SEMINAR ON NUMERICAL ANALYSIS AND COMPUTATIONAL SCIENCE

Investigation of some transmission problems with sign changing coefficients. Application to metamaterials.

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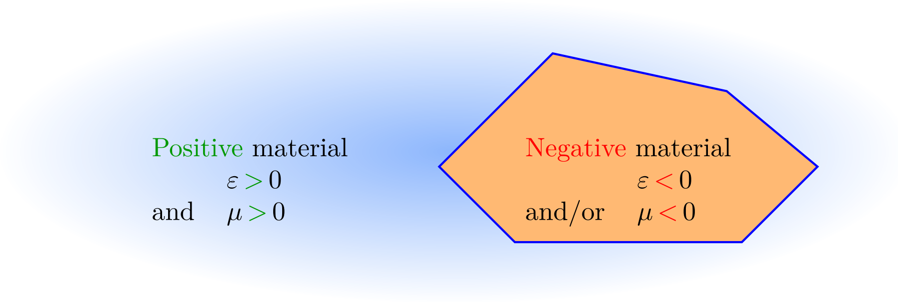
AALTO UNIVERSITY, APRIL 26TH, 2013

Introduction: objective

Scattering by a negative material in electromagnetism in 3D in time-harmonic regime (at a given frequency):



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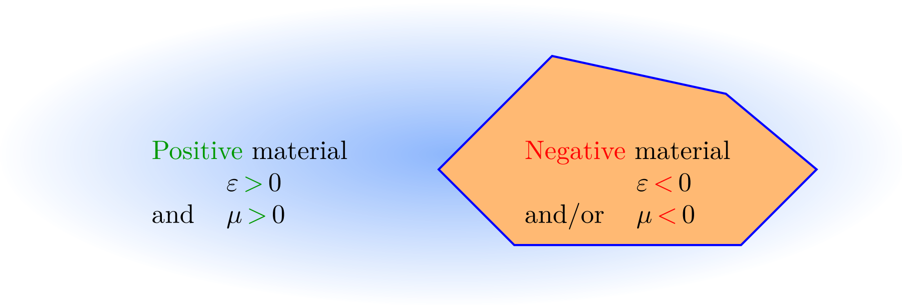

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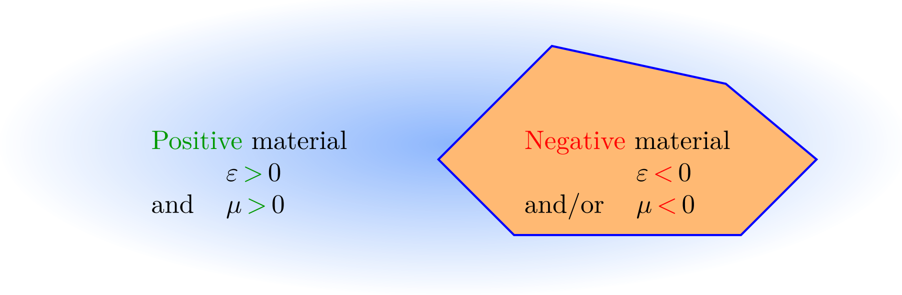

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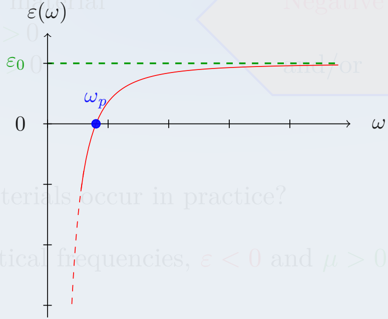
$$\varepsilon(\omega) = \varepsilon_0 \left(1 - \frac{{\omega_p}^2}{\omega^2}\right),$$

where ω_p is the plasma frequency.



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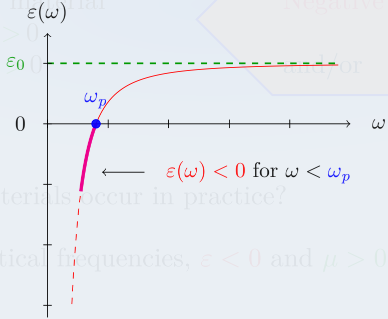

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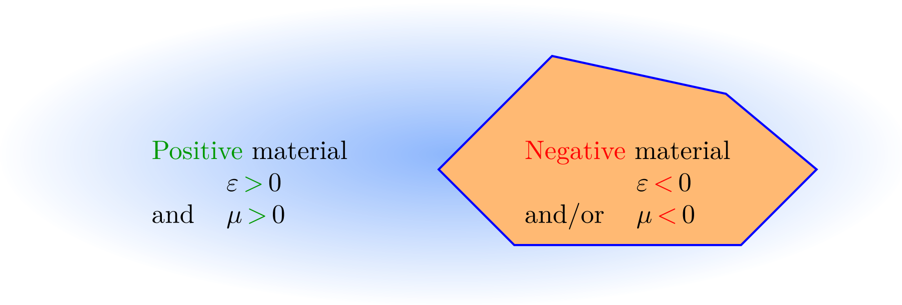

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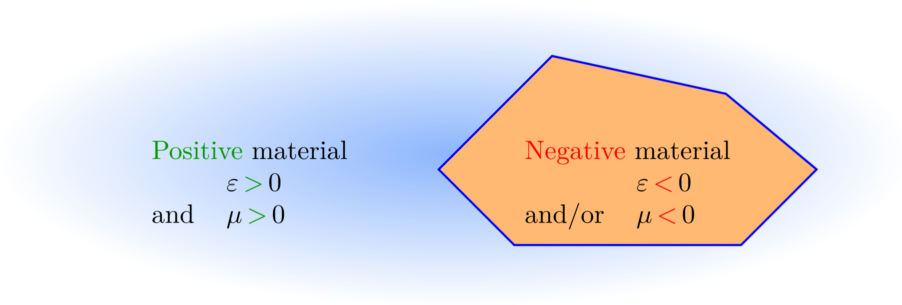

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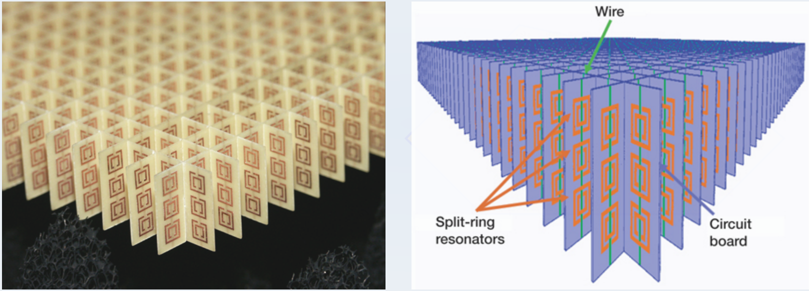
Zoom on a metamaterial: practical realizations of metamaterials are achieved by a periodic assembly of small resonators.



