Localized plasmonic resonances and the Neumann-Poincaré operator: homogenization and bowties

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Foreword: Localized plasmonic resonances (I)

A localized plasmon resonance is a phenomenon caused by the interaction between an electromagnetic wave and a nanoparticle in a dielectric medium.

The Lycurgus cup is encrusted with gold nanoparticles. It looks (left) green when seen in reflection, and (right) red when seen in transmission.

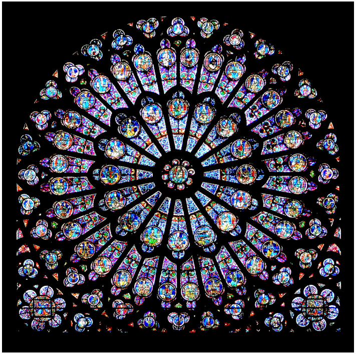
Foreword: Localized plasmonic resonances (II)

Localized plasmon resonances are characterized by:

- A strong enhancement of the rates of absorption and scattering of energy of the particle;
- A blow up of the electric field in the vicinity of the particle.

They occur under very specific circumstances:

- The size of the particle has to be much shorter than the incoming wavelength;
- The dielectric permittivity of the particle has to be negative (as in metals at optical frequency).



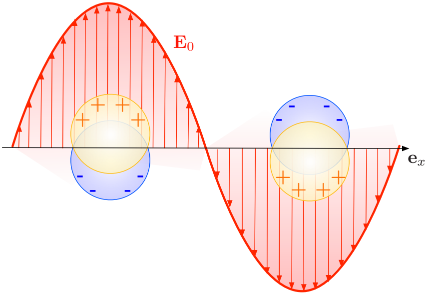
The vivid colors of the stained glass in Notre-Dame de Paris are obtained by colloids of gold nanoparticles.

A simple model for plasmonic resonances (I)

- A nanoparticle D undergoes an electric field $\mathbf{E}_0$ with wavelength much larger than the size of D.

$$\Rightarrow \mathbf{E}_0 \text{ is approximately constant at the level of } D.$$

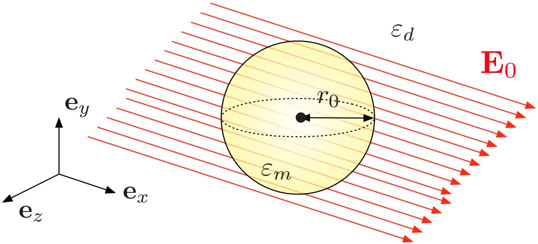
- The electric field $\mathbf{E}_0$ causes a delocalization of the electrons in the valence shell.
- A dipole moment is created, depending on the shape of the particle.
- This restoring force may induce resonance.



A simple model for plasmonic resonances ([Ma], Chap. 5) (II)

- The nanoparticle $D \subset \mathbb{R}^3$ is a sphere with radius r_0 and permittivity ε_m.
- The dielectric permittivity of the ambient medium is ε_d.
- The imposed electric field $\mathbf{E}_0 = E_0 \mathbf{e}_x$ is approximately constant at the scale of the particle $\Rightarrow$ electrostatic situation.
- The total electric field reads $\mathbf{E} = -\nabla\phi$, where the potential ϕ is the solution to:

$$\begin{cases} -\Delta\phi = 0 & \text{in } D \cup (\mathbb{R}^3 \setminus \overline{D}), \\ \phi^- = \phi^+ & \text{on } \partial D, \\ \varepsilon_m \frac{\partial \phi^-}{\partial n} = \varepsilon_d \frac{\partial \phi^+}{\partial n} & \text{on } \partial D, \\ \mathbf{E} = -\nabla\phi \to \mathbf{E}_0 & \text{as } |x| \to \infty. \end{cases}$$



- Elementary calculations using separation of variables yield:

$$\phi(x) = \begin{cases} -\frac{3\varepsilon_d}{\varepsilon_m+2\varepsilon_d} E_0 r \cos\theta & \text{if } |x| < r_0 \\ -E_0 r \cos\theta + \frac{\varepsilon_m-\varepsilon_d}{\varepsilon_m+2\varepsilon_d} E_0 r_0^3 \frac{\cos\theta}{r^2} & \text{otherwise,} \end{cases}$$

where θ is the angle between the position vector and $\mathbf{e}_x$.

- Outside D, the potential ϕ is the superposition of
  - The background potential (i.e. if D were absent) $-E_0 r \cos\theta$;
  - The potential induced by the dipole moment

$$\mathbf{p} = 4\pi\varepsilon_0\varepsilon_d r_0^3 \frac{\varepsilon_m - \varepsilon_d}{\varepsilon_m + 2\varepsilon_d}\mathbf{E}_0.$$

- The total electric field $\mathbf{E} = -\nabla\phi$ reads:

$$\mathbf{E}(x) = \begin{cases} \frac{3\varepsilon_d}{\varepsilon_d+2\varepsilon_m}\mathbf{E}_0 & \text{if } |x| < r_0, \\ \mathbf{E}_0 + \frac{3\mathbf{n}(\mathbf{n}\cdot\mathbf{p})-\mathbf{p}}{4\pi\varepsilon_0\varepsilon_d r^3} & \text{otherwise } (\mathbf{n} \equiv \frac{\mathbf{x}}{|\mathbf{x}|}). \end{cases}$$

