Plasmonic Resonances and their Effect on Scattering

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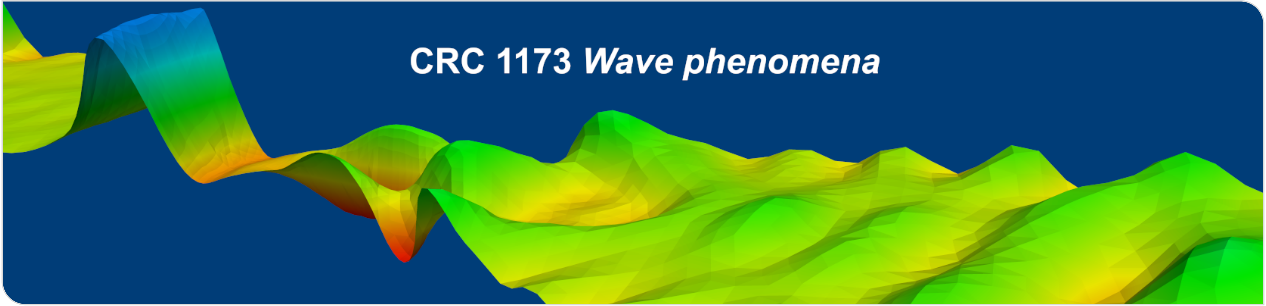


Optical metamaterial cavities

Optical metamaterial cavities:

- Great interest in strongly confining and controlling light.
- Metallic cavity at a nano-scale.
- The permittivity is $\varepsilon_\mathrm{c} < 0$.
  - For the transverse magnetic polarization existence of surface plasmons.
- Applications: surface-enhanced Raman spectroscopy, sensing, antennas, high-resolution imaging, cloaking, etc.

For classic cavities ($\varepsilon_\mathrm{c} > 0$), we have instabilities due to resonances (*Black box scattering*).

▶ **Goal:** extend this to metamaterial cavities.

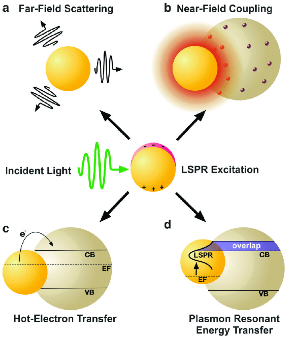
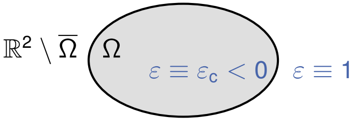


Figure: Erwin, Zarick, Talbert, and Bardhan, *Light trapping in mesoporous solar cells with plasmonic nanostructures*, Energy Environ. Sci., 2016.

Scattering by a 2D transparente cavity



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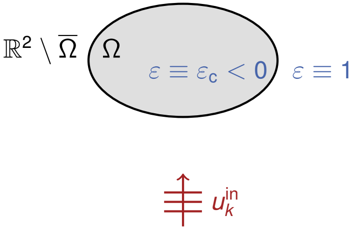
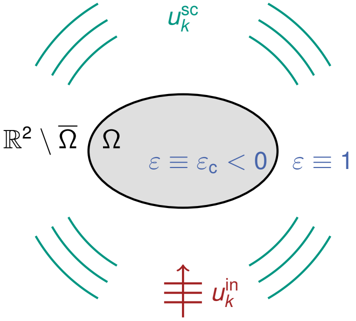


Given:

- a wavenumber $k > 0$
- an incident field $u_k^{\text{in}}(x, y) = e^{iky}$

Scattering by a 2D transparente cavity



Given:

- a wavenumber $k > 0$
- an incident field $u_k^{in}(x, y) = e^{iky}$

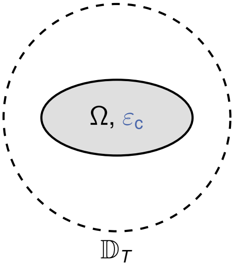
Find: the scattered field $u_k^{sc} \in H^1_{loc}(\mathbb{R}^2)$ such that $u = u_k^{in} + u_k^{sc}$ and

$$\begin{cases} -\operatorname{div}\left(\varepsilon^{-1}\nabla u\right) - k^2 u = 0 & \text{in } \mathbb{R}^2 \\ [u]_{\partial\Omega} = 0 \quad \text{and} \quad \left[\varepsilon^{-1}\partial_{\mathbf{n}} u\right]_{\partial\Omega} = 0 & \text{across } \partial\Omega \\ u_k^{sc} \text{ is } k\text{-outgoing} & \end{cases}$$

u_k^{sc} is k-outgoing: in polar coordinates (r, θ) with $r > \sup_{x\in\Omega}|x|$, we have

$$u_k^{sc}(r, \theta) = \sum_{m\in\mathbb{Z}} \left(a_m H_m^{(1)}(k\,r) + \underbrace{b_m}_{=0} H_m^{(2)}(k\,r)\right) e^{im\theta}$$

