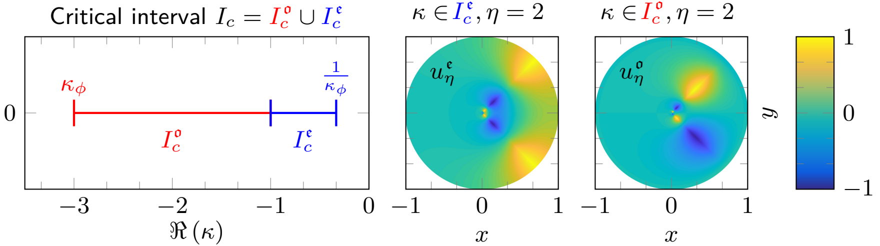


Corner of angle ϕ There is a **critical interval** I_c such that

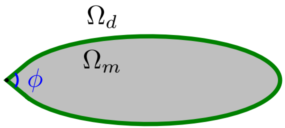
$$\kappa \in I_c \Leftrightarrow \exists!\, \eta > 0 : \; u_\eta(r,\theta) = e^{i\eta \ln r}\Phi_\eta(\theta) \text{ solves } (\star),$$

for some $\Phi_\eta \in H^1_{\text{per}}(-\pi,\pi)$. Crucially $u_\eta \notin H^1_{\text{loc}}$ (strongly-oscillating).



Objectives and outline

Objective Compute complex resonances and embedded eigenvalues for particles with corners.



Outline

1. Definition of complex plasmonic resonances
2. Applicability of corner complex scaling
3. Numerical results using corner perturbations

Continuation of the resolvent: summary of Mellin analysis

Starting point Let $\Omega \subset \mathbb{R}^2$ bounded, $\partial\Omega$ smooth except for one corner.

$$\operatorname{div}\left[\varepsilon_r(\kappa)^{-1}\nabla u\right] = f,\; u_{|\partial\Omega} = 0 \quad (\Im(\kappa) > 0)\,.$$

Lax-Milgram yields a bounded resolvent $R(\kappa) : H^{-1}(\Omega) \to H^1_0(\Omega)$.

⚠ As $\kappa \to I_c^{\mathfrak{o}} \cup I_c^{\mathfrak{e}}$, $\|R(\kappa)f\|_{H^1(\Omega)} \to \infty$.

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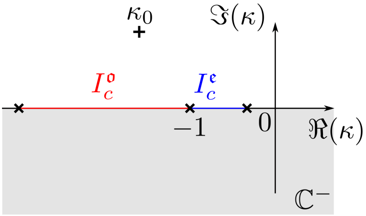

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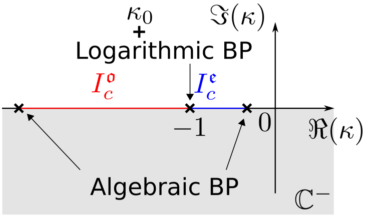

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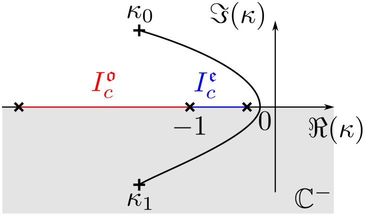

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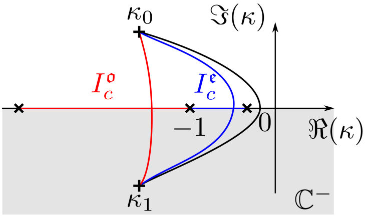

Definition A **complex plasmonic (CP) resonance** is a pole of $\kappa \to R^{|\mathfrak{e}}(\kappa)$ or $\kappa \to R^{|\mathfrak{o}}(\kappa)$ in $\mathbb{C}^-$.