- $\mathbf{E}(x)$ blows up under the Fröhlich resonance condition:

$$\mathrm{Re}(\varepsilon_m) = -2\varepsilon_d \text{ and } |\mathrm{Im}(\varepsilon_d)| \ll 1.$$

A simple model for plasmonic resonances ([Ma], Chap. 5) (IV)

Now, if D is illuminated by a (time-dependent) plane wave $\mathbf{E}_0(x)e^{i\omega t}$ such that:

- The frequency ω is very small: $\mathbf{E}_0(x)$ is approximately constant around D,
- The permittivity $\varepsilon_m \equiv \varepsilon_m(\omega)$ satisfies the Fröhlich condition,

the electric and magnetic fields

$$\mathbf{E}(t,x) = \mathbf{E}(x)e^{i\omega(t)}, \text{ and } \mathbf{H}(t,x) = \mathbf{H}(x)e^{i\omega t}$$

can be calculated as those induced by the electrostatic dipole $\mathbf{p}$.

- Both fields $\mathbf{E}(t,x)$ and $\mathbf{H}(t,x)$ blow up near D; the blow up is even more dramatic for $\mathbf{E}$.
- Blow up of the scattering and absorption cross sections of the particle (i.e. the rates at which energy is removed from $\mathbf{E}_0$ by scattering or absorption).

Similar observations hold when the size of D is no longer so small with respect to the excitation wavelength: Mie theory.

Negative permittivity: the Drude's model (I)

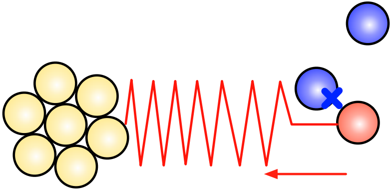
Negative electric permittivity occurs at optical frequency for metals like silver or gold.

This is predicted by the classical Drude's model for the dielectric properties of materials. In this model, each electron of the particle is subjected to:

- The electric force $e\mathbf{E}$ induced by the imposed electric field $\mathbf{E} = E_x\mathbf{e}_x$;
- A repelling force $-kx\mathbf{e}_x$ binding the electron to the nuclei;
- A viscous damping force $-m\gamma x'(t)\mathbf{e}_x$ cause by the mutual interaction between electrons.

The position $x(t)$ of the electron on the axis $\mathbf{e}_x$ is then given by:

$$mx''(t) = eE_0 - kx(t) - m\gamma x'(t).$$



Negative permittivity: the Drude's model (II)

- The polarization $\mathbf{P}$ in the medium then reads:

$$\mathbf{P} = \mathbf{P}(\omega) = Nx(\omega)\mathbf{e}_x.$$

- The dielectric permittivity is defined by

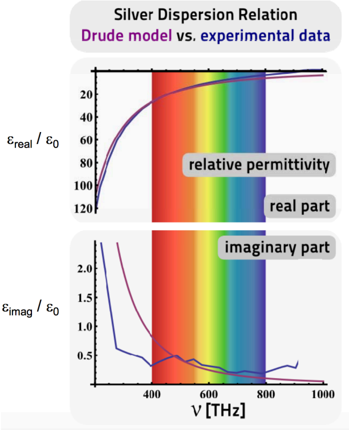
$$\varepsilon(\omega)\mathbf{E} = \varepsilon_0\mathbf{E} + \mathbf{P}.$$

  After calculations, it comes:

$$\varepsilon(\omega) = \varepsilon_0 + \frac{\varepsilon_0\omega_p^2}{\omega_0^2 - \omega^2 + i\omega\gamma},$$

  where $\omega_0 = \sqrt{k/m}$ and ω_p is the plasma frequency of the material.

- For a metal, the electrons have loose bonds with the core: $\omega_0 \approx 0$.



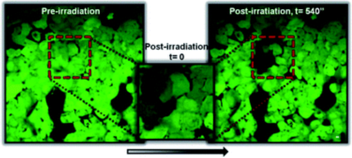
Applications of plasmonic resonances

The strong field enhancement near metallic nanoparticles at plasmonic resonances has been used e.g.

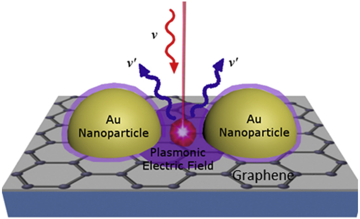
- To selectively produce heat by absorption in photothermal cancer therapy;
- To create intense, localized fields in Surface Enhanced Raman Spectroscopy.

Their great sensitivity to the shape and the local environment of the particle has been used to devise accurate imaging processes:

- Spectroscopy devices in biochemistry, to image molecular adsorption on DNA, polymers, etc.
- Biosensors, gold nanoparticles being harmless for health.



Selective release of a chemotherapeutic agent (from [VolSig])



Enhancement of the Raman effect using silver particles (from [GouDas])

Mathematical model for plasmonic resonances (I)

- In the previous calculation, the resonance is caused by the existence of a non trivial solution u to the homogeneous equation:

$$\begin{cases} -\Delta u = 0 & \text{in } D \cup (\mathbb{R}^3 \setminus \overline{D}), \\ u^- = u^+ & \text{on } \partial D, \\ \varepsilon_m \frac{\partial u^-}{\partial n} = \varepsilon_d \frac{\partial u^+}{\partial n} & \text{on } \partial D, \\ |u(x)| \to 0 & \text{as } |x| \to \infty. \end{cases}$$

in the particular case where $\varepsilon_m = -2\varepsilon_d$: $u(x) = \begin{cases} r\cos\theta & \text{if } r < r_0, \\ \frac{r_0^3}{r^2}\cos\theta & \text{if } r > r_0. \end{cases}$

- The quasi-static plasmonic resonances of the (rescaled) particle D are the values of the ratio

$$\lambda_\varepsilon := \frac{\varepsilon_m + \varepsilon_d}{2(\varepsilon_m - \varepsilon_d)}$$

such that the above system has a non trivial solution u.