Scattering by a 2D transparente cavity: well posedness



Lemma: Bonnet-Ben Dhia, Chesnel, and Ciarlet 2012

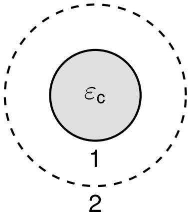
If

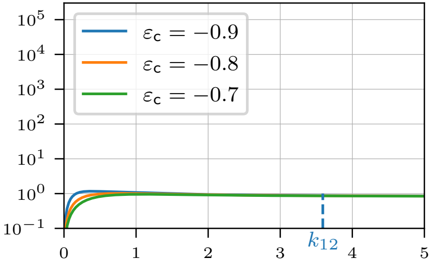
- Ω is smooth
- $\varepsilon_c(\gamma) \neq -1$, for $\gamma \in \partial\Omega$

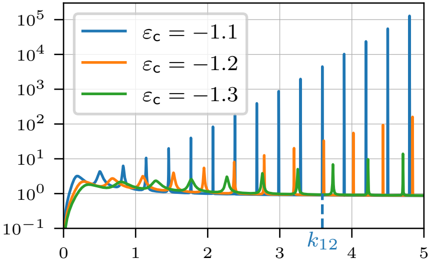
then the scattering problem is well posed and, for a disk $\mathbb{D}_T \supset \Omega$, there exists a constant $C(k) > 0$ such that

$$\frac{\|u_k^{\mathrm{sc}}\|_{L^2(\mathbb{D}_T)}}{\|u_k^{\mathrm{in}}\|_{L^2(\mathbb{D}_T)}} \leq C(k).$$

Disk with $\varepsilon_c \equiv$ cst: plot of $k \mapsto \dfrac{\|u_k^{sc}\|_{L^2(\mathbb{D}_2)}}{\|u_k^{in}\|_{L^2(\mathbb{D}_2)}}$







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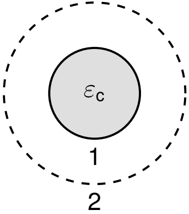
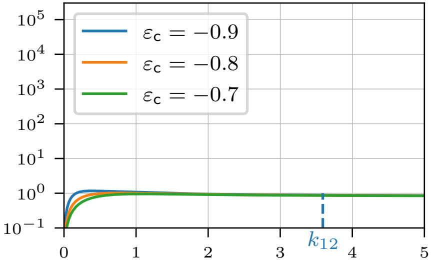
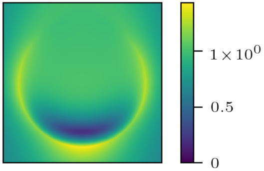
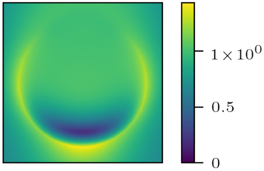
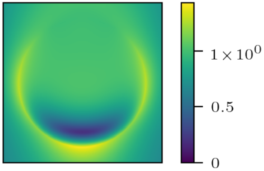




$|u_k^{sc}|$

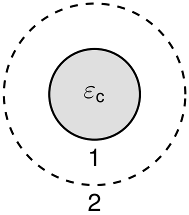




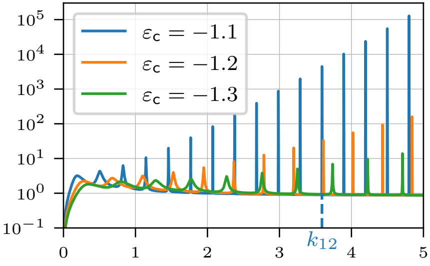


k $\quad k_{12} - 0.01 \quad k_{12} \quad k_{12} + 0.01$

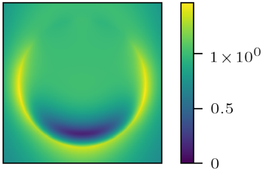
Disk with $\varepsilon_c \equiv$ cst: plot of $k \mapsto \dfrac{\|u_k^{\mathrm{sc}}\|_{L^2(\mathbb{D}_2)}}{\|u_k^{\mathrm{in}}\|_{L^2(\mathbb{D}_2)}}$

