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

DeFI working group (INRIA-CMAP) 7th December 2020

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in collaboration with

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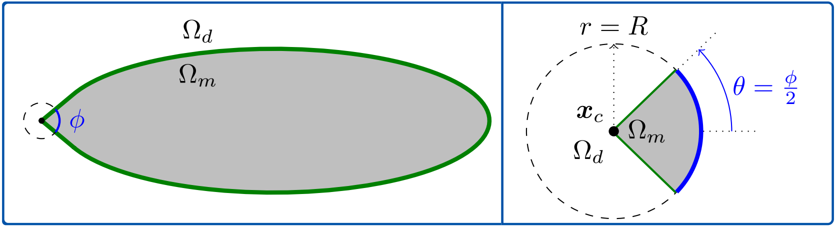
Objective

Context: Waves in "negative" materials, i.e. $\epsilon_m(\omega) < 0$, $\mu_m(\omega) < 0$

Particle: Boundary $\partial\Omega_m$ has one straight corner of angle $\phi \in (0, 2\pi)\backslash\pi$



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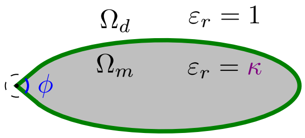
Plasmonic Eigenvalue Problem (PEP)

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

$$\mathrm{div}\left[\varepsilon_r^{-1}\nabla u\right] = 0 \quad \text{in } \mathcal{D}'(\mathbb{R}^2)$$

with piecewise-constant permittivity:

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



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PEP is self-adjoint in $L^2(\mathbb{R}^2)$ with $\kappa < 0 \Rightarrow$ **sign-changing interface**.

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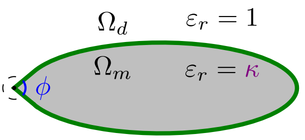

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Objective Investigate existence of solutions $(u_{\text{res}}, \kappa_{\text{res}})$ with

$$\kappa_{\text{res}} \in \mathbb{C}\backslash\mathbb{R}, \; u_{\text{res}} \notin L^2_{\text{loc}}(\mathbb{R}^2).$$

Next: why a corner?

Smooth boundary: H^1 plasmons (discrete spectrum)

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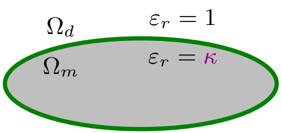
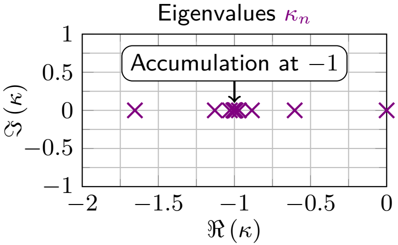
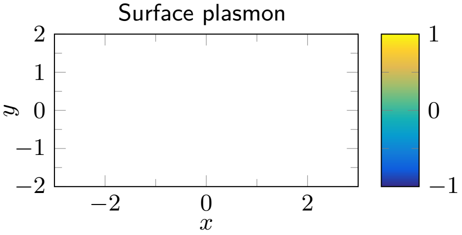


Point spectrum in $H^1_{\text{loc}}(\mathbb{R}^2)$: $\kappa_n < 0$, $\kappa_n \to -1$ (Grieser 2014, Thm. 1)





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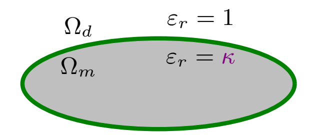

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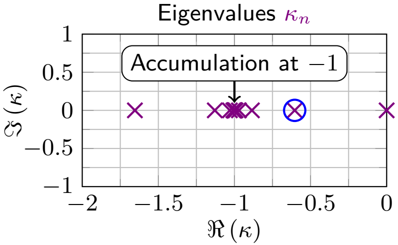

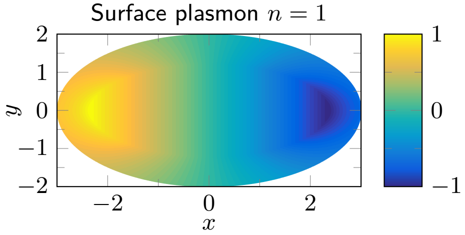

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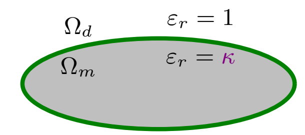

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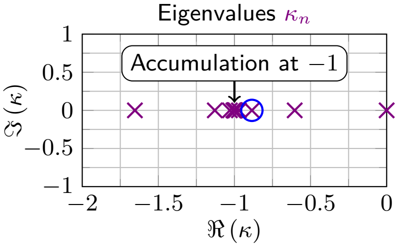

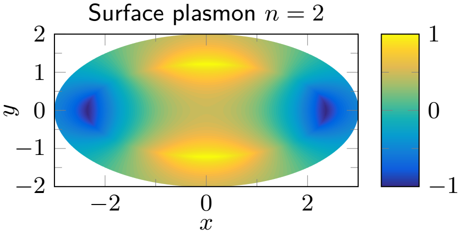

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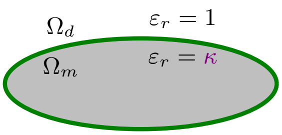

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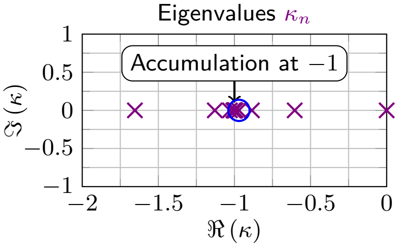

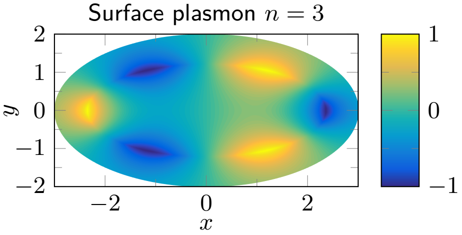

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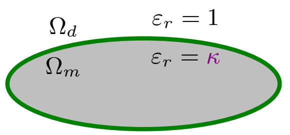

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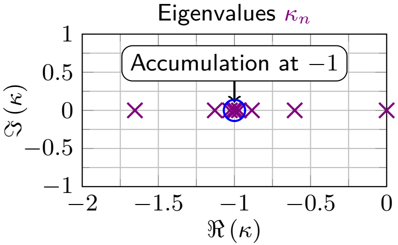

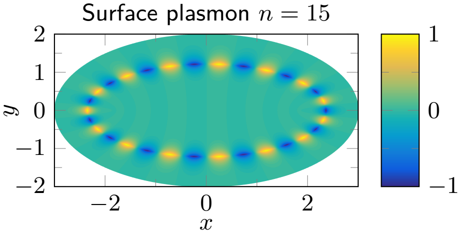

Next: effect of corner on plasmons?