$\Rightarrow$ Eigenvalue problem for the Neumann-Poincaré operator $\mathcal{K}_D^*$.

Beyond electrostatics: Maxwell's equations (I)

- A nanoparticle $D_\delta := \delta D$ with size $\delta \ll 1$ is illuminated by an indicent plane wave $(\mathbf{E}^i, \mathbf{H}^i)$.

- The total field $(\mathbf{E}, \mathbf{H})$ is the solution to the time-harmonic Maxwell system:

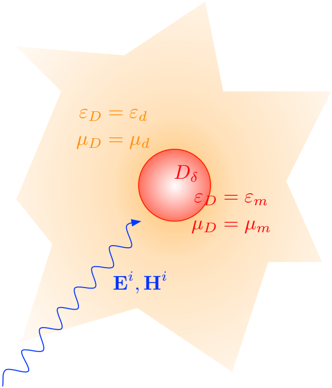
$$\begin{cases} \nabla \times \mathbf{E} = i\omega\mu_D \mathbf{H} & \text{in } \mathbb{R}^3 \setminus \partial D_\delta, \\ \nabla \times \mathbf{H} = -i\omega\varepsilon_D \mathbf{E} & \text{in } \mathbb{R}^3 \setminus \partial D_\delta, \end{cases}$$

complemented with the jump conditions

$$[\mathbf{n} \times \mathbf{E}] = [\mathbf{n} \times \mathbf{H}] = 0 \text{ on } \partial D,$$

and the Silver-Müller radiation condition at infinity:

$$\lim_{|x| \to \infty} |x| \left(\sqrt{\mu_d}(\mathbf{H} - \mathbf{H}^i) \times \mathbf{n} - \sqrt{\varepsilon_d}(\mathbf{E} - \mathbf{E}^i) \right) = 0.$$



Defining the ratios between the permittivity and permeability inside and outside D_δ,

$$\lambda_\varepsilon := \frac{\varepsilon_d + \varepsilon_m}{2(\varepsilon_m - \varepsilon_d)}, \text{ and } \lambda_\mu = \frac{\mu_d + \mu_m}{2(\mu_m - \mu_d)},$$

we define a measure of the distance between the actual situation and the quasi-static plasmonic resonances of D:

$$d_\sigma := \max\left(d\left(\lambda_\varepsilon, \sigma(\mathcal{K}_D^*)\right), d\left(\lambda_\mu, \sigma(\mathcal{K}_D^*)\right)\right).$$

Theorem 1 ([AmDeMi]).

As $\delta \to 0$ and $d_\sigma \to 0$,

- *The electric field $\mathbf{E}$ blows up;*
- *The absorption and scattering cross sections of the particle D_δ blow up.*

See [AmMiRuiZha, AmRuiYuZha] for additional properties and similar statements in the case of the Helmholtz equation.

Mathematical study of plasmonic resonances

- The (simplified) study of plasmonic resonances boils down to that of the two-phase conductivity equation featuring a domain $D \subset \mathbb{R}^d$ and $k < 0$:

$$\text{Search for } u \text{ s.t. } \begin{cases} -\text{div}(a(x)\nabla u) = 0 & \text{in } \mathbb{R}^d, \\ |u(x)| \to 0 & \text{as } |x| \to \infty, \end{cases}$$

$$\text{where } a(x) := \begin{cases} k & \text{if } x \in D, \\ 1 & \text{otherwise.} \end{cases}$$

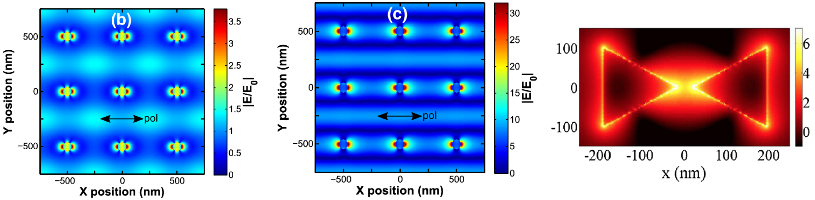
- Of particular interest are those values of $k < 0$ making the problem ill-posed.
- *Variants*: The above system could be posed inside a bounded macroscopic domain Ω, with Dirichlet, Neumann boundary conditions on $\partial\Omega$, etc.
- Several angles of attack:
  - The T-coercivity method, a variant of the inf-sup condition, relying on the construction of inf-sup operators [DhiaCiaZwo];
  - Variational approaches *a la* Agmon-Douglis-Nirenberg [Ng];
  - Layer potential techniques.

Goals of the presentation

Two questions are investigated in this presentation:

1. Collective effects: how do several nanoparticles interact with each other?
2. Observations report further localization and field enhancement phenomena in the presence of corners

$\Rightarrow$ Study of one such singular situation: bowtie-shaped antennas.