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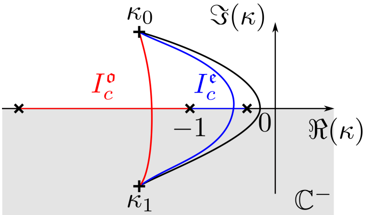


Characterization If κ_{res} is a CP resonance, the associated function blows up at the corner like

$$u_{\text{res}}(r,\theta) \underset{r\to 0}{=} c_\eta\, e^{i\eta \ln r}\, \Phi_\eta(\theta) + c_0 + \mathcal{O}\left(r^{-\eta_\star}\right) \quad (\Im(\eta) > 0,\ \eta_\star < 0)\,,$$

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

Corner complex scaling: formulation and uncovered region

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

κ complex plasmonic resonance of PEP $\iff$ κ eigenvalue of PEPα .

Intuitively, we would like

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

$$\downarrow$$

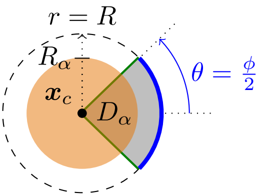
$$\text{(PEP}\alpha\text{)} \qquad u_{\text{res},\alpha} \underset{r\to 0}{\sim} e^{i\frac{\eta}{\alpha}\ln r}\,\Phi_{\eta}(\theta) + c_0 \qquad \left(\Im\left(\frac{\eta}{\alpha}\right) < 0\right)$$

Definition of PEPα. Substitution

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

around the corner.

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



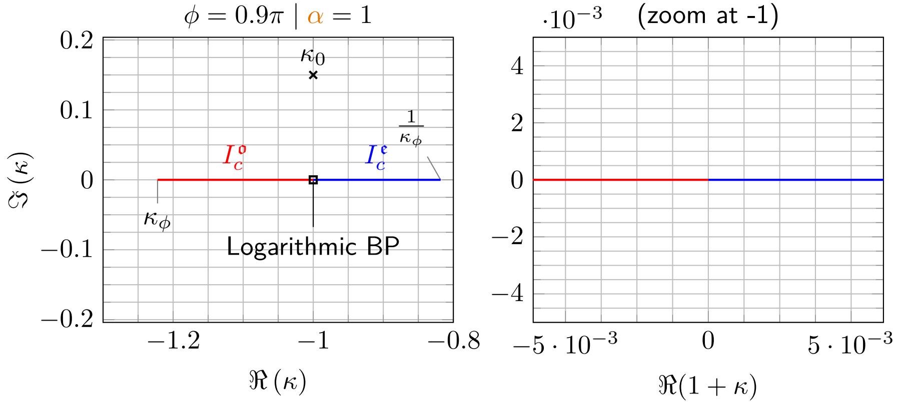
Domain of validity?

Corner complex scaling: formulation and 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,

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



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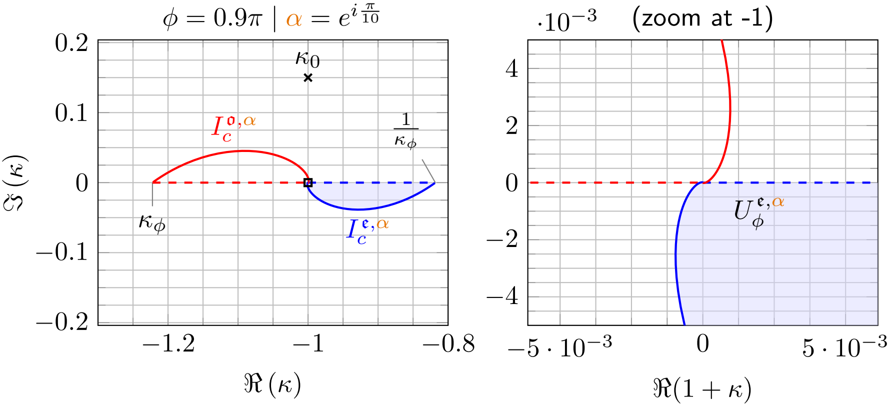