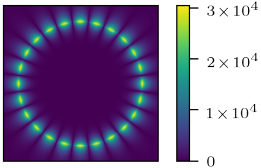


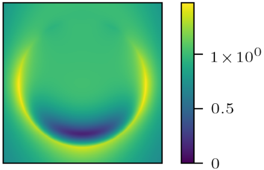
Surface Plasmon Wave (SPW)



$|u_k^{\mathrm{sc}}|$







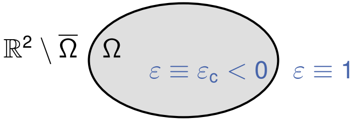
k	$k_{12} - 0.01$	k_{12}	$k_{12} + 0.01$

Scattering resonances of transparente cavities

Ω is smooth

$\varepsilon \neq 0$, discontinuous across $\partial\Omega$

- $\varepsilon \equiv \varepsilon_c < 0$ is $\mathscr{C}^\infty$ in the cavity $\overline{\Omega}$
- $\varepsilon \equiv 1$ in $\mathbb{R}^2 \setminus \overline{\Omega}$



Resonances problem: Find $(\ell^2, u) \in \mathbb{C} \times \mathrm{H}^1_{\mathrm{loc}}(\mathbb{R}^2)$ such that $u \not\equiv 0$ and

$$\begin{cases} -\operatorname{div}(\varepsilon^{-1}\, \nabla u) = \ell^2\, u & \text{in } \mathbb{R}^2 \\ [u]_{\partial\Omega} = 0 \quad \text{and} \quad \left[\varepsilon^{-1}\, \partial_{\mathbf{n}} u\right]_{\partial\Omega} = 0 & \text{across } \partial\Omega \\ u \text{ is } \ell\text{-outgoing} \end{cases}$$

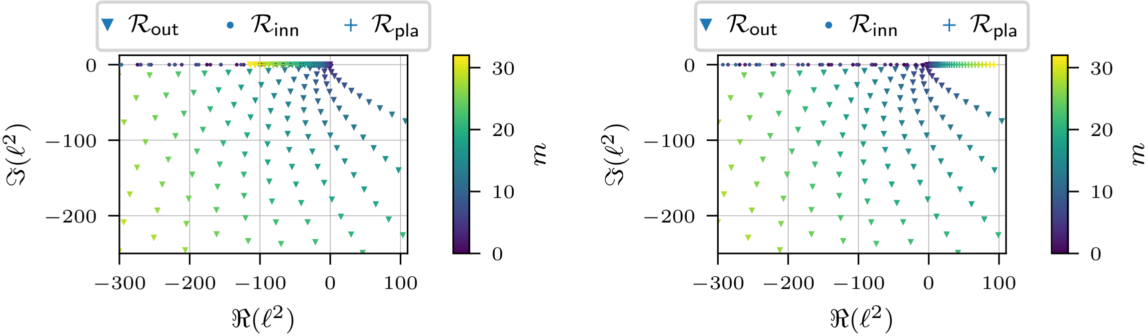
Lemma.

If $\varepsilon_c(\gamma) \neq -1$, for all $\gamma \in \partial\Omega$, on $\partial\Omega$ then the operator $-\operatorname{div}(\varepsilon^{-1}\, \nabla\, \cdot)$ is self-adjoint and

- discrete spectrum $\subset \mathbb{R}^*_-$;
- essential spectrum $= \mathbb{R}_+$;
- resonances $\subset \{z \in \mathbb{C} \mid \Im(z) < 0\}$.

Proof: Costabel and Stephan 1985 + *Black Box Scattering* Dyatlov and Zworski 2019.