(Left,middle) Two resonant modes associated to a periodic array of nanoparticles (from [KhloLau]); (right) Strong enhancement of the electric field near the tip of a bowtie-shaped particle (from [NiCha]).

The Newtonian potential

- The Newtonian potential, or free space Green's function $G(x,y)$ is the fundamental solution to the Laplace operator:

$$\Delta_x G(x,y) = \delta_{x=y} \text{ in } \mathbb{R}^d.$$

It is defined by:

$$\forall x \neq y, \quad G(x,y) = \begin{cases} \frac{1}{2\pi} \log|x-y| & \text{if } d = 2, \\ \frac{|x|^{2-d}}{(2-d)\omega_d} & \text{otherwise,} \end{cases}$$

where ω_d is the area of the unit sphere in $\mathbb{R}^d$.

- Physically, $G(x,y)$ is the electric potential generated at x by a point source with (negative) unit intensity located at y.

- Other types of Green's functions exist, with different boundary conditions, e.g.
  - The fundamental solution of the Laplace operator with homogeneous Dirichlet or Neumann conditions on the boundary of a 'hold-all' domain Ω;
  - Periodic Green's functions.

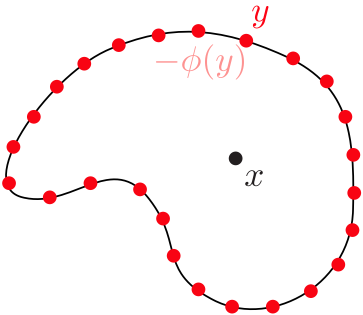
The single layer potential

Let $D \subset \mathbb{R}^d$ be a bounded domain of class $\mathcal{C}^2$.

The single layer potential associated to a function $\phi \in \mathcal{C}(\partial D)$ is defined by:

$$\forall x \notin \partial D, \;\; \mathcal{S}_D\phi(x) = \int_{\partial D} G(x,y)\phi(y)\, ds(y).$$

Intuitively, $\mathcal{S}_D\phi(x)$ is the potential induced at x by a distribution of charges at points $y \in \partial D$ with intensity $-\phi(y)$.



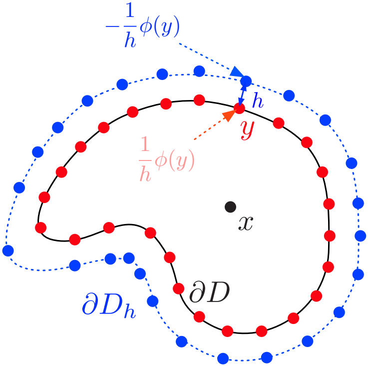
The double layer potential

The double layer potential associated to $\phi \in \mathcal{C}(\partial D)$ is:

$$\forall x \notin \partial D, \;\; \mathcal{D}_D\phi(x) = \int_{\partial D} \frac{\partial G}{\partial n_y}(x,y)\phi(y)\, ds(y).$$

Physically, $\mathcal{D}_D\phi(x)$ is the potential induced at x by two close layers of charge densities,

- One of them distributed along ∂D, with intensity $\frac{1}{h}\phi(y)$;
- The other one being distributed on the offset surface ∂D_h, with intensity $-\frac{1}{h}\phi(y)$.



Properties of layer potentials

- Both $\mathcal{S}_D\phi$ and $\mathcal{D}_D\phi$ are harmonic in D and $\mathbb{R}^d \setminus \overline{D}$.
- Decay at infinity:
  - If $d \geq 3$, $|\mathcal{S}_D\phi(x)| \leq C|x|^{2-d}$ as $|x| \to \infty$.
  - If $d = 2$, one only has: $|\mathcal{S}_D\phi(x)| \leq C|\log|x||$ as $|x| \to \infty$.
  - If $d = 2$ and in addition $\int_{\partial D} \phi \, ds = 0$, one has $|\mathcal{S}_D\phi(x)| \leq C|x|^{-1}$.
  - It is often required that $\int_{\partial D} \phi \, ds = 0$ if $d = 2$.
- More interesting is their behavior when $x \to \partial D$.

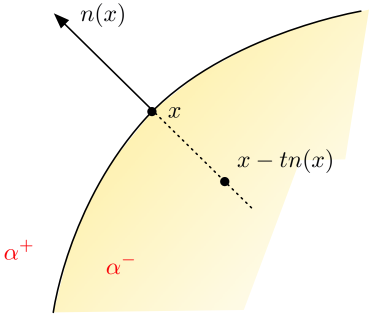
Notation: The one-sided limits of a function α at $x \in \partial D$ are:

$$\alpha^+(x) = \lim_{t\downarrow 0} \alpha(x + tn(x)),$$

$$\alpha^-(x) = \lim_{t\downarrow 0} \alpha(x - tn(x)),$$

and the jump of α across ∂D is:

$$[\alpha](x) := \alpha^+(x) - \alpha^-(x).$$



Jump relations

Theorem 2.

The single layer potential $\mathcal{S}_D\phi$

- *Has continuous trace across* ∂D*: for* $x \in \partial D$, $\quad \mathcal{S}_D\phi^-(x) = \mathcal{S}_D\phi^+(x)$.
- *Has jumping normal derivative across* ∂D*:*

$$\text{For } x \in \partial D,\ \ \frac{\partial}{\partial n}(\mathcal{S}_D\phi)^{\pm}(x) = \pm\frac{1}{2}\phi(x) + \mathcal{K}_D^*\phi(x).$$

Theorem 3.