Corner: strongly-oscillating plasmons (essential spectrum)

Let $\partial\Omega_m$ have one corner at $\boldsymbol{x}_c$ and $D := \{|\boldsymbol{x} - \boldsymbol{x}_c| < R\}$.

Even (odd) **local solutions** with separated variables are:

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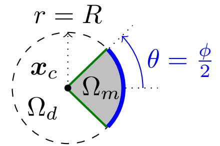

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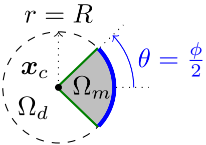

Analysis of $f_\phi^{\mathfrak{e}(\mathfrak{o})}$ yields **critical interval** $I_c = I_c^{\mathfrak{e}} \cup I_c^{\mathfrak{o}}$: (Bonnet-Ben Dhia et al. 2016)

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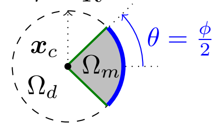

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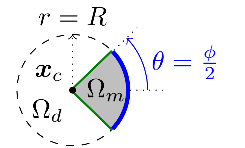

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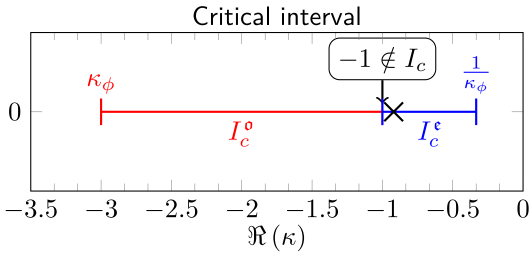

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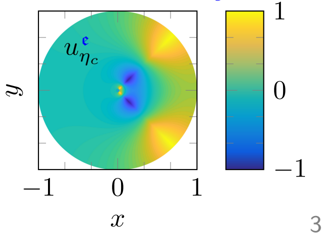

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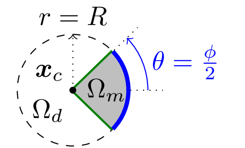

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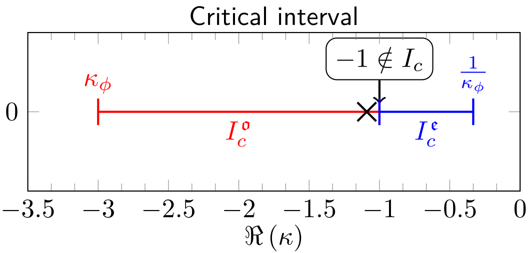

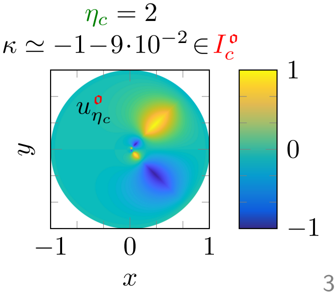

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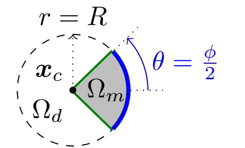

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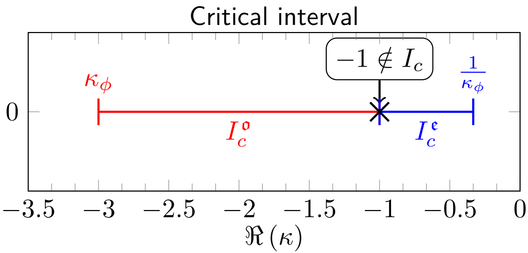

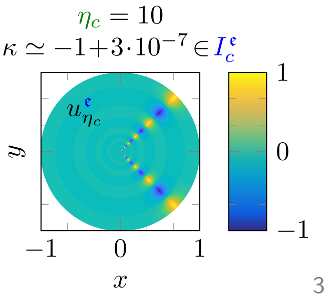

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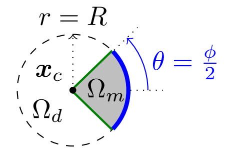

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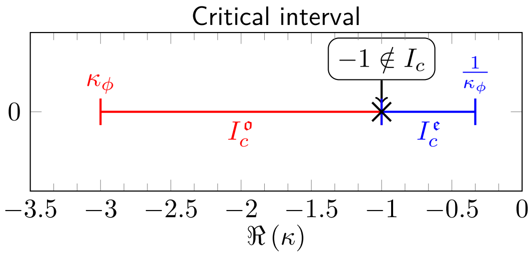

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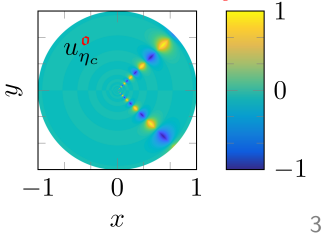

Definition of complex plasmonic (CP) resonances: strategy

Tentative definition: A contrast $\kappa \in \mathbb{C} \backslash \mathbb{R}$ is a *CP resonance* if there is $u_{\text{res}} : \mathbb{R}^2 \to \mathbb{C}$ such that (u_{res}, κ) solves the PEP.

⚠ $u_{\text{res}} \notin L^2_{\text{loc}}(\mathbb{R}^2)$, since the PEP is self-adjoint.

Objective Characterize the behavior of u_{res} when $r \to 0$.

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Starting point: Let $\kappa \in \mathbb{C}^+$ and $u(\kappa) \in H^1(D)$ local solution: $\forall \eta_\star < 0$,

$$u(r,\theta;\kappa) \underset{r\to 0}{=} c_0 + \sum_{\mathfrak{p}\in\{\mathfrak{e},\mathfrak{o}\}} \sum_{\substack{\eta \in \widehat{H}_\phi^{\mathfrak{p}}(\kappa) \\ \eta_\star < \Im(\eta)}} c_\eta^{\mathfrak{p}}\, u_\eta^{\mathfrak{p}}(r,\theta) + \mathcal{O}\left(r^{-\eta_\star}\right) \qquad (1)$$

Strategy Obtain a continuation of (1) by studying the continuation to $\mathbb{C}^-$ of the map

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

Continuation of set of stable zeros: key results

Zeros: $\mathbb{C} \ni \kappa \mapsto H_{\phi}^{\mathfrak{e}(\mathfrak{o})}(\kappa)$, Stable zeros: $\mathbb{C}^{+} \ni \kappa \mapsto \widehat{H}_{\phi}^{\mathfrak{e}(\mathfrak{o})}(\kappa)$

Lemma (analyticity). For any $\kappa \in U := \mathbb{C} \backslash \{\kappa_\phi, {}^1/_{\kappa_\phi}\}$, each element η of $H_{\phi}^{\mathfrak{e}(\mathfrak{o})}(\kappa)$ depends analytically upon $\kappa \in U$.

The map $\mathbb{C} \ni \kappa \mapsto H_{\phi}^{\mathfrak{e}(\mathfrak{o})}(\kappa)$ is single-valued, but...