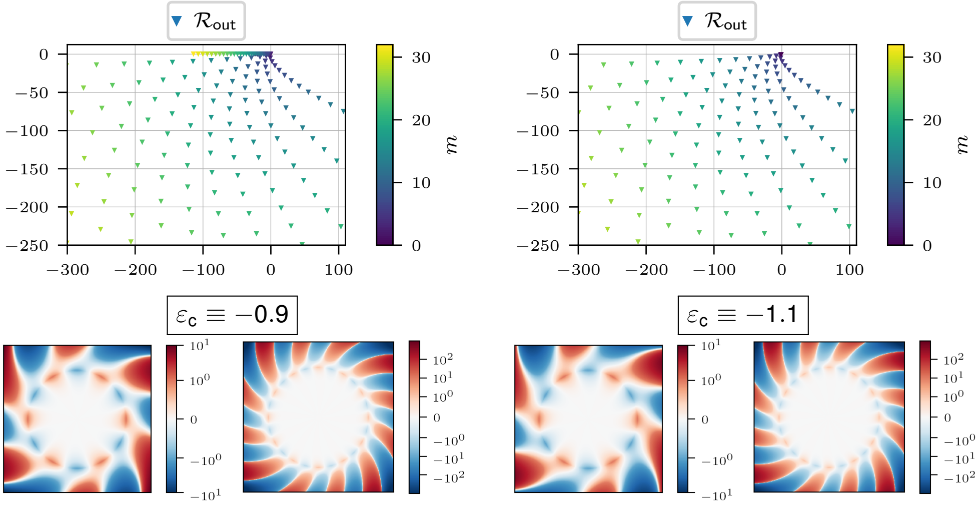
Disk with $\varepsilon_c \equiv$ cst: resonance spectrum



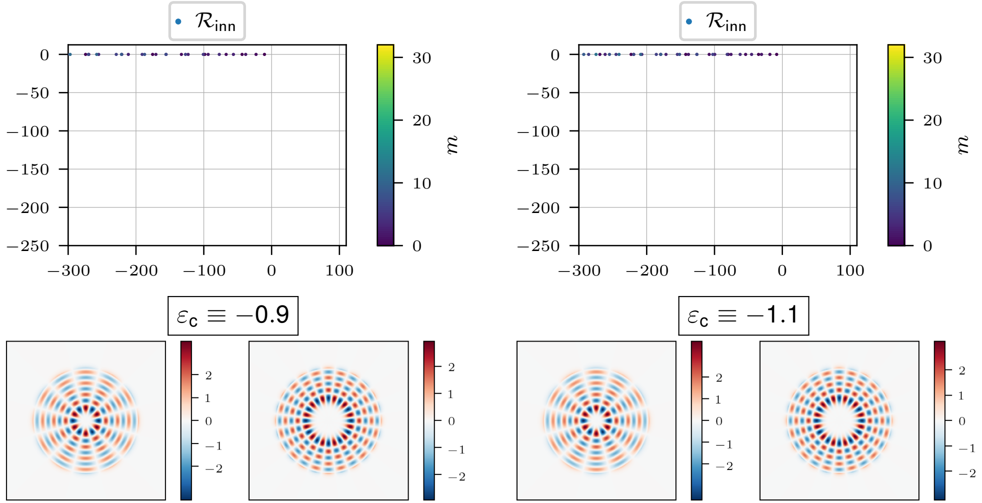
$\varepsilon_c \equiv -0.9$

$\varepsilon_c \equiv -1.1$

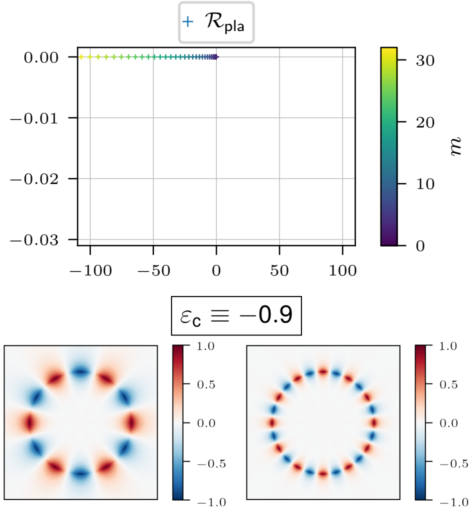
Disk with $\varepsilon_c \equiv$ cst: outer resonances

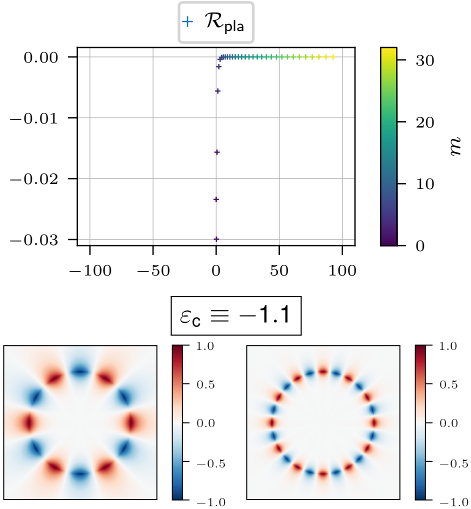


Disk with $\varepsilon_c \equiv$ cst: inner resonances



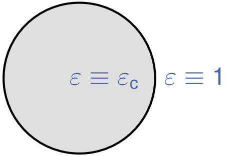
Disk with $\varepsilon_c \equiv$ cst: Surface Plasmon Wave resonances