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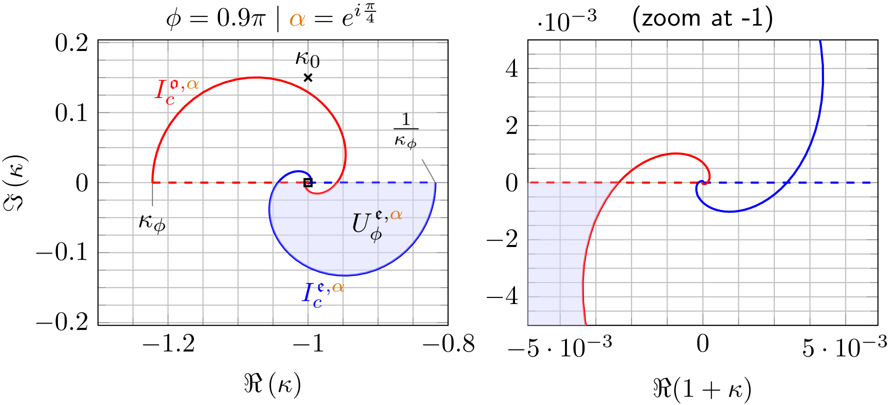
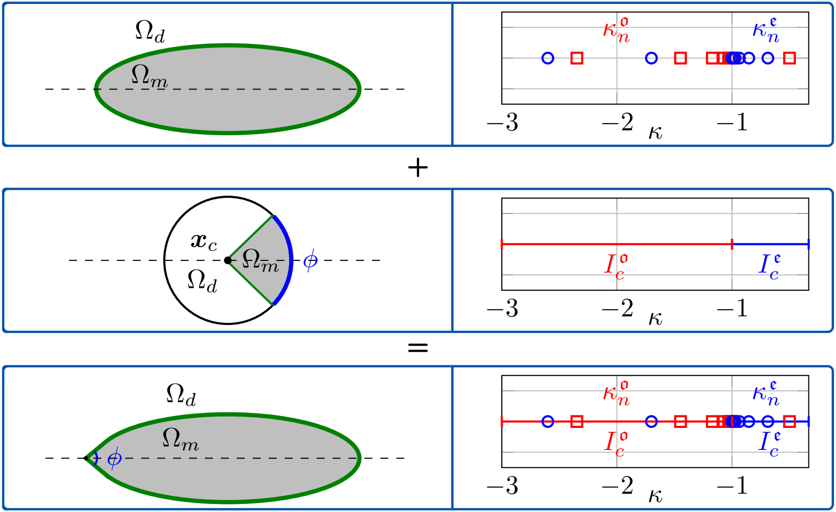


How to obtain complex resonances?

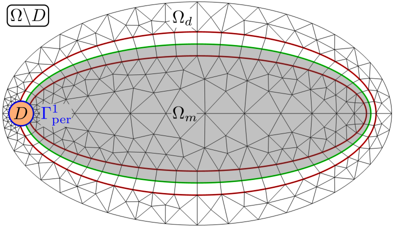
Perturbation of elliptical Ω_m by corner along major axis.

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

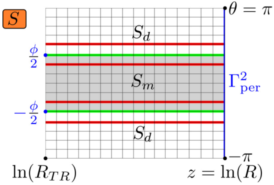


Geometry, weak formulation, Mesh

$\partial\Omega_m$ = 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 $(z = \ln(r), \theta)$.

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

Solution space:

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

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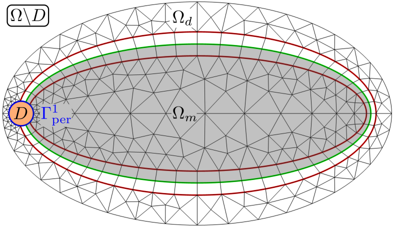

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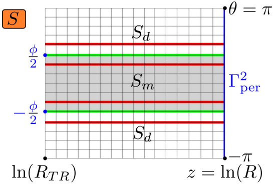

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Discretization with H^1-conforming elements (isoparametric P^2/Q^2).
Find $(\kappa, U) \in \mathbb{C} \times \mathbb{C}^N$:

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

where all matrices are real.