The double layer potential $\mathcal{D}_D\phi$

- *Has jumping trace across* ∂D*:*

$$\text{For } x \in \partial D,\ \ \mathcal{D}_D\phi^{\pm}(x) = \mp\frac{1}{2}\phi(x) + \mathcal{K}_D\phi(x).$$

- *Has continuous normal derivative across* ∂D*:*

$$\frac{\partial}{\partial n}(\mathcal{S}_D\phi)^{-} = \frac{\partial}{\partial n}(\mathcal{S}_D\phi)^{+}.$$

Jump relations and the Neumann-Poincaré operator

- The operator $\mathcal{K}_D\phi : \mathcal{C}(\partial D) \to \mathcal{C}(\partial D)$ is defined by:

$$\forall x \in \partial D, \ \ \mathcal{K}_D\phi(x) = \int_{\partial D} \frac{\partial G}{\partial n_y}(x,y)\phi(y)\, ds(y).$$

- Its $L^2(\partial D)$ adjoint $\mathcal{K}_D^*\phi : \mathcal{C}(\partial D) \to \mathcal{C}(\partial D)$, given by

$$\forall x \in \partial D, \ \ \mathcal{K}_D^*\phi(x) = \int_{\partial D} \frac{\partial G}{\partial n_x}(x,y)\phi(y)\, ds(y)$$

is the Neumann-Poincaré operator.

- That these operators are indeed well-defined is not trivial; it relies on the $\mathcal{C}^2$ character of ∂D (see below).

Other settings

- Other functional settings than that of densities $\phi \in \mathcal{C}(\partial D)$:
  - One defines $\mathcal{K}_D$, $\mathcal{K}_D^* : L^2(\partial D) \to L^2(\partial D)$.
  - A more natural setting is that of energy spaces; see [McLe]: the single and double layer potentials $\mathcal{S}_D$, $\mathcal{D}_D$ extend as

    $$\mathcal{S}_D : H_0^{-1/2}(\partial D) \to W_0^{1,-1}(\mathbb{R}^d), \text{ and } \mathcal{D}_D : H^{1/2}(\partial D) \to W_0^{1,-1}(\mathbb{R}^d).$$

    Likewise, one extends:

    $$\mathcal{K}_D : H^{1/2}(\partial D) \to H^{1/2}(\partial D), \text{ and } \mathcal{K}_D^* : H^{-1/2}(\partial D) \to H^{-1/2}(\partial D).$$

- Other 'physical' settings than that of potentials u on the whole space $\mathbb{R}^d$, with adapted versions of layer potentials (and the associated Green's function):
  - Potentials u defined on a bounded domain $\Omega \subset \mathbb{R}^d$, imposing homogeneous Dirichlet or Neumann boundary conditions on $\partial\Omega$
  - One could consider periodic potentials u.

- Consider the two-phase conductivity equation:

$$\begin{cases} -\Delta u = 0 & \text{in } D \cup (\mathbb{R}^d \setminus \overline{D}), \\ u^- = u^+ & \text{on } \partial D, \\ k\frac{\partial u^-}{\partial n} = \frac{\partial u^+}{\partial n} & \text{on } \partial D, \\ u(x) \to H(x) & \text{as } |x| \to \infty, \end{cases}$$

where $H(x)$ is a given harmonic function on $\mathbb{R}^d$.

- The unique variational solution can be represented by a single layer potential:

$$u(x) = H(x) + \mathcal{S}_D\phi(x),$$

with density $\phi \in H_0^{-1/2}(\partial D)$, to be identified (s.t. $\int_{\partial D} \phi \, ds = 0$ if $d = 2$).

- The jump relations imply the following Fredholm equation:

Search for $\phi \in H_0^{-1/2}(\partial D)$ s.t. $\lambda\phi - \mathcal{K}_D^*\phi = (k-1)\dfrac{\partial H}{\partial n}$, with $\lambda := \dfrac{1}{2}\dfrac{k+1}{k-1}$.

$\Rightarrow$ The plasmonic resonances of D are determined by the spectrum $\sigma(\mathcal{K}_D^*)$.

Theorem 4.

If D is of class $\mathcal{C}^2$, the Neumann-Poincaré operator $\mathcal{K}_D^* : L^2(\partial D) \to L^2(\partial D)$ is compact.

Sketch of proof:

- For an arbitrary potential $\phi \in L^2(\partial D)$,

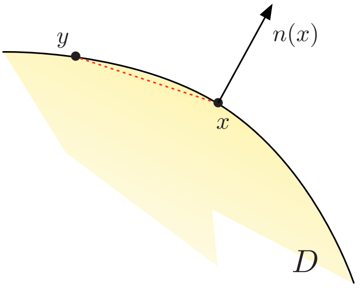
$$\mathcal{K}_D^*\phi(x) = \int_{\partial D} K^*(x,y)\phi(y)\, ds(y),$$

$$\text{where } K^*(x,y) := \frac{(x-y)\cdot n(x)}{\omega_d |x-y|^d}.$$

- *Key point:* Since ∂D is smooth, there is a constant $C > 0$ such that for $x, y \in \partial D$,

$$|(x-y)\cdot n(x)| \le C|x-y|^2,$$

$$\text{and so } \boxed{|K^*(x,y)| \le \frac{C}{|x-y|^{d-2}}}.$$



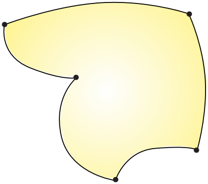
- Hence, $\mathcal{K}_D^*$ is (nearly) a Hilbert-Schmidt operator on $L^2(\partial D)$.