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Proposition. The map $\mathbb{C}^+ \ni \kappa \mapsto \widehat{H}_\phi^{\mathfrak{e}(\mathfrak{o})}(\kappa)$ has three branch points:

$$\kappa = \kappa_\phi \text{ (algebraic)}, \ \kappa = -1 \text{ (logarithmic)}, \ \kappa = {}^1/\kappa_\phi \text{ (algebraic)}.$$

Proof. Follows from asymptotic expansions of the critical exponent η_c. □

By crossing $\mathbb{R}$ **once** we obtain **three continuations** of $\widehat{H}_\phi(\kappa)$ to $\mathbb{C}^-$:

$$\widehat{H}_\phi(\kappa), \ \widehat{H}_\phi^{|\mathfrak{e}}(\kappa), \ \widehat{H}_\phi^{|\mathfrak{o}}(\kappa).$$

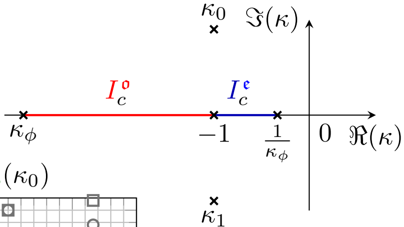
Next: let us plot each of these three continuations.

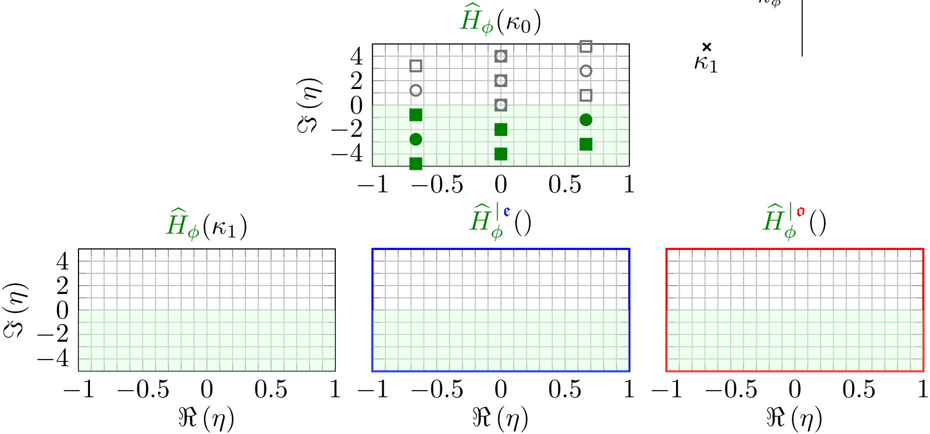
Continuation of set of stable zeros: illustration

Let's compare three paths satisfying

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

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





Next: definition of complex plasmonic resonances using $\widehat{H}_\phi^{|\mathfrak{e}(\mathfrak{o})}$.

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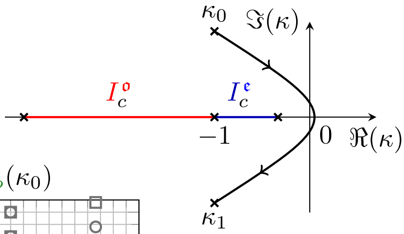

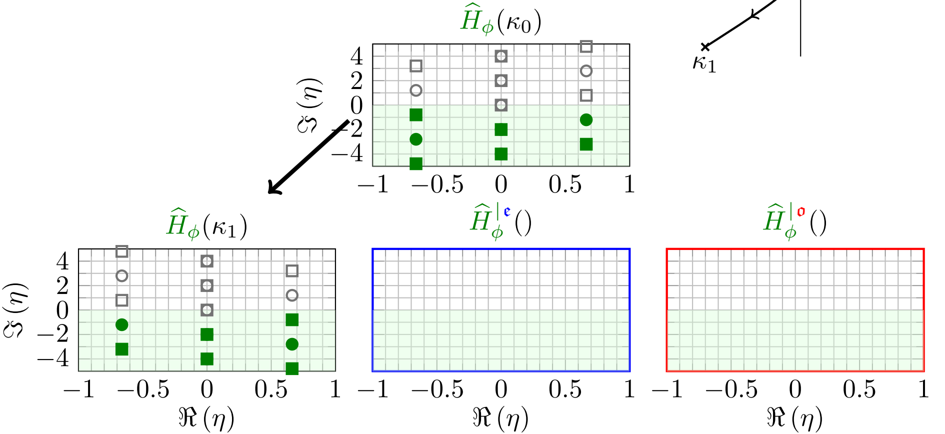

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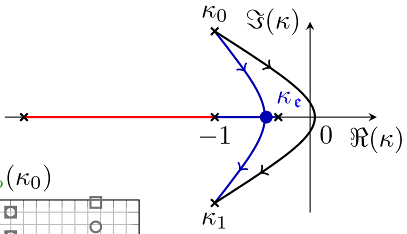

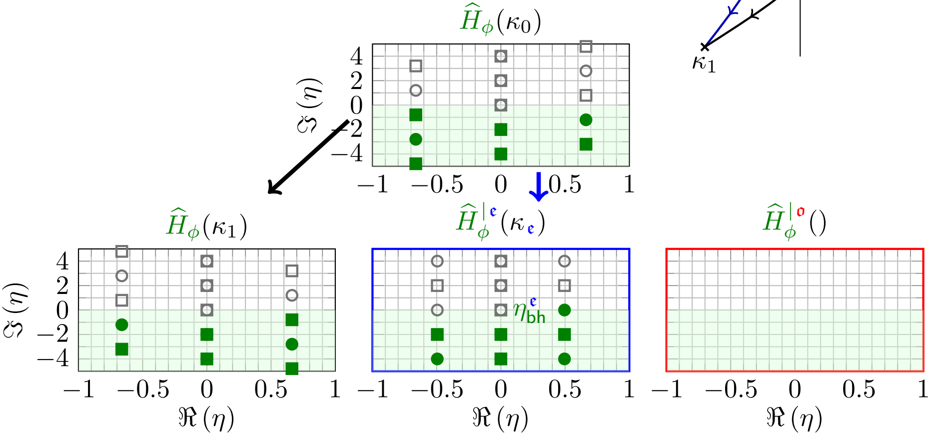

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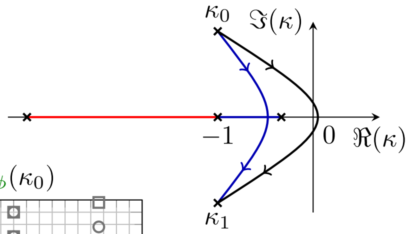