Geometry, weak formulation, Mesh

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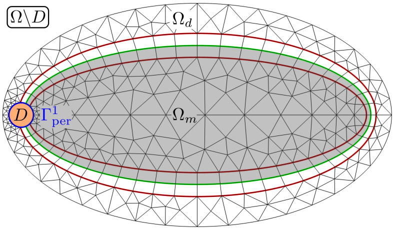

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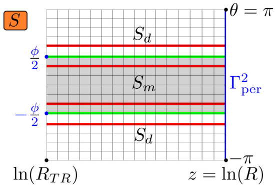

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⚠ Mesh symmetry at $\partial\Omega_m$ to avoid spurious plasmons.
Proof for polygonal interfaces: (Bonnet-Ben Dhia, Carvalho, and Ciarlet 2018).

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

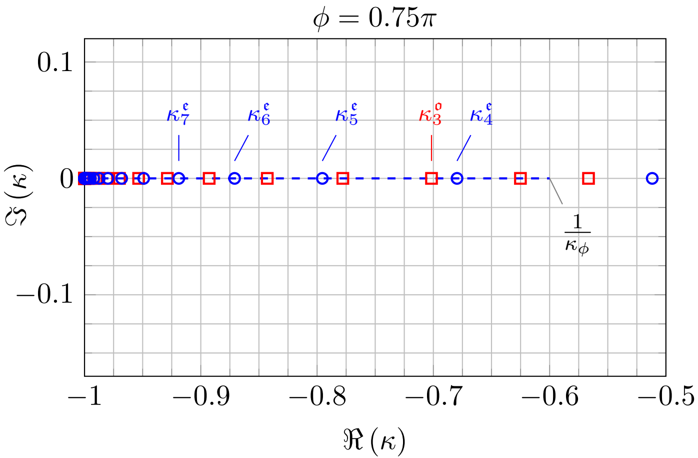

Fig. Spectrum for increasing values of $\arg(\alpha)$.
(○,□): unperturbed eigenvalues $\kappa_n^{\mathfrak{e}}$ and $\kappa_n^{\mathfrak{o}}$, (– –): critical interval $I_c^{\mathfrak{e}}$,

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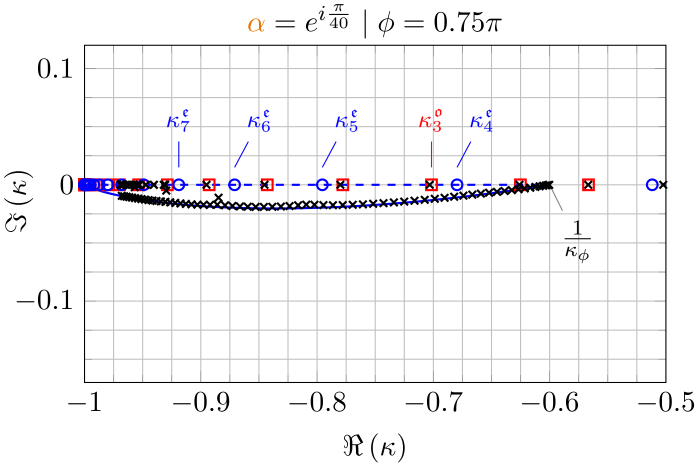

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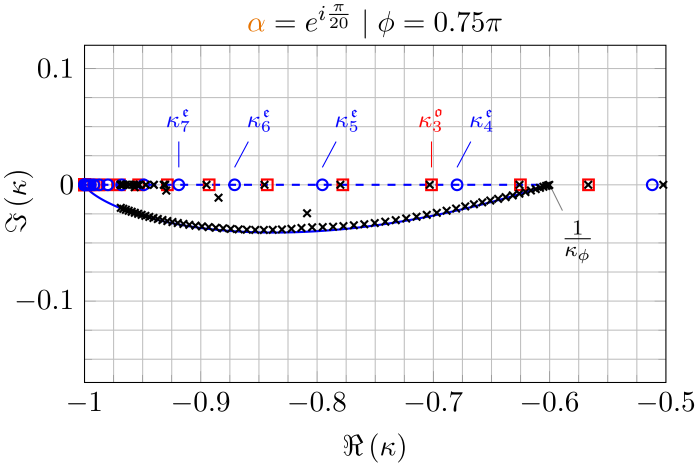