Spectrum of the Neumann-Poincaré operator

- In the above situation, it also holds that $\mathcal{K}_D^* : H^{-1/2}(\partial D) \to H^{-1/2}(\partial D)$ is compact [Kre].
- Provided D is $\mathcal{C}^2$, the spectrum $\sigma(\mathcal{K}_D^*)$ is only composed of a discrete sequence of eigenvalues, accumulating at 0:
$$-\frac{1}{2} < \lambda_1^- \leq \lambda_2^- \leq \ldots < 0 < \ldots \leq \lambda_2^+ \leq \lambda_1^+ \leq \frac{1}{2}.$$
- The Neumann-Poincaré operator is not self-adjoint, but it can be symmetrized with respect to a different inner product than the usual one on $H^{-1/2}(\partial D)$.

The Neumann-Poincaré operator of a non smooth domain

Let us now assume that D is only Lipschitz (e.g. a piecewise smooth domain with corners).



- The *definition* of the operators $\mathcal{K}_D$ and $\mathcal{K}_D^*$ poses difficulty, since in this case,

$$K^*(x,y) = \frac{(x-y)\cdot n(x)}{|x-y|^d} = \mathcal{O}\left(\frac{1}{|x-y|^{d-1}}\right).$$

- A difficult result allows to give them a meaning as Cauchy principal value integrals [CoiMcInMe].
- The jump relations remain valid in this context [Cos, Ver].
- However, the compactness of $\mathcal{K}_D$ and $\mathcal{K}_D^*$ fails.

An adapted functional space for exterior problems: $W^{1,-1}(\mathbb{R}^d)$

- Following [Ne], we define the functional space adapted to exterior problems:

$$W^{1,-1}(\mathbb{R}^2) = \left\{ u,\ \frac{u}{(1+|x|^2)^{\frac{1}{2}} \log(2+|x|^2)} \in L^2(\mathbb{R}^2),\ \nabla u \in L^2(\mathbb{R}^2)^2 \right\}.$$

and in 3d,

$$W^{1,-1}(\mathbb{R}^3) = \left\{ u,\ \frac{u}{(1+|x|^2)^{\frac{1}{2}}} \in L^2(\mathbb{R}^3),\ \nabla u \in L^2(\mathbb{R}^3)^3 \right\}.$$

- In 2d, the space $W^{1,-1}(\mathbb{R}^2)$ contains the constant functions. It is customary to consider instead:

$$W_0^{1,-1}(\mathbb{R}^2) := W^{1,-1}(\mathbb{R}^2)/\mathbb{R}$$

which is formally the subspace of functions in $W^{1,-1}(\mathbb{R}^2)$ vanishing at infinity.

- The following inner product is considered on $W_0^{1,-1}(\mathbb{R}^d)$:

$$\langle u, v \rangle_{W^{1,-1}(\mathbb{R}^d)} = \int_{\mathbb{R}^d} \nabla u \cdot \nabla v \, dx.$$

The Poincaré variational principle

Let $D \subset \mathbb{R}^d$ be a bounded, Lipschitz domain.

The original work of Poincaré, recently revisited by [KhaPuSha], gives an energetic flavor to layer potential theory.

Definition 1.

The Poincaré variational operator

$$T_D : W_0^{1,-1}(\mathbb{R}^d) \to W_0^{1,-1}(\mathbb{R}^d)$$

associates, to any $u \in W_0^{1,-1}(\mathbb{R}^d)$, the unique $T_D u \in W_0^{1,-1}(\mathbb{R}^d)$ such that:

$$\forall v \in W_0^{1,-1}(\mathbb{R}^d), \ \int_{\mathbb{R}^d} \nabla(T_D u) \cdot \nabla v \, dx = \int_D \nabla u \cdot \nabla v \, dx.$$

Roughly speaking, $T_D u$ describes the fraction of the energy of u which lies inside D.

The Poincaré variational principle

- Let us consider the two-phase conductivity equation:

Search for $u \in W_0^{1,-1}(\mathbb{R}^d)$ s.t. $-\operatorname{div}(a(x)\nabla u) = f,$

$$\text{where } a(x) := \begin{cases} k & \text{if } x \in D, \\ 1 & \text{otherwise,} \end{cases} \quad \text{and } f \in (W_0^{1,-1}(\mathbb{R}^d))^*.$$

- The associated variational formulation is: search for $u \in W_0^{1,-1}(\mathbb{R}^d)$ s.t.

$$\forall v \in W_0^{1,-1}(\mathbb{R}^d), \quad \int_{\mathbb{R}^d} a(x)\nabla u \cdot \nabla v \, dx = \langle f, v \rangle_{(W_0^{1,-1}(\mathbb{R}^d))^*, W_0^{1,-1}(\mathbb{R}^d)}$$

- A simple calculation reveals that u is solution to the above equation if and only if:

$$(\lambda \mathrm{Id} - T_D)u = \lambda g,$$

where $\lambda = \frac{1}{1-k}$ and $g \in W_0^{1,-1}(\mathbb{R}^d)$ is the representative of f supplied by the Riesz representation theorem:

$$\forall v \in W_0^{1,-1}(\mathbb{R}^d), \quad \int_{\mathbb{R}^2} \nabla g \cdot \nabla v \, dx = \langle f, v \rangle_{(W_0^{1,-1}(\mathbb{R}^d))^*, W_0^{1,-1}(\mathbb{R}^d)}.$$

The Poincaré variational principle

Let $D_1, ..., D_N$ be the connected components of D.