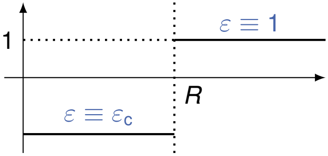




Disk with $\varepsilon_c \equiv$ cst: Angular Fourier Modes

Disk of radius R





Axisymmetry $\Longrightarrow$ angular Fourier decomposition: $\boxed{u(r,\theta) = \sum_{m\in\mathbb{Z}} w_m(r)\,\mathrm{e}^{\mathrm{i}m\theta}}$

$\Longrightarrow$ Family of problems indexed by $m \in \mathbb{Z}$: Find $(\ell, w) \in \mathbb{C} \times \mathrm{H}^1_{\mathrm{loc}}(\mathbb{R}^*_+, r\,\mathrm{d}r)$ such that $w \neq 0$ and

$$\begin{cases} -\dfrac{1}{r}\left(\varepsilon(r)^{-1}\, r\, w_m'\right)' + \varepsilon(r)^{-1}\dfrac{m^2}{r^2}\, w_m = \ell_m^2\, w_m & \text{in } (0,+\infty) \\ [w_m]_{\{R\}} = 0 \quad \text{and} \quad \left[\varepsilon^{-1} w_m'\right]_{\{R\}} = 0 & \text{across } \{R\} \\ w_m(r) = \mathrm{H}^{(1)}_m(\ell_m\, r) & r > R \end{cases}$$

Disk with $\varepsilon_c \equiv$ cst: the Schrödinger Analogy

We transform

$$-\frac{1}{r}\left(\varepsilon(r)^{-1}\, r\, w_m'\right)' + \varepsilon(r)^{-1}\frac{m^2}{r^2}\, w_m = \ell_m^2\, w_m$$

into

$$-m^{-2}\,\mathscr{L} w_m + V\, w_m = \operatorname{sgn}(\varepsilon)\,\lambda\, w_m \qquad \text{where} \begin{cases} m^{-1} & \text{the semiclassical parameter} \\ \lambda = m^{-2}\ell^2 & \text{the spectral parameter} \\ \mathscr{L} w = \dfrac{1}{r}\left(|\varepsilon(r)|^{-1}\, r\, w'\right)' & \text{“Laplacian like”} \\ V(r) = \dfrac{1}{|\varepsilon(r)|\, r^2} & \text{the potential} \end{cases}$$

Disk with $\varepsilon_\mathrm{c} \equiv$ cst: leading term as $m \to +\infty$

The resonances problem become

$$-m^{-2}\mathscr{L} w_m^- + V^- w_m^- = -\lambda w_m^-$$

$$w_m^- = w_m^+$$

$$\varepsilon_\mathrm{c}^{-1}\partial_r w_m^- = \partial_r w_m^+$$

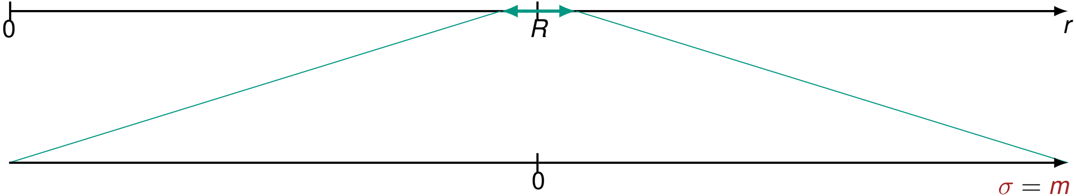
$$-m^{-2}\mathscr{L} w_m^+ + V^+ w_m^+ = \lambda w_m^+$$

Disk with $\varepsilon_c \equiv$ cst: leading term as $m \to +\infty$

The resonances problem become

$$w_m^- = w_m^+$$

$$-m^{-2}\mathscr{L} w_m^- + V^- w_m^- = -\lambda w_m^- \qquad \varepsilon_c^{-1}\partial_r w_m^- = \partial_r w_m^+ \qquad -m^{-2}\mathscr{L} w_m^+ + V^+ w_m^+ = \lambda w_m^+$$



$$\sigma = m\left(\frac{r}{R} - 1\right)$$

$$\varphi^{\pm}(\sigma) = w_m^{\pm}(r)$$

Disk with $\varepsilon_c \equiv$ cst: leading term as $m \to +\infty$

The resonances problem become

$$-m^{-2}\mathscr{L}w_m^- + V^- w_m^- = -\lambda w_m^- \qquad \begin{array}{c} w_m^- = w_m^+ \\ \varepsilon_c^{-1}\partial_r w_m^- = \partial_r w_m^+ \end{array} \qquad -m^{-2}\mathscr{L}w_m^+ + V^+ w_m^+ = \lambda w_m^+$$