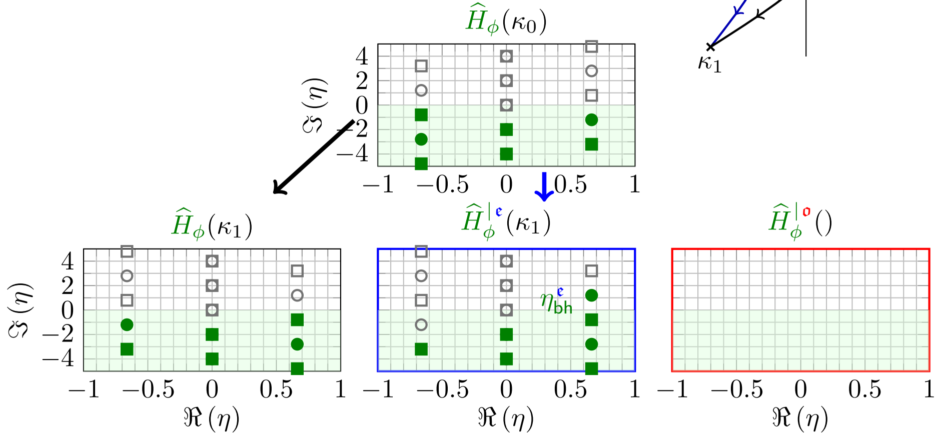

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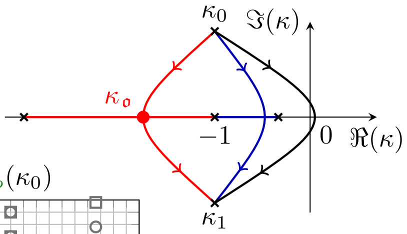

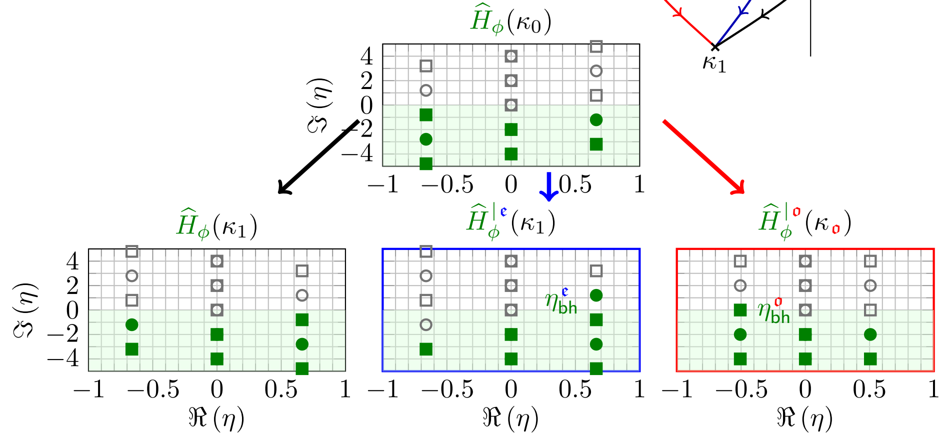

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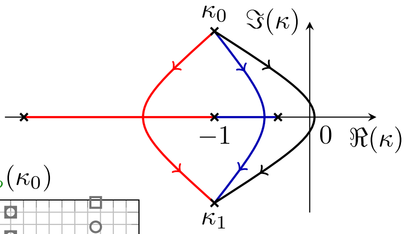

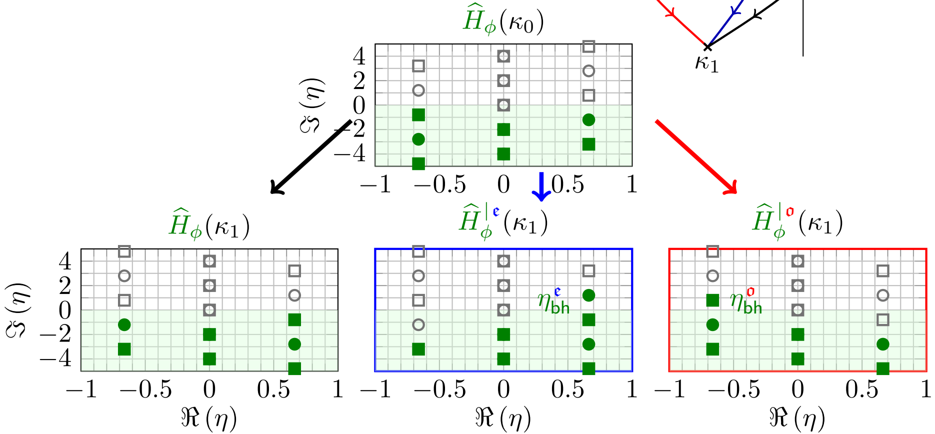

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Definition of complex plasmonic (CP) resonances

The continuation of $\widehat{H}_\phi(\kappa)$ across $I_c^{\mathfrak{e}}$ is

$$\widehat{H}_\phi^{|\mathfrak{e}}(\kappa) = \widehat{H}_\phi^{\mathfrak{e}|\mathfrak{e}}(\kappa) \cup \widehat{H}_\phi^{\mathfrak{o}|\mathfrak{e}}(\kappa).$$

This suggests...

Even-critical complex plasmonic resonance:

Contrast $\kappa_{\text{res}} \in \mathbb{C}^-$ associated with $u_{\text{res}} \notin L^2_{\text{loc}}(\mathbb{R}^2)$.

$$u_{\text{res}}(r,\theta) \underset{r\to 0}{=} c_0 + \sum_{\mathfrak{p}\in\{\mathfrak{e},\mathfrak{o}\}} \sum_{\substack{\eta\in\widehat{H}_\phi^{\mathfrak{p}|\mathfrak{e}}(\kappa_{\text{res}}),\\ \eta_\star<\Im(\eta)}} c_\eta^{\mathfrak{p}}\, u_\eta^{\mathfrak{p}}(r,\theta) + \mathcal{O}\left(r^{-\eta_\star}\right)$$

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$$\underset{r\to 0}{\sim} c_0 + c_\eta^{\mathfrak{e}}\, r^{i\eta}\, \Phi_\eta^{\mathfrak{e}}(\theta) \quad \text{with } \eta = \eta_{\text{bh}}^{\mathfrak{e}}\left(\kappa_{\text{res}}\right),$$

where the blow-up rate is

$$\Im\left(\eta_{\text{bh}}^{\mathfrak{e}}\left(\kappa_{\text{res}}\right)\right) > 0.$$

Next: applicability of corner complex scaling (Bonnet-Ben Dhia, Carvalho, Chesnel, and Ciarlet 2016).