- T_D is a self-adjoint, positive operator with norm $||T_D|| \leq 1$.
- Its kernel $\mathrm{Ker}(T_D)$ is:
$$\mathrm{Ker}(T_D) = \left\{ u \in W_0^{1,-1}(\mathbb{R}^d), \;\; u = c_j \text{ on } D_j, \;\; j = 1, ..., N \right\}.$$
- The eigenspace $\mathrm{Ker}(\mathrm{Id} - T_D)$ is:
$$\mathrm{Ker}(\mathrm{Id} - T_D) = \left\{ u \in W_0^{1,-1}(\mathbb{R}^d), \;\; u \equiv 0 \text{ on } \mathbb{R}^d \setminus \overline{D} \right\}.$$
- The following orthogonal decomposition holds:
$$W_0^{1,-1}(\mathbb{R}^d) = \mathrm{Ker}(T_D) \oplus \mathfrak{h} \oplus \mathrm{Ker}(\mathrm{Id} - T_D), \;\text{ where}$$

$$\mathfrak{h} = \left\{ u \in W_0^{1,-1}(\mathbb{R}^d), \;\; \Delta u = 0 \text{ on } D \cup (\mathbb{R}^d \setminus \overline{D}), \right.$$
$$\left. \int_{\partial D_j} \frac{\partial u^+}{\partial n} \, ds = 0, j = 1, ..., N \right\}.$$

The space of single layer potentials

We actually consider the slightly larger space of single layer potentials:

$$\mathfrak{h}_S = \left\{ u \in W_0^{1,-1}(\mathbb{R}^d),\ \ \Delta u = 0 \text{ on } D \cup (\mathbb{R}^d \setminus \overline{D}) \right\},$$

and the induced operator $T_D : \mathfrak{h}_S \to \mathfrak{h}_S$.

Proposition 5.

The mapping

$$H_0^{-1/2}(\partial D) \ni \phi \longmapsto \mathcal{S}_D\phi \in \mathfrak{h}_S$$

is an isomorphism, with inverse:

$$\mathfrak{h}_S \ni u \longmapsto \left[\frac{\partial u}{\partial n}\right] \in H_0^{-1/2}(\partial D).$$

Reminder: For $\phi \in H_0^{-1/2}(\partial D)$, $\mathcal{S}_D\phi$ is the unique solution $u \in W_0^{1,-1}(\mathbb{R}^d)$ to the variational problem:

$$\forall v \in W_0^{1,-1}(\mathbb{R}^d),\ \int_{\mathbb{R}^d} \nabla u \cdot \nabla v \, dx = -\int_{\partial D} \phi v \, ds.$$

T_D and the NP

The Neumann-Poincaré operator is related to (a shift of) the restriction $T_D : \mathfrak{h}_S \to \mathfrak{h}_S$.

Theorem 6.

The operator $R_D := T_D - \frac{1}{2}\mathrm{Id} : \mathfrak{h}_S \to \mathfrak{h}_S$ satisfies:

$$R_D = -\mathcal{S}_D \circ \mathcal{K}_D^* \circ \mathcal{S}_D^{-1}.$$

Sketch of proof: From the definition, for $u \in \mathfrak{h}_S$, one has, for all $v \in W_0^{1,-1}(\mathbb{R}^d)$,

$$\begin{aligned} \int_{\mathbb{R}^d} \nabla(R_D u) \cdot \nabla v \, dx &= \frac{1}{2}\int_D \nabla u \cdot \nabla v \, dx - \frac{1}{2}\int_{\mathbb{R}^d \setminus \overline{D}} \nabla u \cdot \nabla v \, dx \\ &= \frac{1}{2}\int_{\partial D} \left(\frac{\partial u^+}{\partial n} + \frac{\partial u^-}{\partial n} \right) v \, ds \end{aligned}$$

Introducing $\phi \in H_0^{-1/2}(\partial D)$ such that $u = \mathcal{S}_D \phi$, the jump relations read:

$$\frac{\partial u^\pm}{\partial n} = \pm \frac{1}{2}\phi + \mathcal{K}_D^* \phi,$$

and so:

$$\int_{\mathbb{R}^d} \nabla(R_D u) \cdot \nabla v \, dx = \int_{\partial D} (\mathcal{K}_D^* \phi) \, v \, ds \Leftrightarrow R_D u = \mathcal{S}_D(\mathcal{K}_D^* \phi).$$

Min-Max formulas

The usual min-max formulas for a compact, self-adjoint operator read in this case:

Proposition 7 ([BonTri, KhaPuSha]).