EXAMPLE OF METAMATERIAL (NASA)

Mathematical justification of the homogenized model (`Bouchitté, Bourel, Felbacq 09`).

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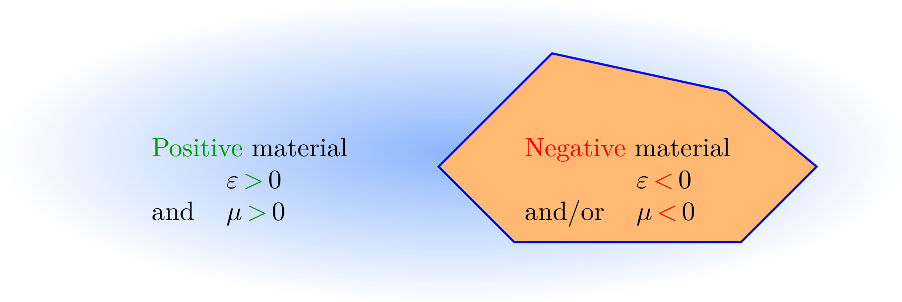

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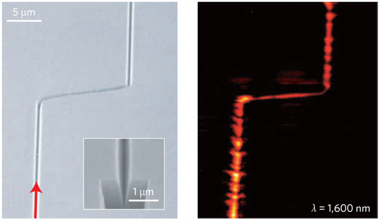
- Surface Plasmons Polaritons that propagate at the interface between a metal and a dielectric can help reducing the size of computer chips.



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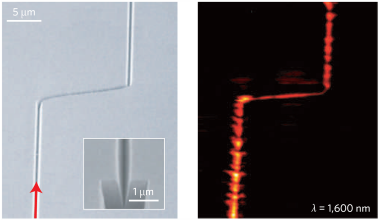

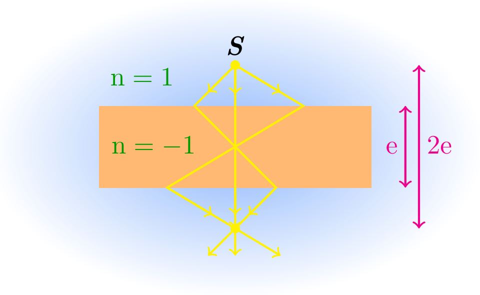

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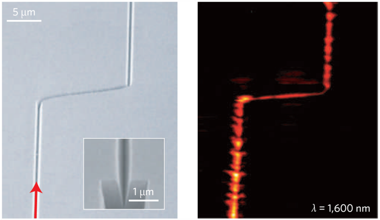

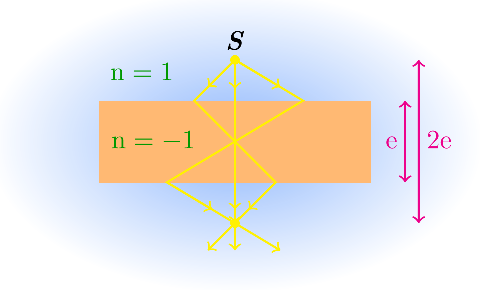

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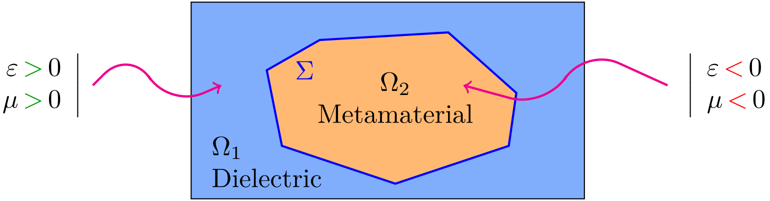
Interfaces between negative materials and dielectrics occur in all (exciting) applications...

Introduction: in this talk

Problem set in a bounded domain $\Omega \subset \mathbb{R}^3$:



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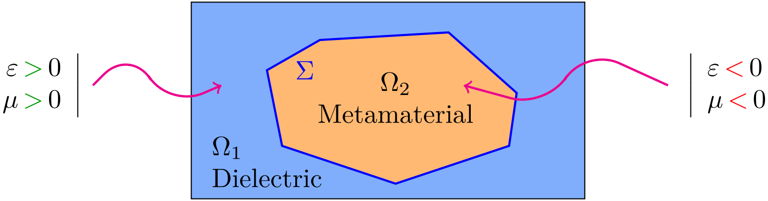

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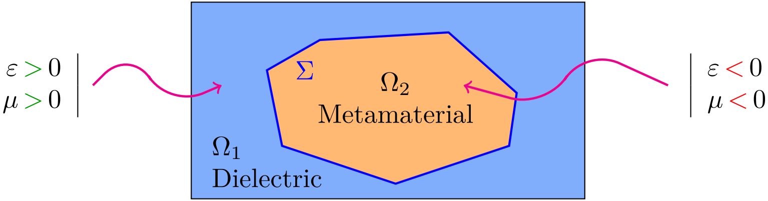

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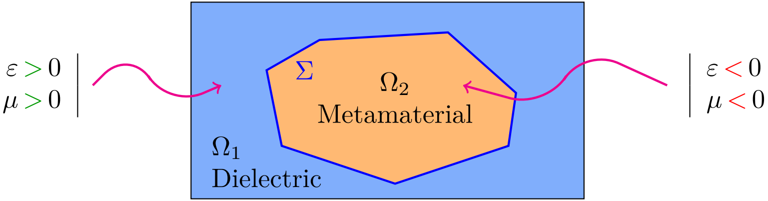

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Σ

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Metamaterial

Ω_1
Dielectric

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The relevant question is then: what happens if dissipation is neglected ?

- Does well-posedness still hold?
- What is the appropriate functional framework?
- What about the convergence of approximation methods?