0 R r

$$-\partial_\sigma^2\varphi^- + \varphi^- = \varepsilon_c R^2\check{\lambda}\varphi^- \qquad \begin{array}{c} \varphi^- = \varphi^+ \\ \varepsilon_c^{-1}\partial_\sigma\varphi^- = \partial_\sigma\varphi^+ \end{array} \qquad -\partial_\sigma^2\varphi^+ + \varphi^+ = R^2\check{\lambda}\varphi^+ \qquad [+\mathcal{O}(m^{-1})]$$

0

$$\sigma = m\left(\tfrac{r}{R} - 1\right)$$

$$\varphi^\pm(\sigma) = w_m^\pm(r)$$

Disk with $\varepsilon_c \equiv$ cst: leading term as $m \to +\infty$

The resonances problem become

$$w_m^- = w_m^+$$

$$-m^{-2}\mathscr{L} w_m^- + V^- w_m^- = -\lambda w_m^- \qquad \varepsilon_c^{-1}\partial_r w_m^- = \partial_r w_m^+ \qquad -m^{-2}\mathscr{L} w_m^+ + V^+ w_m^+ = \lambda w_m^+$$

0 R r

$$\varphi^- = \varphi^+$$

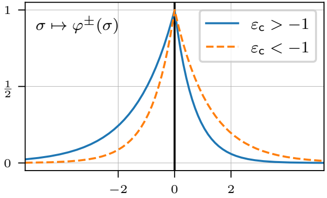
$$-\partial_\sigma^2 \varphi^- + \varphi^- = \varepsilon_c R^2 \check{\lambda} \varphi^- \qquad \varepsilon_c^{-1}\partial_\sigma \varphi^- = \partial_\sigma \varphi^+ \qquad -\partial_\sigma^2 \varphi^+ + \varphi^+ = R^2 \check{\lambda} \varphi^+ \qquad [+\mathcal{O}(m^{-1})]$$

$$\sigma = m\left(\tfrac{r}{R} - 1\right)$$

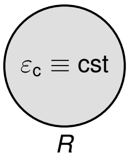
$$\varphi^\pm(\sigma) = w_m^\pm(r)$$

$$\lambda = R^{-2}\left(1 + \varepsilon_c^{-1}\right)$$

$$\varphi^\pm(\sigma) = \exp\left(-\sqrt{|\varepsilon_c|}^{\mp 1}\,|\sigma|\right)$$



Asymptotic expansion of quasi-SPW resonances

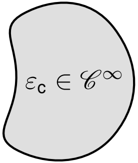


Theorem.

If $\varepsilon_c \neq -1$, then there exists quasi-pair $\left(\underline{\ell}_m^2, \underline{u}_m\right)_{m\geq 1}$ of $u \mapsto -\operatorname{div}(\varepsilon^{-1}\nabla u)$ meaning that

- $\underline{\ell}_m^2 = \left(\frac{m}{R}\right)^2 P\left(R\, m^{-1}\right)$ where P is a **real** function and $P(0) = 1 + \varepsilon_c^{-1}$
- $\|\underline{u}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = 1$ and $\operatorname{supp}\left(\underline{u}_m\right)$ is compact (indep. m)
- $\left\|-\operatorname{div}(\varepsilon^{-1}\nabla \underline{u}_m) - \underline{\ell}_m^2 \underline{u}_m\right\|_{\mathrm{L}^2(\mathbb{R}^2)} = \mathcal{O}\left(m^{-\infty}\right)$ as $m \to +\infty$

Asymptotic expansion of quasi-SPW resonances

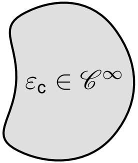


Theorem. Carvalho and Moitier 2020

If Ω is smooth and $\varepsilon_c(\gamma) \neq -1$, for $\gamma \in \partial\Omega$, then there exists quasi-pair $\left(\underline{\ell}_m^2, \underline{u}_m\right)_{m\geq 1}$ of $u \mapsto -\operatorname{div}(\varepsilon^{-1} \nabla u)$ meaning that