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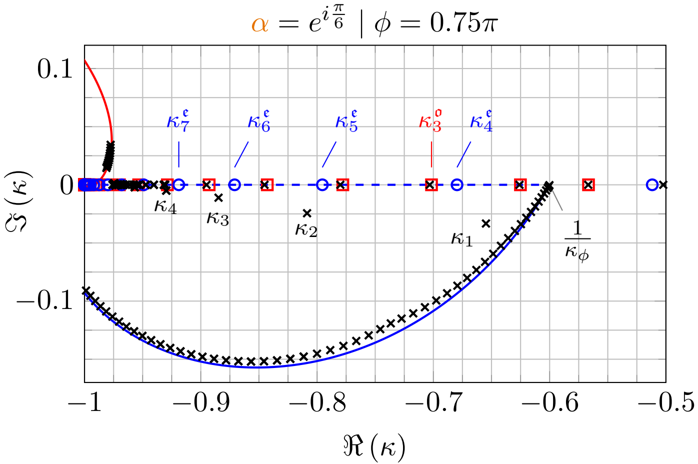

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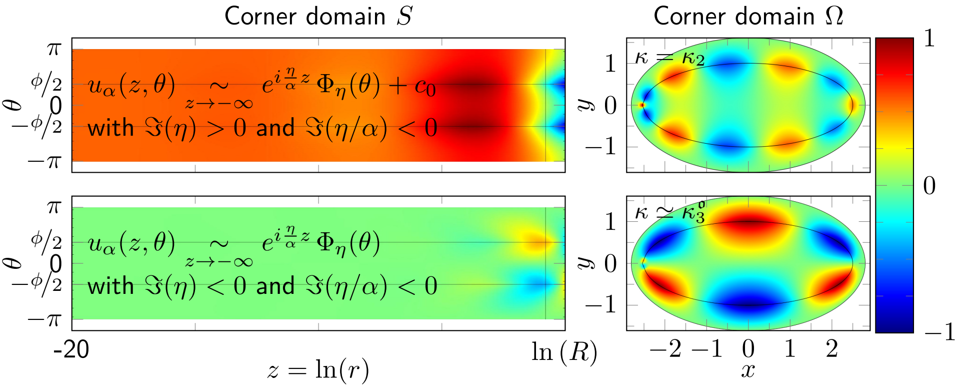
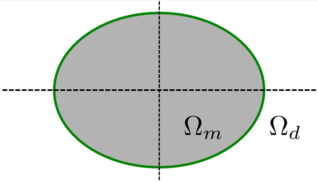
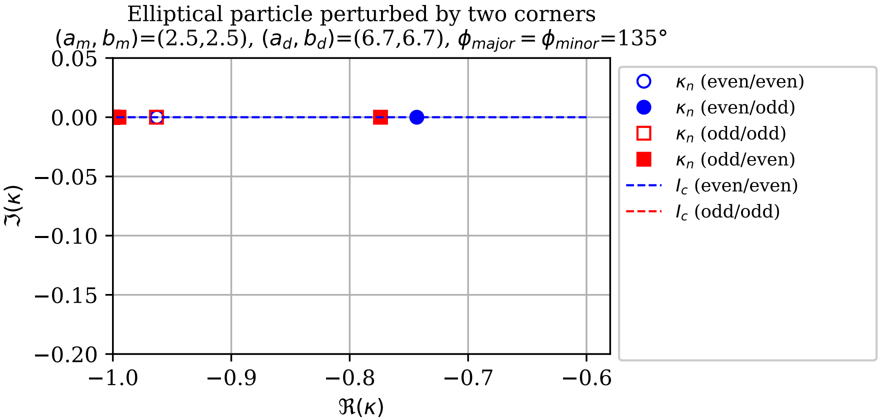


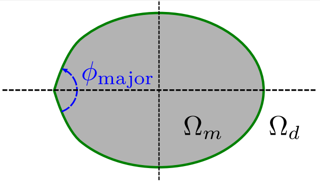
Fig. Eigenfunctions $\Re(u_\alpha)/\|u_\alpha\|_\infty$ of PEP-α with $\alpha = e^{i\frac{\pi}{6}}$.
(Top row) $\kappa = \kappa_2 \simeq 0.8086 - 0.02445i$, complex plasmonic resonance,
(Bottom row) $\kappa \simeq 0.70313 - 8.0357 \cdot 10^{-8}i \simeq \kappa_3^0$, embedded eigenvalue.