Outline of the talk

1. The coerciveness issue for the scalar case

We develop a T-coercivity method based on geometrical transformations to study $\mathbf{div}(\mu^{-1}\nabla\cdot) : \mathbf{H}^1_0(\Omega) \rightarrow \mathbf{H}^{-1}(\Omega)$ (improvement over `Bonnet-Ben Dhia et al. 10`, `Zwölf 08`).

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2. A new functional framework in the critical interval

We propose a new functional framework when $\mathbf{div}(\mu^{-1}\nabla\cdot):\mathbf{X}\to\mathbf{Y}$ is not Fredholm for $\mathrm{X}=\mathrm{H}^1_0(\Omega)$ and $\mathrm{Y}=\mathrm{H}^{-1}(\Omega)$ (extension of `Dauge, Texier 97`, `Ramdani 99`).

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3. A curious instability phenomenon

We prove a curious instability phenomenon for a rounded corner when the rounding parameter tends to zero.

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A scalar model problem

Problem for E_z in 2D in case of an invariance with respect to z:

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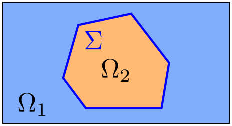

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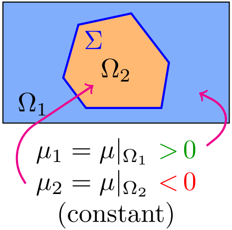

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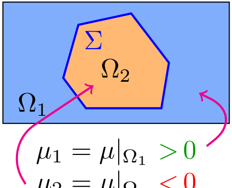

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with $a(u,v) = \displaystyle\int_\Omega \mu^{-1}\,\nabla u \cdot \nabla v$ and $l(v) = \langle f, v\rangle_\Omega$.

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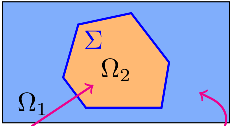

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Definition. We will say that the problem $(\mathscr{P})$ is well-posed if the operator $A = \operatorname{div}(\mu^{-1}\nabla\cdot)$ is an isomorphism from $\mathrm{H}^1_0(\Omega)$ to $\mathrm{H}^{-1}(\Omega)$.

Mathematical difficulty

- Classical case $\mu > 0$ everywhere:

$$a(u,u) = \int_\Omega \mu^{-1} |\nabla u|^2 \geq \min(\mu^{-1}) \, \|u\|^2_{\mathrm{H}^1_0(\Omega)} \qquad \text{coercivity}$$

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  - When $\mu_2 = -\mu_1$, $(\mathscr{P})$ is always ill-posed (`Costabel-Stephan 85`). For a symmetric domain (w.r.t. Σ) we can build a kernel of infinite dimension.

Idea of the `T`-coercivity 1/2

Let `T` be an isomorphism of $\mathrm{H}^1_0(\Omega)$.

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Goal: Find $\mathtt{T}$ such that a is $\mathtt{T}$-coercive: $\displaystyle\int_\Omega \mu^{-1} \nabla u \cdot \nabla(\mathtt{T}u) \geq C \, \|u\|^2_{\mathrm{H}^1_0(\Omega)}$.

In this case, Lax-Milgram $\Rightarrow$ $(\mathscr{P}_V^{\mathtt{T}})$ (and so $(\mathscr{P}_V)$) is well-posed.

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In this case, Lax-Milgram $\Rightarrow$ $(\mathscr{P}_V^{\mathtt{T}})$ (and so $(\mathscr{P}_V)$) is well-posed.

① Define $\mathtt{T}_1 u = \left| \begin{array}{ll} u_1 & \text{in } \Omega_1 \\ -u_2 + ... & \text{in } \Omega_2 \end{array} \right.$

Idea of the T-coercivity 1/2

Let $\mathtt{T}$ be an isomorphism of $\mathrm{H}^1_0(\Omega)$.

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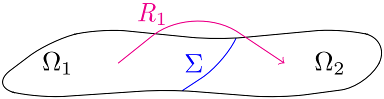

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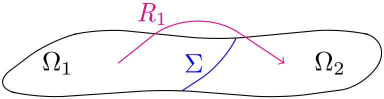

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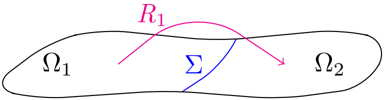

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On Σ, we have $-u_2 + 2R_1 u_1 = -u_2 + 2u_1 = u_1 \Rightarrow \mathtt{T}_1 u \in \mathrm{H}^1_0(\Omega)$.

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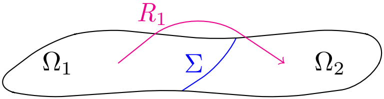

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❸ One has $a(u, \mathtt{T}_1 u) = \displaystyle\int_\Omega |\mu|^{-1} |\nabla u|^2 - 2 \int_{\Omega_2} \mu_2^{-1} \nabla u \cdot \nabla (R_1\, u_1)$

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⑤ Conclusion:

THEOREM. If the contrast $\kappa_\mu = \mu_2/\mu_1 \notin [-\|R_1\|^2; -1/\|R_2\|^2]$, then the operator $\mathrm{div}\,(\mu^{-1}\,\nabla\cdot)$ is an isomorphism from $\mathrm{H}^1_0(\Omega)$ to $\mathrm{H}^{-1}(\Omega)$.

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The interval depends on the norms of the transfer operators

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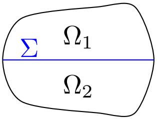
Choice of R_1,R_2?

- A simple case: symmetric domain



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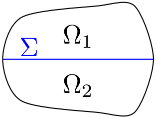

$$R_1 = R_2 = S_{\Sigma}$$

so that $\|R_1\| = \|R_2\| = 1$

$(\mathscr{P})$ well-posed $\Leftrightarrow$ $\kappa_\mu \neq -1$

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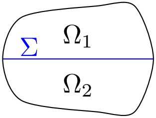

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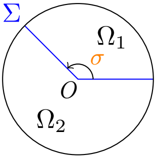
- Interface with a 2D corner



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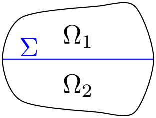

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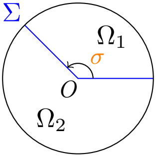

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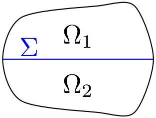

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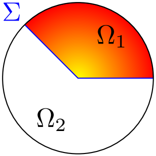

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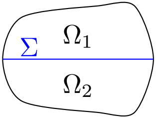

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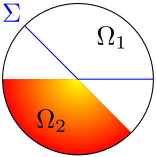

Action of R_1: symmetry w.r.t θ

Choice of R_1,R_2?