- $\underline{\ell}_m^2 = \left(\frac{2\pi m}{|\partial\Omega|}\right)^2 P\left(\frac{|\partial\Omega|}{2\pi} m^{-1}\right)$ where P is a **real** function and
$$P(0) = \left[\frac{1}{|\partial\Omega|} \int_{\partial\Omega} \left[1 + \varepsilon_c|_{\partial\Omega}^{-1}\right]^{-\frac{1}{2}} \mathrm{d}s\right]^{-2}$$
- $\|\underline{u}_m\|_{\mathrm{L}^2(\mathbb{R}^2)} = 1$ and $\operatorname{supp}(\underline{u}_m)$ is compact (indep. m)
- $\left\|-\operatorname{div}(\varepsilon^{-1} \nabla \underline{u}_m) - \underline{\ell}_m^2 \underline{u}_m\right\|_{\mathrm{L}^2(\mathbb{R}^2)} = \mathcal{O}\left(m^{-\infty}\right)$ as $m \to +\infty$

Asymptotic expansion of quasi-SPW resonances



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If Ω is smooth and $\varepsilon_{\mathrm{c}}(\gamma) \neq -1$, for $\gamma \in \partial\Omega$, then there exists quasi-pair $\left(\underline{\ell}_m^2, \underline{u}_m\right)_{m \geq 1}$ of $u \mapsto -\operatorname{div}(\varepsilon^{-1}\, \nabla u)$ meaning that

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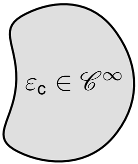
$$P(0) = \left[\frac{1}{|\partial\Omega|}\int_{\partial\Omega}\left[1 + \varepsilon_{\mathrm{c}}|_{\partial\Omega}^{-1}\right]^{-\frac{1}{2}} \mathrm{d}s\right]^{-2}$$
- $\left\|\underline{u}_m\right\|_{\mathrm{L}^2(\mathbb{R}^2)} = 1$ and $\operatorname{supp}\left(\underline{u}_m\right)$ is compact (indep. m)
- $\left\|-\operatorname{div}(\varepsilon^{-1}\, \nabla \underline{u}_m) - \underline{\ell}_m^2 \underline{u}_m\right\|_{\mathrm{L}^2(\mathbb{R}^2)} = \mathcal{O}\left(m^{-\infty}\right)$ as $m \to +\infty$

Proof: Construction of power series using matching asymptotic expansion / semi-WKB + Borel summation.

Asymptotic expansion of quasi-SPW resonances



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If Ω is smooth and $\varepsilon_c(\gamma) \neq -1$, for $\gamma \in \partial\Omega$, then there exists quasi-pair $\left(\underline{\ell}_m^2, \underline{u}_m\right)_{m\geq 1}$ of $u \mapsto -\operatorname{div}(\varepsilon^{-1}\nabla u)$ meaning that

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$$P(0) = \left[\frac{1}{|\partial\Omega|}\int_{\partial\Omega}\left[1 + \varepsilon_c|_{\partial\Omega}^{-1}\right]^{-\frac{1}{2}} \mathrm{d}s\right]^{-2}$$
- $\left\|\underline{u}_m\right\|_{\mathrm{L}^2(\mathbb{R}^2)} = 1$ and $\operatorname{supp}\left(\underline{u}_m\right)$ is compact (indep. m)
- $\left\|-\operatorname{div}(\varepsilon^{-1}\nabla \underline{u}_m) - \underline{\ell}_m^2 \underline{u}_m\right\|_{\mathrm{L}^2(\mathbb{R}^2)} = \mathcal{O}\left(m^{-\infty}\right)$ as $m \to +\infty$

- m: number of oscillation along $\partial\Omega$.
- inner and outer boundary layer $\sim m^{-1}$.
- The Taylor coefficient of P can be computed with by computer algebra system (for example: SymPy).

Effect on scattering

Recall the definition of the stability constant $C(k)$, if Ω is smooth and $\varepsilon_{\mathrm{c}}(\gamma) \neq -1$, for $\gamma \in \partial\Omega$, we have

$$\frac{\| u_k^{\mathrm{sc}} \|_{\mathrm{L}^2(\mathbb{D}_T)}}{\| u_k^{\mathrm{in}} \|_{\mathrm{L}^2(\mathbb{D}_T)}} \leq C(k).$$

Theorem: Carvalho and Moitier 2020

If Ω is smooth and $\varepsilon_{\mathrm{c}}(\gamma) < -1$, for $\gamma \in \partial\Omega$, then, as $m \to +\infty$, for all $N \geq 0$ there exists $c_N > 0$ such that

$$C\left(\underline{\ell}_m = \frac{2\pi m}{|\partial\Omega|} \sqrt{P\left(\frac{|\partial\Omega|}{2\pi m}\right)}\right) \geq c_N\, m^N.$$

- The peaks occur for the Surface Plasmon Waves.