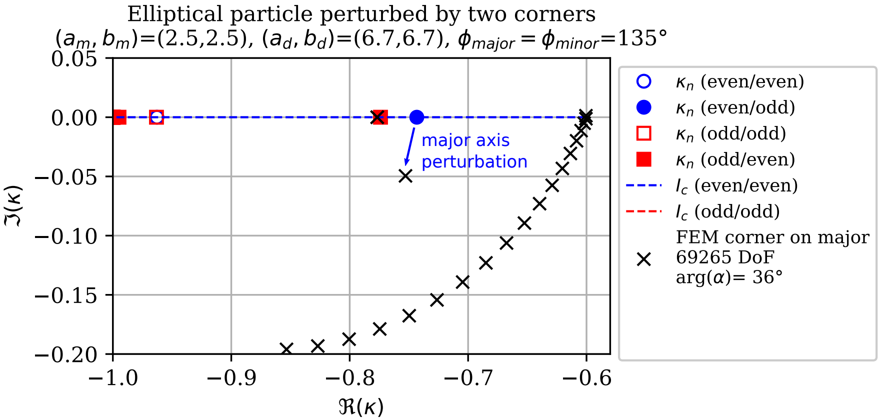
Results: corner perturbations along both major/minor axes



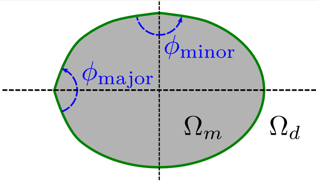


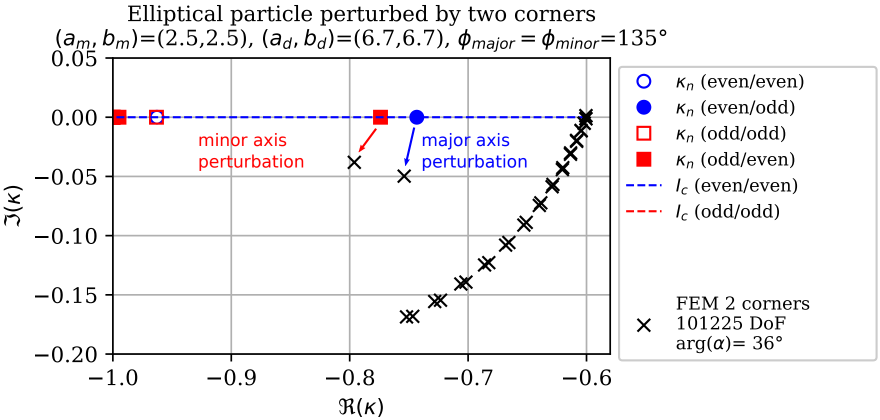
Results: corner perturbations along both major / minor axes





Results: corner perturbations along both major / minor axes





Conclusions & outlook

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Takeaways

- Complex plasmonic (CP) resonances
  - Analogous to scattering resonances: ”Infinity $\Leftrightarrow$ Corner”
- Corner complex scaling (Bonnet-Ben Dhia, Carvalho, Chesnel, and Ciarlet 2016)
  - Linear eigenvalue problem in κ, valid in uncovered region U_ϕ^α
- Numerical results
  - Meshing strategy for curvilinear sign-changing interface
  - Corroborate mechanism described in (Li and Shipman 2019)

Outlook

- Interest of working with $\alpha(\kappa)$? (Nannen and Wess 2018)
- Drop quasi-static assumption. (Demésy et al. 2020)
- Expansion using quasi-normal surface plasmons? (Truong et al. 2020)
- Extension to $\Omega_m \subset \mathbb{R}^3$.
  (Helsing and Perfekt 2018) (Li, Perfekt, and Shipman 2020)

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Thanks for your attention. Any questions?

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