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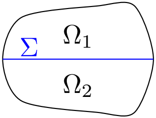

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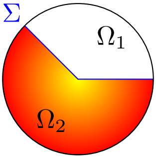

Action of R_1: symmetry + dilatation w.r.t θ

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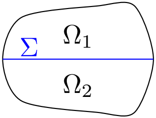

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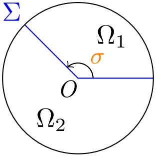

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$$\|R_1\|^2 \qquad = \mathcal{R}_\sigma := (2\pi - \sigma)/\sigma$$

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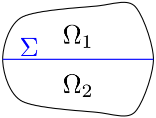

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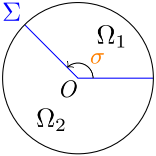

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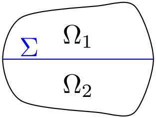

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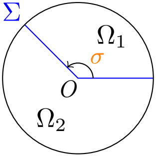

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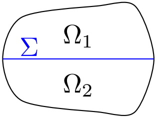

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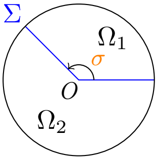

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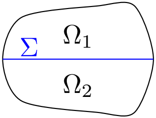

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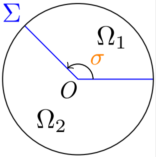
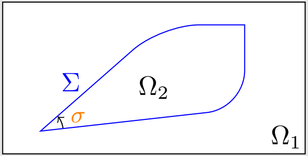
$\neq -1$

- Interface with





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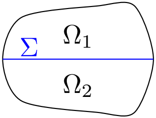

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$= 1$

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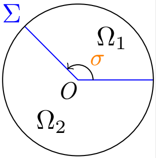

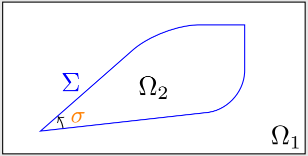

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- By localization techniques, we prove

Proposition. ($\mathscr{P}$) is well-posed in the Fredholm sense for a curvilinear polygonal interface iff $\kappa_\mu \notin [-\mathcal{R}_\sigma; -1/\mathcal{R}_\sigma]$ where σ is the smallest angle.

⇒When Σ is smooth, ($\mathscr{P}$) is well-posed in the Fredholm sense iff $\kappa_\mu \neq -1$.

Extensions for the scalar case

- The `T`-coercivity approach can be used to deal with non constant μ_1, μ_2 and with the Neumann problem.

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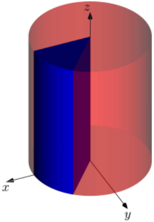
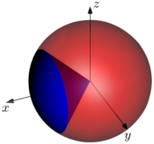
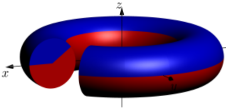
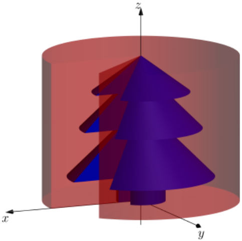
- 3D geometries can be handled in the same way.

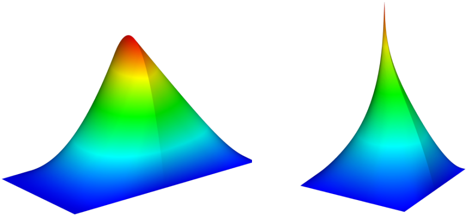








- The `T`-coercivity technique allows to justify convergence of standard finite element method for simple meshes (`Bonnet-Ben Dhia et al. 10`, `Nicaise, Venel 11`, `Chesnel, Ciarlet 12`).



Digression: the result for Maxwell's equations

Consider $\boldsymbol{F} \in \mathbf{L}^2(\Omega)$ such that div $\boldsymbol{F} \in \mathbf{L}^2(\Omega)$.

THEOREM. Suppose

$$(\varphi, \varphi') \mapsto \int_\Omega \varepsilon \nabla\varphi \cdot \nabla\varphi' \text{ is T-coercive on } \mathrm{H}^1_0(\Omega); \qquad (\mathcal{A}_\varepsilon)$$

$$(\varphi, \varphi') \mapsto \int_\Omega \mu \nabla\varphi \cdot \nabla\varphi' \text{ is T-coercive on } \mathrm{H}^1(\Omega)/\mathbb{R}. \qquad (\mathcal{A}_\mu)$$

Then, the problem for the magnetic field

$$\left| \begin{array}{ll} \text{Find } \boldsymbol{H} \in \mathbf{H}(\mathbf{curl}\,;\Omega) \text{ such that:} & \\ \mathbf{curl}\,(\varepsilon^{-1}\mathbf{curl}\,\boldsymbol{H}) - \omega^2\mu\boldsymbol{H} = \boldsymbol{F} & \text{in } \Omega \\ \varepsilon^{-1}\mathbf{curl}\,\boldsymbol{H} \times \boldsymbol{n} = 0 & \text{on } \partial\Omega \\ \mu\boldsymbol{H} \cdot \boldsymbol{n} = 0 & \text{on } \partial\Omega. \end{array} \right.$$

is well-posed for all $\omega \in \mathbb{C}\backslash\mathscr{S}$ where $\mathscr{S}$ is a discrete (or empty) set of $\mathbb{C}$.

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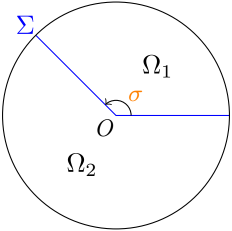
- This result (with the same assumptions) is also true for the problem for the electric field.

Transition: from variational methods to Fourier/Mellin techniques

❓ For the corner case, what happens when the contrast lies inside the criticial interval, *i.e.* when $\kappa_\mu \in [-\mathcal{R}_\sigma; -1/\mathcal{R}_\sigma]$???



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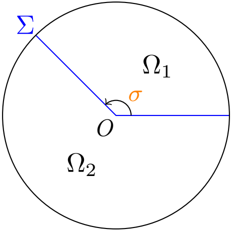


Idea: we will study precisely the regularity of the “solutions” using the Kondratiev’s tools, *i.e.* the Fourier/Mellin transform (`Dauge, Texier 97`, `Nazarov, Plamenevsky 94`).