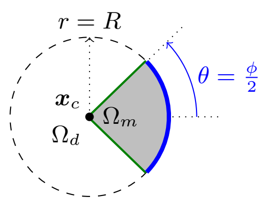
Corner complex scaling: formulation (Bonnet-Ben Dhia et al. 2016)

(PEP) Find $(u, \kappa) \in U \times \mathbb{C}$:

$$\frac{1}{r^2} r\partial_r \left[\varepsilon^{-1} r\partial_r u\right] + \frac{1}{r^2}\partial_\theta \left[\varepsilon^{-1}\partial_\theta u\right] = 0.$$

Local solutions

$$u_\eta^{\mathfrak{e}(\mathfrak{o})}(r,\theta) = r^{i\eta}\Phi_\eta^{\mathfrak{e}(\mathfrak{o})}(\theta), \quad \eta \in H_\phi^{\mathfrak{e}(\mathfrak{o})}(\kappa)$$



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 .

Intuition: Pick α such that if $u_{\text{res}} \sim r^{i\eta}$ then $u_{\text{res},\alpha} \sim r^{i\frac{\eta}{\alpha}}$ with $\Im\left(\frac{\eta}{\alpha}\right) < 0$.

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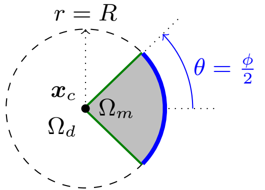

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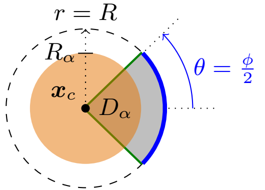
(PEP-α) Find $(u, \kappa) \in U \times \mathbb{C}$:

$$\frac{\alpha(r)}{r^2} r\partial_r \left[\varepsilon^{-1}\alpha(r) r\partial_r u\right] + \frac{1}{r^2}\partial_\theta \left[\varepsilon^{-1}\partial_\theta u\right] = 0$$

with purely-radial scaling $\alpha(r) = \alpha \mathbb{1}_{D_\alpha} + \mathbb{1}_{\mathbb{R}^2\setminus\overline{D_\alpha}}$.

Local solutions (same dispersion relation)

$$u_{\eta,\alpha}^{\mathfrak{e}(\mathfrak{o})}(r,\theta) = r^{i\frac{\eta}{\alpha}}\Phi_\eta^{\mathfrak{e}(\mathfrak{o})}(\theta), \quad \eta \in H_\phi^{\mathfrak{e}(\mathfrak{o})}(\kappa)$$



Corner complex scaling: analysis of uncovered region

Where can complex plasmonic resonances be computed?

For any scaling $\alpha \in \mathbb{C}^*$, the **uncovered region** is

$$U_\phi^{\mathfrak{e}(\mathfrak{o}),\alpha} := \left\{ \kappa \in \overline{\mathbb{C}^-} \,\middle|\, \forall \eta \in \widehat{H}_\phi^{|\mathfrak{e}(\mathfrak{o})}(\kappa),\ \Im\left(\frac{\eta}{\alpha}\right) < 0 \right\}.$$

Plotting the uncovered region is crucial to post-process results because of...

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Proposition. Let $\alpha \in \mathbb{C}\backslash\mathbb{R}$ and (u_α, κ) be a solution of PEPα. If

$$\kappa \in U_\phi^{\mathfrak{e},\alpha}$$

then κ is an even-critical CP resonance associated with

$$u_{\text{res}}(\boldsymbol{x}) := u_\alpha(\boldsymbol{x}) \qquad \left(\boldsymbol{x} \in \mathbb{R}^2\backslash\overline{D_\alpha}\right)$$

$$u_{\text{res}}(r,\theta) := u_\alpha(r^\alpha,\theta) \quad ((r,\theta) \in D_\alpha)\,.$$

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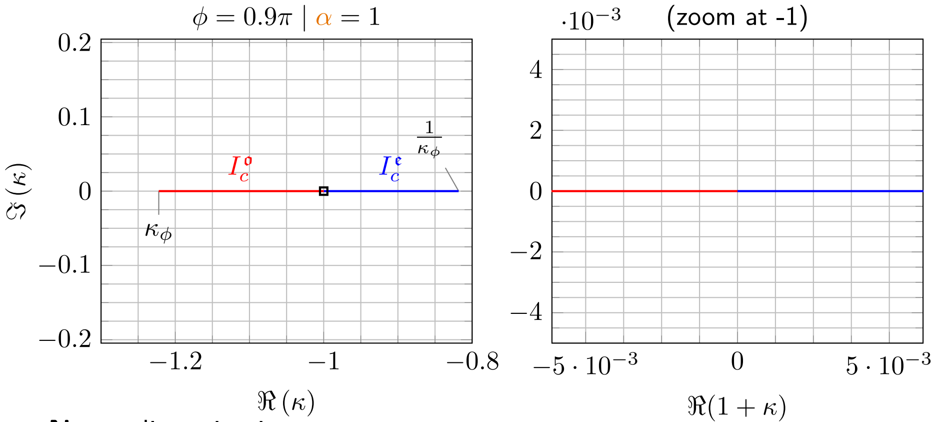

Next: discretization

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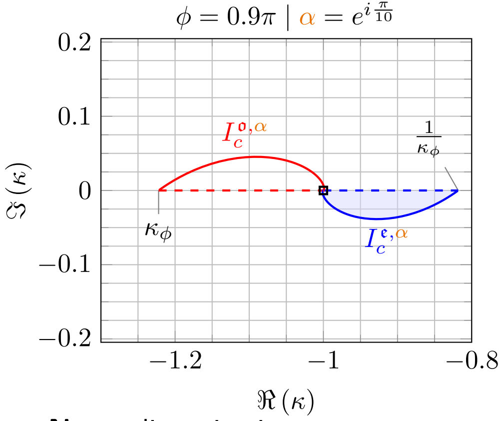