Final remarks

Karlsruhe Institute of Technology

Conclusion:

- We have characterized the SPW for metamaterial cavities via asymptotic.
- If $\varepsilon_{\mathrm{c}} < -1$, the scattering problem is well posed but has sharp instabilities.

Future works:

- What happends when the cavity has corners.
- Change the mathematical settings to 3D Helmholtz and 3D Maxwell.

Bibliography

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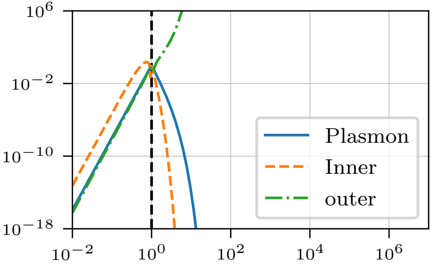
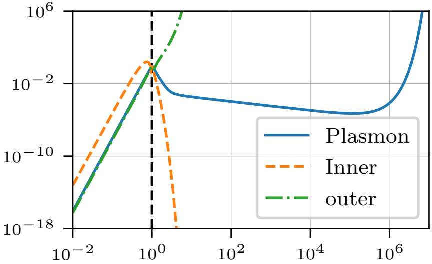
Thank you for your attention

Comparaison resonances modes

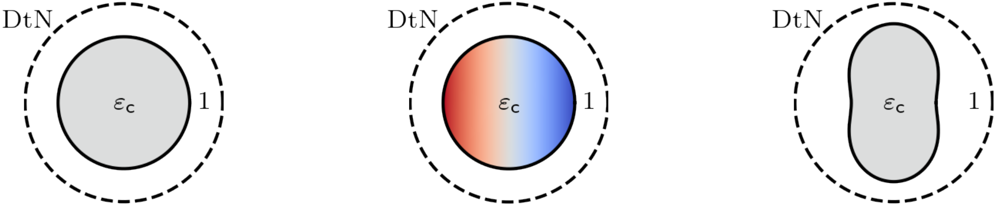


$\varepsilon_c \equiv -0.9$

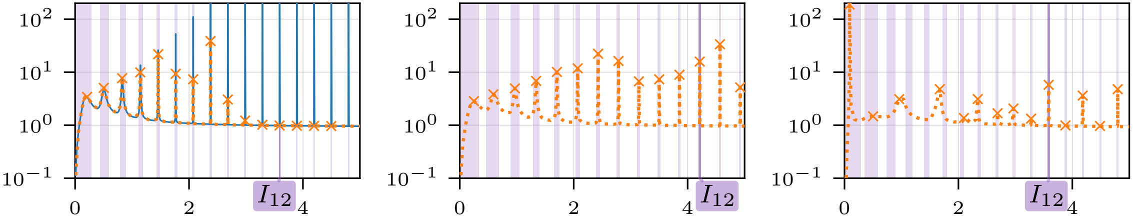


$\varepsilon_c \equiv -1.1$

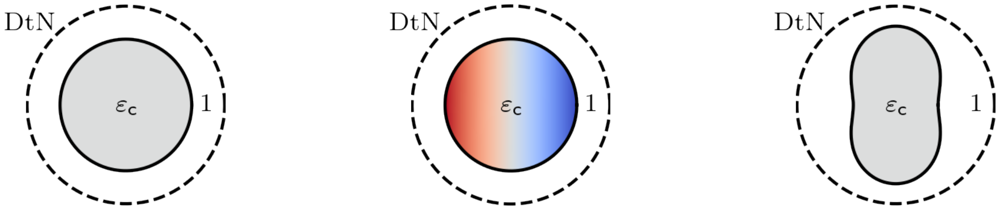
Numerical results by general cavity: $\varepsilon_c < -1$



FEM with XLiFE++: geometry degree 3 (GMSH), FE degree 7, DOFs $\sim$ 23000, k-grid $\sim$ 230 points.



Numerical results by general cavity: $\varepsilon_c > -1$



FEM with XLiFE++: geometry degree 3 (GMSH), FE degree 7, DOFs $\sim$ 23000, *k*-grid 230 points.