1. The coerciveness issue for the scalar case

2. A new functional framework in the critical interval

   ⇒ collaboration with `X. Claeys` (LJLL Paris VI).

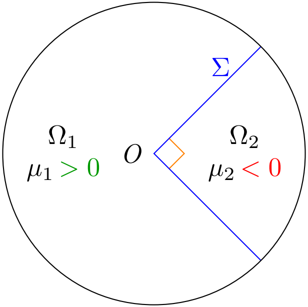
3. A curious instability phenomenon

Problem considered in this section

- We recall the problem under consideration

$$(\mathscr{P}) \left| \begin{array}{l} \text{Find } u \in \mathrm{H}^1_0(\Omega) \text{ such that:} \\ -\mathrm{div}(\mu^{-1}\nabla u) = f \quad \text{in } \Omega. \end{array} \right.$$

- To simplify the presentation, we work on a particular configuration.



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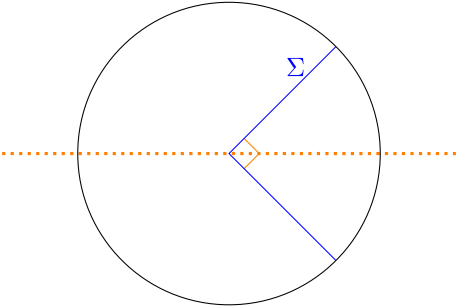

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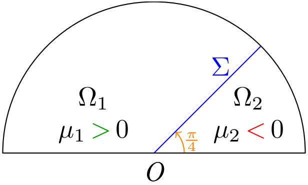

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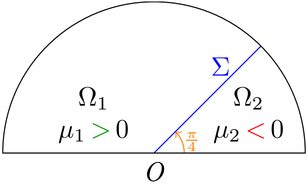

- Using the variational method of the previous section, we prove the

PROPOSITION. The problem $(\mathscr{P})$ is well-posed as soon as the contrast $\kappa_\mu = \mu_2/\mu_1$ satisfies $\kappa_\mu \notin [-3; -1]$.

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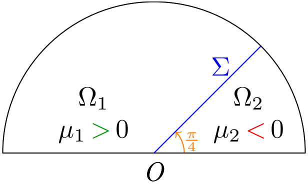

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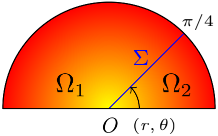
Proposition. The problem $(\mathscr{P})$ is well-posed as soon as the contrast $\kappa_\mu = \mu_2/\mu_1$ satisfies $\kappa_\mu \notin [-3; -1]$.

What happens when $\kappa_\mu \in [-3; -1)$?

Analogy with a waveguide problem

- Bounded sector Ω



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Analogy with a waveguide problem

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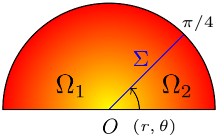

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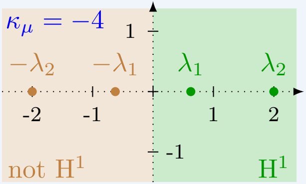
- Singularities in the sector

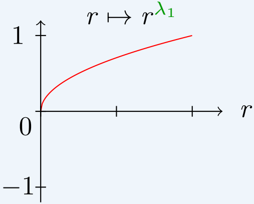
$s(r,\theta) = r^\lambda\varphi(\theta)$

Analogy with a waveguide problem

We compute the singularities $s(r,\theta) = r^{\lambda}\varphi(\theta)$ and we observe two cases:

- Outside the critical interval





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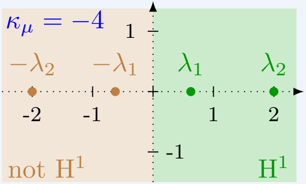

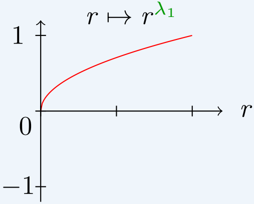

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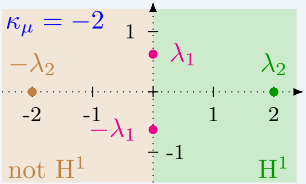

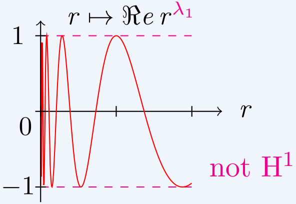

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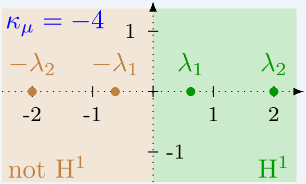

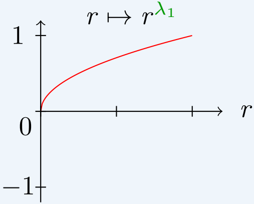

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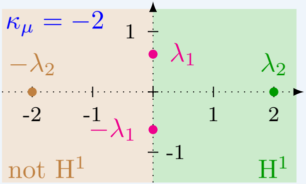
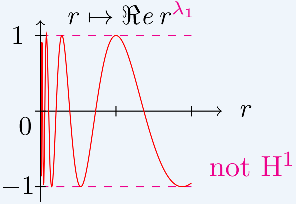
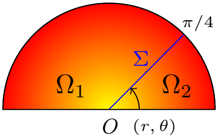




How to deal with the propagative singularities inside the critical interval?

Analogy with a waveguide problem

- Bounded sector Ω



- Equation:

$$\underbrace{-\mathrm{div}(\mu^{-1}\,\nabla u)}_{-r^{-2}(\mu^{-1}(r\partial_r)^2+\partial_\theta\mu^{-1}\partial_\theta)u} = f$$

- Singularities in the sector

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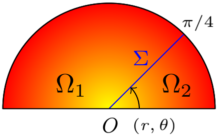
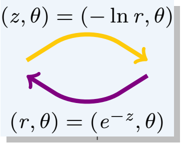
Analogy with a waveguide problem

- Bounded sector Ω





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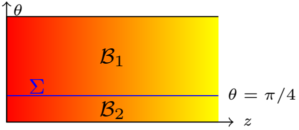
- Half-strip $\mathcal{B}$



Analogy with a waveguide problem

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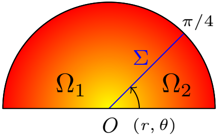

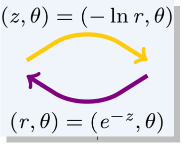

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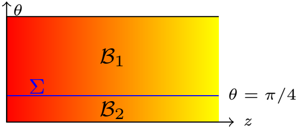