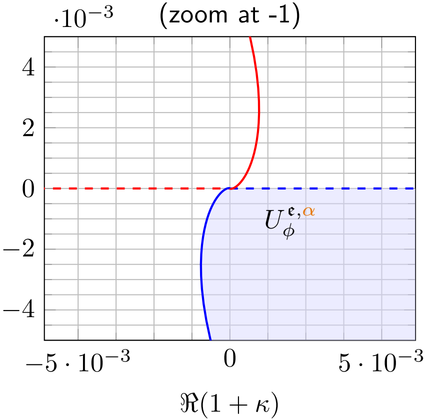

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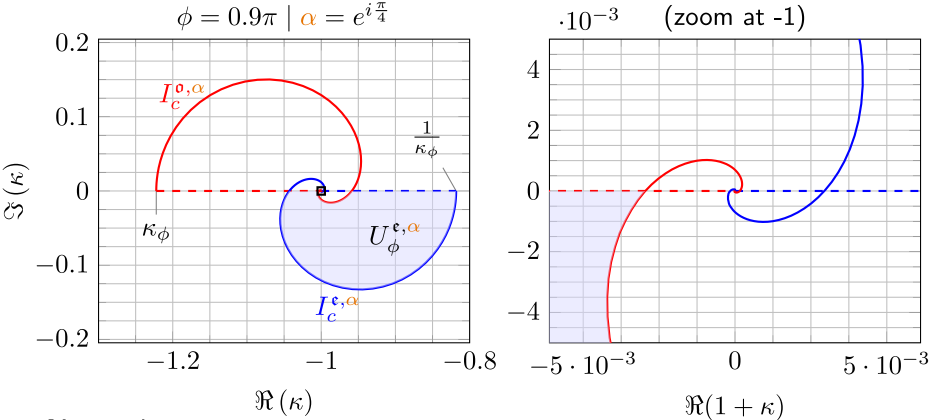
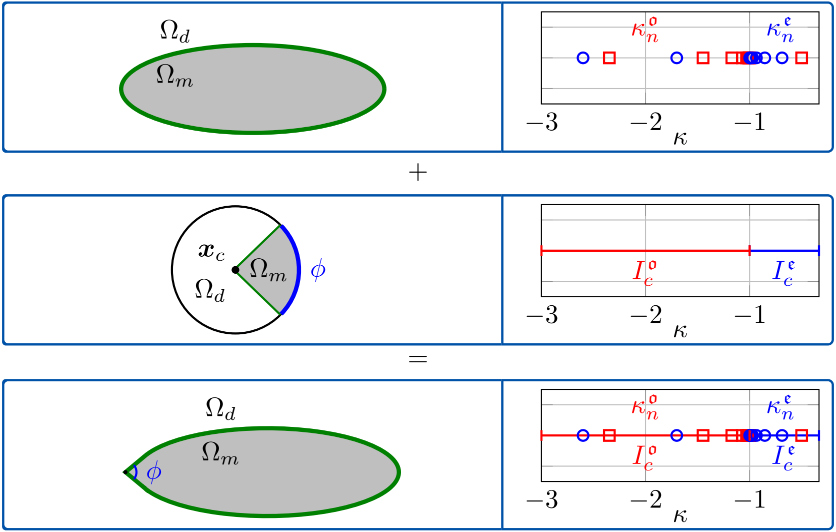


Next: discretization

How to obtain complex plasmonic (CP) resonances?

Strategy based on (Li and Shipman 2019, § 5.2): small perturbation of smooth particle Ω_m by a corner of angle ϕ



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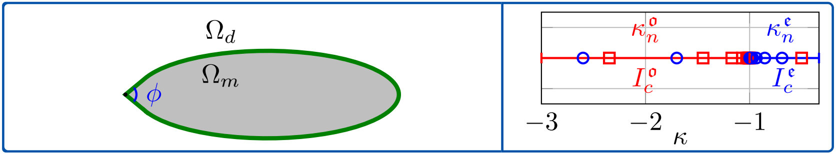


Perturbation mechanism described in (Li and Shipman 2019, § 5.2):

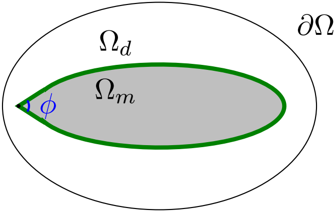
- odd eigenvalues $\kappa_n^{\mathfrak{o}}$ in $I_c^{\mathfrak{e}}$ are perturbed into embedded eigenvalues
- even eigenvalues $\kappa_n^{\mathfrak{e}}$ in $I_c^{\mathfrak{e}}$ are perturbed into complex resonances

Known results from spectral studies of the Neumann-Poincaré operator (double-layer potential) (Khavinson, Putinar, and Shapiro 2007):

- Numerical evidence of embedded eigenvalues κ_n (Helsing, Kang, and Lim 2017)
- Existence theorem for embedded eigenvalues (Li and Shipman 2019) (Perfekt 2019)

Weak formulation: without scaling

Particle: piecewise-smooth boundary $\partial\Omega_m$ of angle $\phi \in (0, \pi)$.



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

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

Discretization N_h-dimensional generalized eigenvalue problem

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

where each matrix is real symmetric and positive (but not definite).

Weak formulation: with complex scaling

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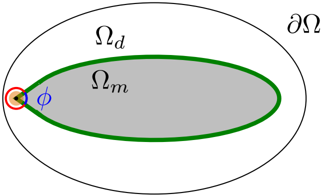
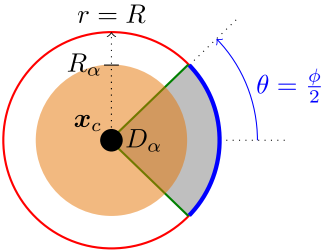


Unknown u in

$$H_e := H_0^1(\Omega)$$



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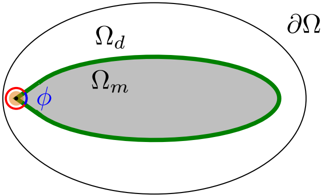

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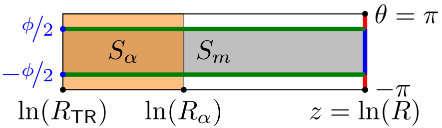
$$H_e := \left\{ u \in H^1(\Omega \backslash \overline{D}) \;\middle|\; u_{|\partial\Omega} = 0 \right\}$$



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

Unknown $\breve{u}$ in

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

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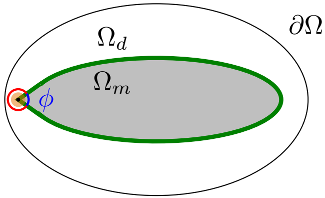

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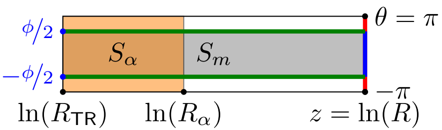

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Solution space with matching condition

$$\{ (u, \breve{u}) \in H_e \times H_c \mid u(x_c + R\cos\theta, R\sin\theta) = \breve{u}(\ln R, \theta) \quad (\theta \in (-\pi, \pi]) \}$$

Discretization yields generalized eigenvalue problem

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

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

Geometry and mesh

⚠ Local mesh symmetry at $\partial\Omega_m$ (Bonnet-Ben Dhia, Carvalho, and Ciarlet 2018).

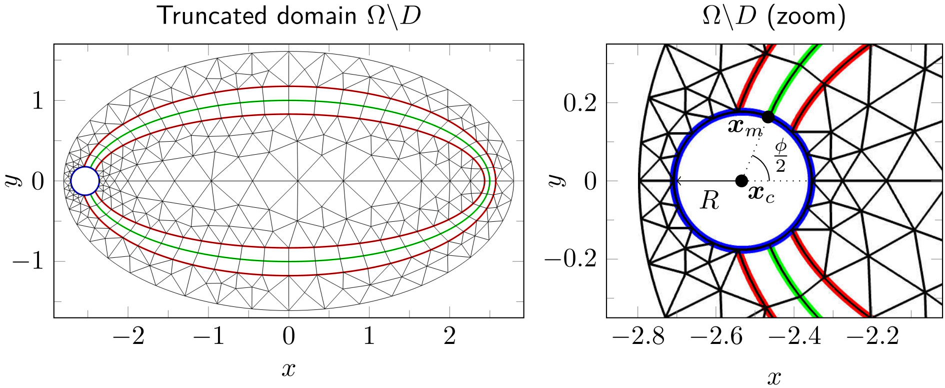

Fig. Mesh topology.

⚠ Corner-ellipse junction at $\boldsymbol{x}_m$ is C^1:

- $\Rightarrow$ boundary $\partial\Omega_m$ uniquely defined by (a_m, b_m, ϕ).
- $\Rightarrow$ perturbation size $R := |\boldsymbol{x}_c - \boldsymbol{x}_m| = f(\phi, a_m, b_m)$

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⚠ Local mesh symmetry at $\partial\Omega_m$ (Bonnet-Ben Dhia, Carvalho, and Ciarlet 2018).

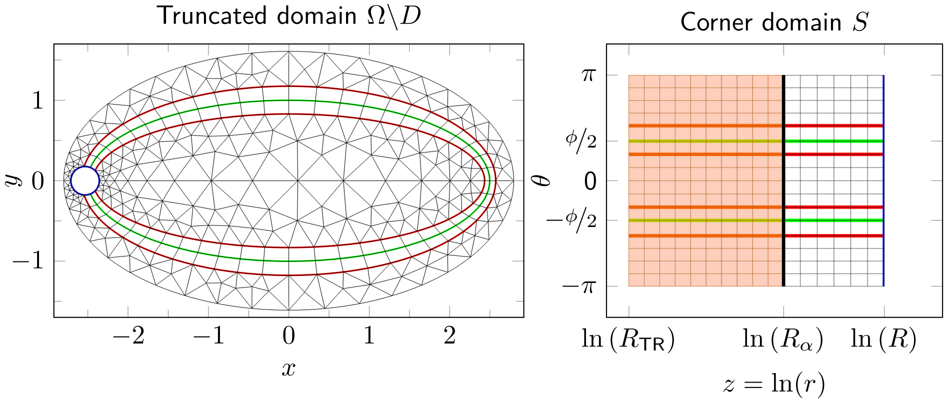

Fig. Mesh topology.

⚠ Corner-ellipse junction at $\boldsymbol{x}_m$ is C^1:

$\Rightarrow$ boundary $\partial\Omega_m$ uniquely defined by (a_m, b_m, ϕ).

$\Rightarrow$ perturbation size $R := |\boldsymbol{x}_c - \boldsymbol{x}_m| = f(\phi, a_m, b_m)$

Results: spectrum

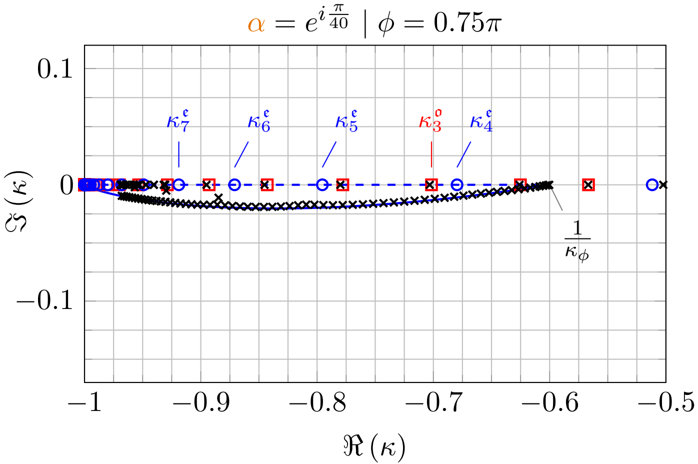

Fig. Spectrum for increasing values of $\arg(\alpha)$.
(×): computed ($N_h = 26345$, $R_\alpha = R/2$, $R_{\text{TR}} = 10^{-50} \cdot R$),
(○): unperturbed even eigenvalues $\kappa_n^{\mathfrak{e}}$, (□): $\kappa_n^{\mathfrak{o}}$,
(—): even critical curve $I_c^{\mathfrak{e},\alpha}$, (—): $I_c^{\mathfrak{o},\alpha}$.

Results: spectrum

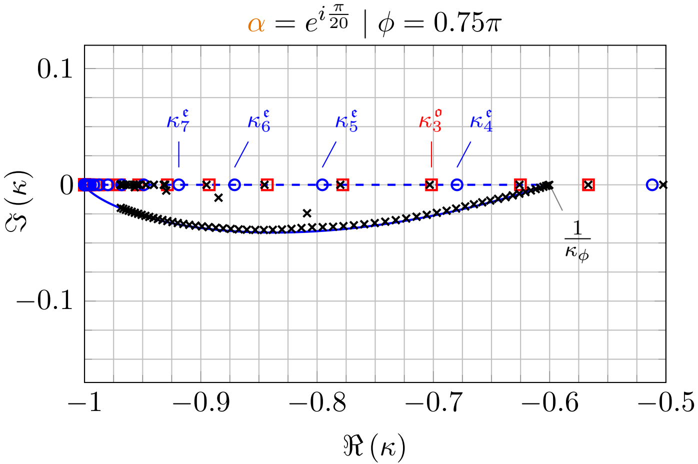

Fig. Spectrum for increasing values of $\arg(\alpha)$.
($\times$): computed ($N_h = 26345$, $R_\alpha = R/2$, $R_{\text{TR}} = 10^{-50} \cdot R$),
($\bigcirc$): unperturbed even eigenvalues $\kappa_n^{\mathfrak{e}}$, ($\square$): $\kappa_n^{\mathfrak{o}}$,
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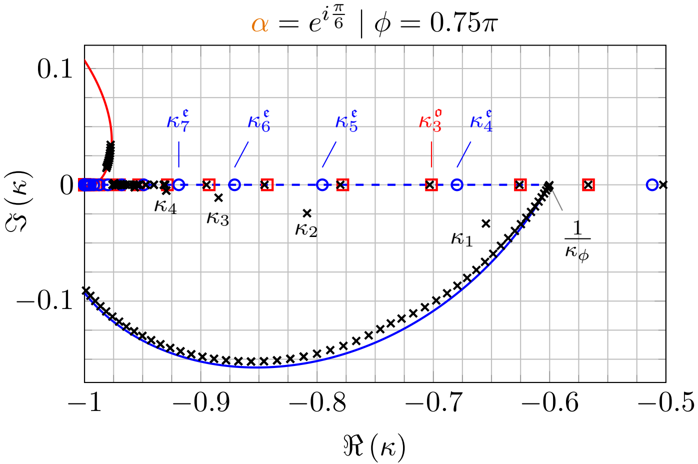