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Analogy with a waveguide problem

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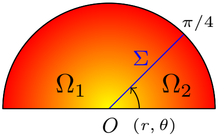

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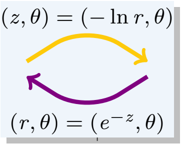

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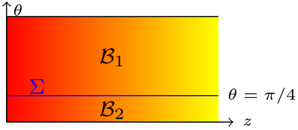

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- Modes in the strip

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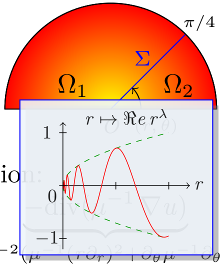
Analogy with a waveguide problem

- Bounded sector Ω



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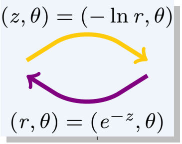

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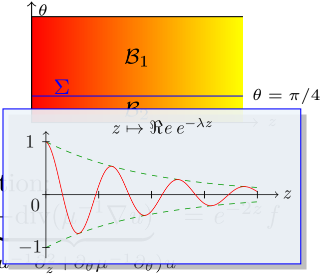

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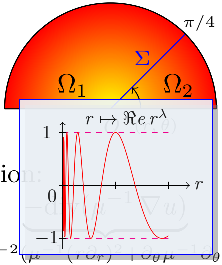
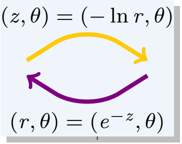
$s \in \mathrm{H}^1(\Omega)$ $\Re e\,\lambda > 0$ m is evanescent

Analogy with a waveguide problem

- Bounded sector Ω





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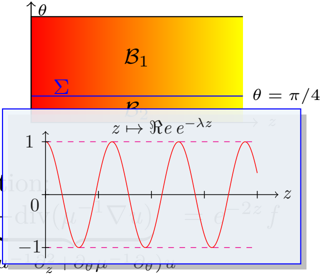

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$$s(r,\theta) = r^{\lambda}\varphi(\theta)$$
$$= \cancel{r^{a}}\,(\cos b\ln r + i\sin b\ln r)\varphi(\theta)$$

- Modes in the strip

$$m(z,\theta) = e^{-\lambda z}\varphi(\theta)$$
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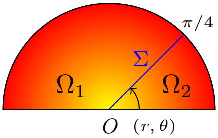
$(\Re e\,\lambda = a,\ \Im m\,\lambda = b)$

$s \in \mathrm{H}^1(\Omega)$	$\Re e\,\lambda > 0$	m is evanescent
$s \notin \mathrm{H}^1(\Omega)$	$\Re e\,\lambda = 0$	m is propagative

Analogy with a waveguide problem

- Bounded sector Ω



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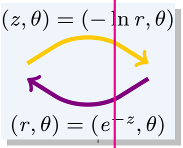
- Singularities in the sector

$$\begin{aligned} s(r,\theta) &= r^{\lambda}\varphi(\theta) \\ &= \cancel{r^{a}}\,(\cos b\ln r + i\sin b\ln r)\varphi(\theta) \end{aligned}$$



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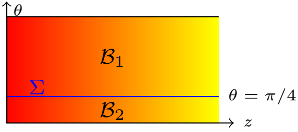


- Equation:

$$\underbrace{-\mathrm{div}(\mu^{-1}\nabla u)}_{-(\mu^{-1}\partial_z^2+\partial_\theta\mu^{-1}\partial_\theta)u} \quad = e^{-2z}f$$

- Modes in the strip

$$\begin{aligned} m(z,\theta) &= e^{-\lambda z}\varphi(\theta) \\ &= \cancel{e^{-az}}\,(\cos bz - i\sin bz)\varphi(\theta) \end{aligned}$$

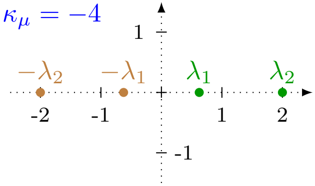
$(\Re e\,\lambda = a,\ \Im m\,\lambda = b)$

$s \in \mathrm{H}^1(\Omega)$ $\qquad \Re e\,\lambda > 0$ $\qquad m$ is evanescent

$s \notin \mathrm{H}^1(\Omega)$ $\qquad \Re e\,\lambda = 0$ $\qquad m$ is propagative

► This encourages us to use modal decomposition in the half-strip.

Modal analysis in the waveguide



- Outside the critical interval. All the modes are exponentially growing or decaying.

→ We look for an exponentially decaying solution. H^1 framework

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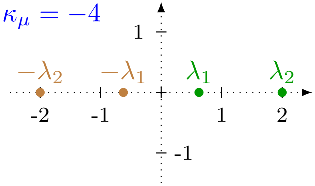

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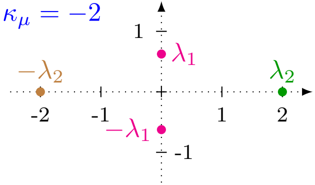

- **Inside the critical interval**. There are exactly two propagative modes.

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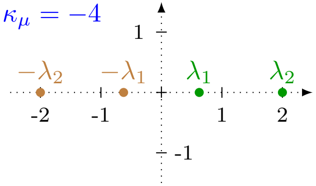

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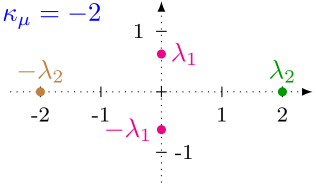

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→ The decomposition on the outgoing modes leads to look for a solution of the form

$$u = \underbrace{c_1\,\varphi_1\,e^{\lambda_1 z}}_{\text{propagative part}} + \underbrace{u_e}_{\text{evanescent part}}.$$

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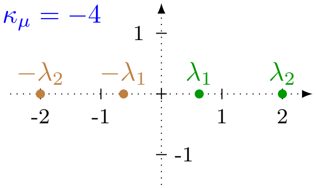

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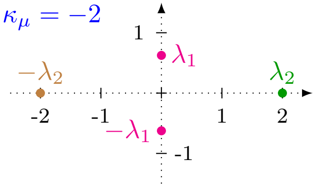

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... but the modal decomposition is not easy to justify because two sign-changing appear in the transverse problem: $\partial_\theta \sigma \partial_\theta \varphi = -\sigma \lambda^2 \varphi$.

The new functional framework

Consider $0 < \beta < 2$, ζ a cut-off function (equal to 1 in $+\infty$) and define

$\mathrm{W}_{-\beta} = \{v \mid e^{\beta z} v \in \mathrm{H}^1_0(\mathcal{B})\}$ space of exponentially decaying functions

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$\mathrm{W}^{+} = \mathrm{span}(\zeta \varphi_1 \, e^{\lambda_1 z}) \oplus \mathrm{W}_{-\beta}$ propagative part + evanescent part
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THEOREM. Let $\kappa_\mu \in (-3; -1)$ and $0 < \beta < 2$. The operator $A^+ : \mathrm{div}(\mu^{-1} \nabla \cdot)$ from W^+ to W^*_β is an isomorphism.

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1. $A_{-\beta} : \mathrm{div}(\mu^{-1}\nabla\cdot)$ from $\mathrm{W}_{-\beta}$ to W^*_β is injective but not surjective.

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4. Limiting absorption principle to select the outgoing mode.

How to approximate the solution?

- Let us try a usual Finite Element Method (P1 Lagrange Finite Element). We solve the problem

$$\boxed{\left|\begin{array}{l}\text{Find } u_h \in \mathrm{V}_h \text{ s.t.:}\\ \displaystyle\int_\Omega \mu^{-1}\,\nabla u_h \cdot \nabla v_h = \int_\Omega f v_h, \quad \forall v \in \mathrm{V}_h,\end{array}\right.}$$

where V_h approximates $\mathrm{H}^1_0(\Omega)$ as $h \to 0$ (h is the mesh size).

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- We display u_h as $h \to 0$.

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THE SEQUENCE (u_h) DOES NOT CONVERGE AS $h \to 0$!!!

- We display u_h as $h \to 0$.

$(\ldots)$ $(\ldots)$

Contrast $\kappa_\mu = -1.001 \in (-3; -1)$.

Remark

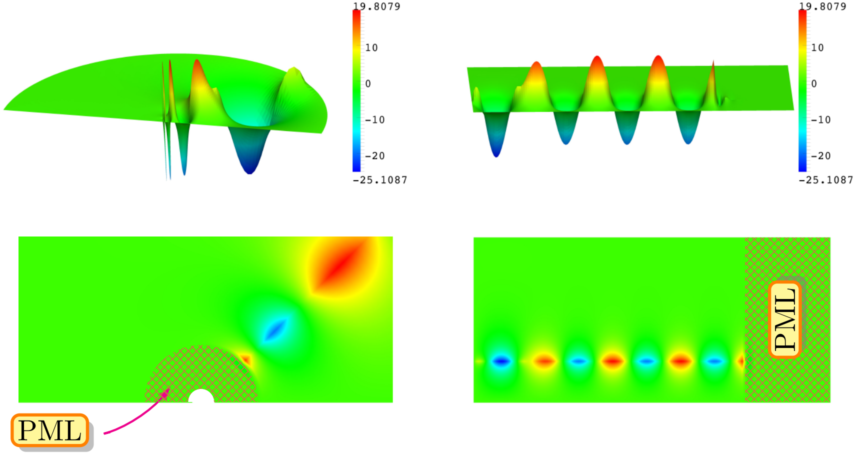
- Outside the critical interval, the sequence (u_h) converges.

$(\dots)$ $(\dots)$

Contrast $\kappa_\mu = -0.999 \notin (-3; -1)$.

A funny use of PMLs

- We use a PML (*Perfectly Matched Layer*) to bound the domain $\mathcal{B}$ + finite elements in the truncated strip



Contrast $\kappa_\mu = -1.001 \in (-3; -1)$.

A black hole phenomenon

- The same phenomenon occurs for the Helmholtz equation.

$$(\boldsymbol{x}, t) \mapsto \Re e\left(u(\boldsymbol{x})e^{-i\omega t}\right) \quad \text{for } \kappa_\mu = -1.3$$

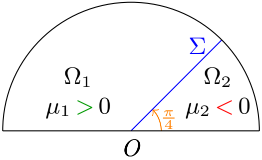
$(\ldots)$ $(\ldots)$

- Analogous phenomena occur in cuspidal domains in the theory of water-waves and in elasticity (`Cardone, Nazarov, Taskinen`).

Summary of the results for the scalar problem

Problem

$$(\mathscr{P}) \quad \left| \begin{array}{l} \text{Find } u \in \mathrm{H}^1_0(\Omega) \text{ s.t.:} \\ -\mathrm{div}\,(\mu^{-1}\nabla u) = f \quad \text{ in } \Omega. \end{array} \right.$$



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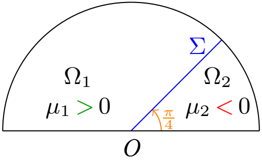
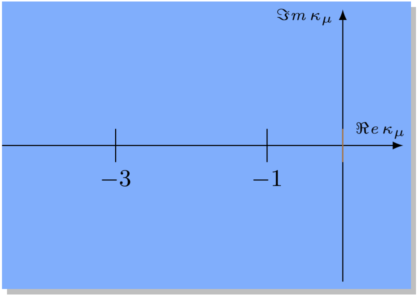


Results

🟦 For $\kappa_\mu \in \mathbb{C}\backslash\mathbb{R}_-$, $(\mathscr{P})$ well-posed in $\mathrm{H}^1_0(\Omega)$ (Lax-Milgram)



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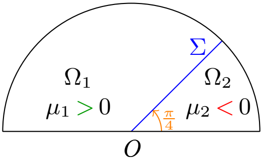

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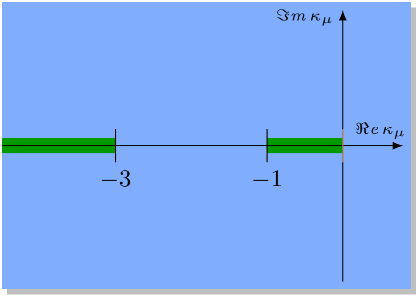

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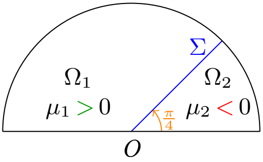