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Results: eigenfunctions

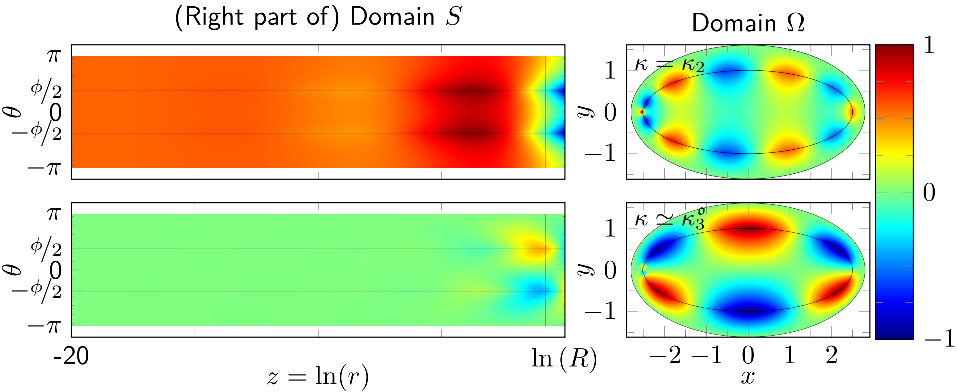

Fig. Eigenfunctions $\Re(u_\alpha)/\|u_\alpha\|_\infty$ of PEP-α with $\alpha = e^{i\frac{\pi}{6}}$.
(Top row) $\kappa = \kappa_2 \simeq 0.8086 - 0.02445i$, complex plasmonic resonance,
(Bottom row) $\kappa \simeq 0.70313 - 8.0357 \cdot 10^{-8}i \simeq \kappa_3^{\mathfrak{o}}$, embedded eigenvalue.

Results: influence of corner angle

$\alpha = e^{i\frac{\pi}{5}} \mid \phi = 0.86\pi$

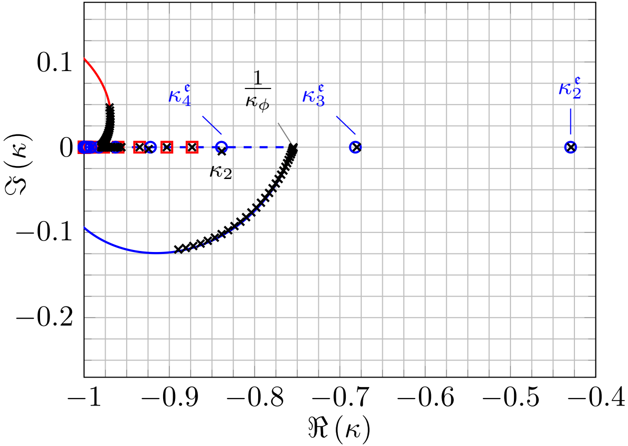

Fig. Spectrum for decreasing values of ϕ (increasing R).
($\times$): computed ($N_h = 35695$, $R_\alpha = R/2$, $R_{\text{TR}} = 10^{-50} \cdot R$),
($\bigcirc$): unperturbed even eigenvalues $\kappa_n^{\mathfrak{e}}$, ($\square$): $\kappa_n^{\mathfrak{o}}$,
(—): even critical curve $I_c^{\mathfrak{e},\alpha}$, (—): $I_c^{\mathfrak{o},\alpha}$.

Results: influence of corner angle

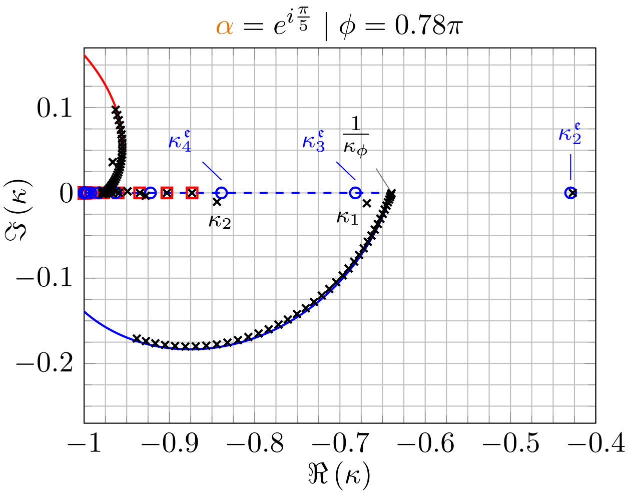

Fig. Spectrum for decreasing values of ϕ (increasing R).
($\times$): computed ($N_h = 35695$, $R_\alpha = R/2$, $R_{\mathsf{TR}} = 10^{-50} \cdot R$),
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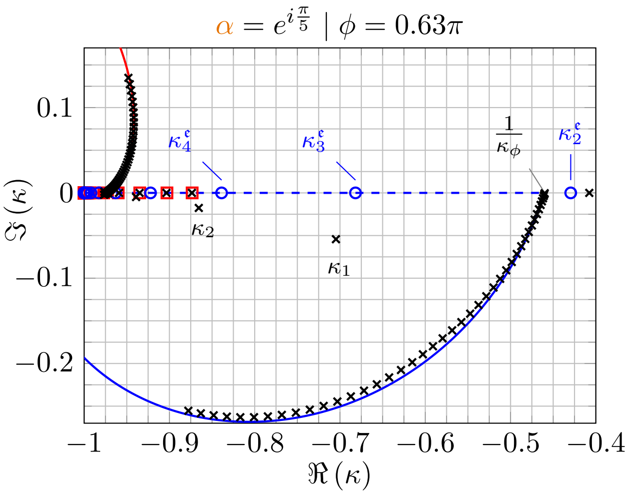
Results: influence of corner angle



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Conclusions & outlook

Takeaways

– Complex plasmonic (CP) resonances

- Defined using multivaluation of set of stable zeros $\kappa \mapsto \widehat{H}_\phi(\kappa)$
- Analogous to complex resonances in scattering: "Infinity $\Leftrightarrow$ Corner"

– Corner complex scaling (Bonnet-Ben Dhia, Carvalho, Chesnel, and Ciarlet 2016)

- Yields a linear eigenvalue problem in κ, valid in uncovered region U_ϕ^α

– Numerical results

- Meshing strategy for ellipse perturbed by corner
- Corroborate mechanism described in (Li and Shipman 2019)

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Takeaways

– Complex plasmonic (CP) resonances

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Outlook

- Drop quasi-static assumption and solve the nonlinear problem in ω
- Interest of working with $\alpha(\kappa)$? (Nannen and Wess 2018)
- Extension to axi-symmetric particles $\Omega_m \subset \mathbb{R}^3$ (Helsing and Perfekt 2018)
- Computation of CP resonances with Boundary Element method? (Helsing, Kang, and Lim 2017) (Helsing and Karlsson 2018)

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

Thanks for your attention. Any questions?

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