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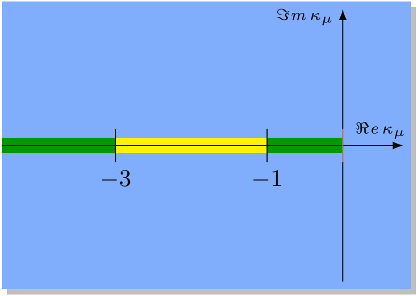

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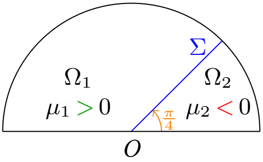

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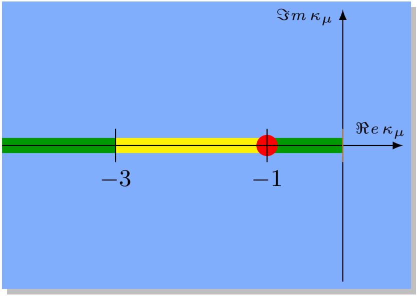
🔴 $\kappa_\mu = -1$, $(\mathscr{P})$ ill-posed in $\mathrm{H}^1_0(\Omega)$



1. The coerciveness issue for the scalar case

2. A new functional framework in the critical interval

3. A curious instability phenomenon

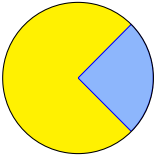
⇒ joint work with `S.A. Nazarov` (IPME RAS St Petersburg).

Problem considered in this section

- We recall the problem under consideration

$$(\mathscr{P}) \left| \begin{array}{l} \text{Find } u \in \mathrm{H}^1_0(\Omega) \text{ such that:} \\ -\mathrm{div}(\mu^{-1}\nabla u) = f \quad \text{ in } \Omega. \end{array} \right.$$

- When the interface has a corner, $(\mathscr{P})$ is well-posed in the Fredholm sense iff $\kappa_\mu \notin I_c$ (the critical interval).



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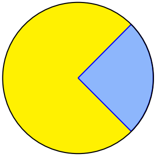

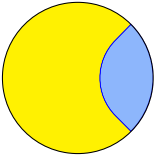

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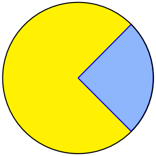

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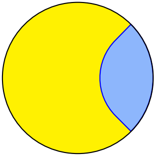
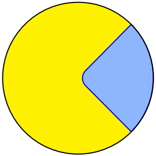


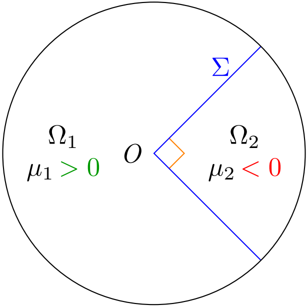
- When the interface is smooth, $(\mathscr{P})$ is well-posed in the Fredholm sense iff $\kappa_\mu \neq -1$.

What happens for a slightly rounded corner when $\kappa_\mu \in I_c \setminus \{-1\}$?



Numerical experiment 1/2

- For the numerical experiment, we round the corner in a particular way.



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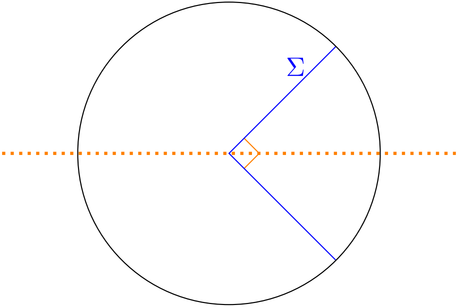

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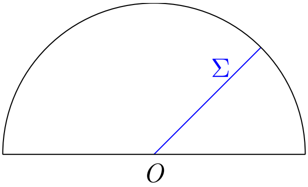

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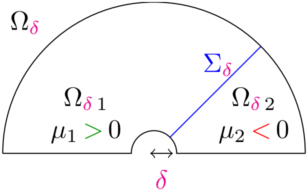

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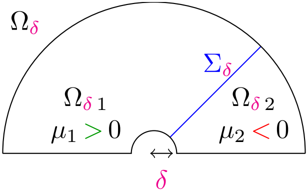

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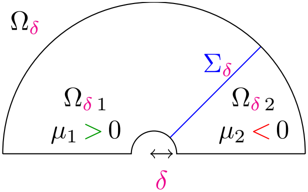

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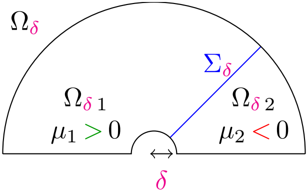

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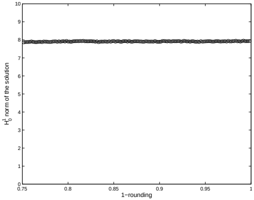

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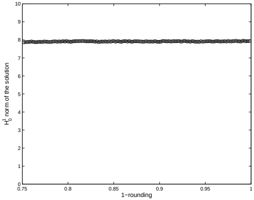

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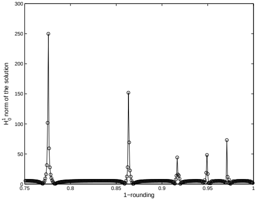

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where $\beta > 0$ and where $\tilde{\mathscr{S}}$ is a neighbourhood of $\mathscr{S}$.

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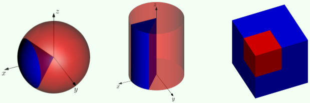
This leads us to question the physical model we are using. What do we lose at the corner?

Future directions

Scalar problem



- Computation of 3D singularities (conical tip, edge, Fichera corner) for the scalar problem. Are the interval obtained by geometrical methods optimal?
- Concerning the approximation of the solution, in practice, usual methods converge. Only partial proofs are available.
- Our new model in the critical interval raises a lot of questions, related to the physics of plasmonics and metamaterials.

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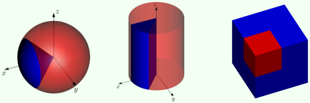

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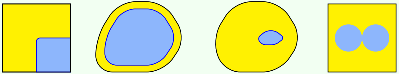

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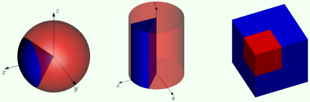

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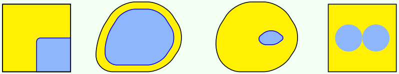

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Maxwell's equations inside the critical interval

- New functional framework for Maxwell's equations taking into account the propagative singularities.
- Approximation of the solution in the new functional framework. We need first to justify an edge element method outside the critical interval...

Thank you for your attention!!!