The spectrum of $T_D : \mathfrak{h}_S \to \mathfrak{h}_S$ is a translate of that $\sigma(\mathcal{K}_D^*)$ of the Neumann-Poincaré operator; it is a discrete sequence of eigenvalues with $\frac{1}{2}$ as unique accumulation point.

$$0 < \lambda_1^- \le \lambda_2^- \le ... \le \frac{1}{2}, \text{ and } \frac{1}{2} \le ... \le \lambda_2^+ \le \lambda_1^+ < 1.$$

If $\{w_i^\pm\}_{i\ge 1}$ are the associated eigenfunctions, they satisfy min-max formulae:

$$\lambda_i^- = \min_{\substack{u\in\mathfrak{h}_S\setminus\{0\} \\ u\perp w_1^-,\dots,w_{i-1}^-}} \frac{\displaystyle\int_D |\nabla u|^2\,dx}{\displaystyle\int_{\mathbb{R}^d} |\nabla u|^2\,dx} = \max_{\substack{F_i\subset\mathfrak{h}_S \\ \dim(F_i)=i-1}} \min_{u\in F_i^\perp\setminus\{0\}} \frac{\displaystyle\int_D |\nabla u|^2\,dx}{\displaystyle\int_{\mathbb{R}^d} |\nabla u|^2\,dx},$$

and:

$$\lambda_i^+ = \max_{\substack{u\in\mathfrak{h}_S\setminus\{0\} \\ u\perp w_1^+,\dots,w_{i-1}^+}} \frac{\displaystyle\int_D |\nabla u|^2\,dx}{\displaystyle\int_{\mathbb{R}^d} |\nabla u|^2\,dx} = \min_{\substack{F_i\subset\mathfrak{h}_S \\ \dim(F_i)=i-1}} \max_{u\in F_i^\perp\setminus\{0\}} \frac{\displaystyle\int_D |\nabla u|^2\,dx}{\displaystyle\int_{\mathbb{R}^d} |\nabla u|^2\,dx}.$$

In a nutshell (I)

$\lambda \in \left(-\frac{1}{2}, \frac{1}{2}\right]$ and $\phi \in H_0^{-1/2}(\partial D)$ are eigenelements of $\mathcal{K}_D^* : \mathcal{K}_D^* \phi = \lambda \phi$

$\beta = \frac{1}{2} - \lambda$, $u = \mathcal{S}_D \phi$ ↓ ↑ $\lambda = \beta + \frac{1}{2}$, $\phi = \left[\frac{\partial u}{\partial n}\right]$

$\beta \in [0, 1)$ and $u \in \mathfrak{h}_S$ are eigenelements of $T_D : T_D u = \beta u$

$k = 1 - \frac{1}{\beta}$ ↓ ↑ $\beta = \frac{1}{1-k}$

$u \in W_0^{1,-1}(\mathbb{R}^d)$ is a non trivial solution to

$$-\mathrm{div}(a(x)\nabla u) = 0 \qquad \text{where} \qquad a(x) = \begin{cases} k & \text{if } x \in D, \\ 1 & \text{otherwise} \end{cases}$$

In a nutshell (II)

The spectrum $\sigma(\mathcal{K}_D^*)$ can be studied from two complementary points of view:

- *Viewpoint of $\mathcal{K}_D^*$:* (Fredholm) integral equations, with explicit (albeit complicated) operators, posed on ∂D,
- *Viewpoint of T_D:* Self-adjoint operator T_D, defined on a fixed functional space, and Laplace equations with sign-changing coefficients.

The Neumann-Poincaré operator is a key tool in the study of many interface problems with various origins; see [Kan] and references therein:

- Detection and imaging of inhomogeneities in an ambient medium,
- Passive cloaking, and cloaking by anomalous localized resonances,
- Analysis of stress concentration between close-to-touching inclusions (metallic particles, elastic fibers, etc.).

Different types of spectrum

- We have hitherto considered particles with smooth shapes D:
  - Plasmonic resonances $\lambda \in \sigma(T_D)$ form a discrete sequence of eigenvalues, accumulating at $\frac{1}{2}$.
  - Numerical calculations reveal that the corresponding eigenfunctions have 'evenly distributed energy' over the space $\mathbb{R}^d$.
- When D is piecewise smooth with corners, T_D also contains essential spectrum:
  - The essential spectrum fills a whole interval, and is therefore easier to excite in practice.
  - Generalized eigenfunctions have strongly localized energy.

Eigenvalues and essential spectrum

Let $T : H \to H$ be a bounded self-adjoint operator on a Hilbert space H.

Definition 2.

- *The discrete spectrum* $\sigma_{\mathrm{disc}}(T)$ *of* T *is the subset of the* $\lambda \in \sigma(T)$ *such that:*
  (i) λ *is isolated in* $\sigma(T)$*: there exists* $\varepsilon > 0$ *such that* $\sigma(T) \cap (\lambda - \varepsilon, \lambda + \varepsilon) = \{\lambda\}$,
  (ii) λ *is an eigenvalue of* T *with finite multiplicity.*
- *The closed set* $\sigma_{\mathrm{ess}}(T) := \sigma(T) \setminus \sigma_{\mathrm{disc}}(T)$ *is the essential spectrum of* T.

Theorem 8 (Weyl criterion).

- $\lambda \in \mathbb{R}$ *belongs to* $\sigma(T)$ *if and only if there exists a sequence* $u_n \in H$ *such that:*

$$||u_n|| = 1 \text{ and } ||\lambda u_n - T u_n|| \xrightarrow{n \to \infty} 0.$$

  Such a sequence is called a Weyl sequence for T *associated to the value* λ.
- $\lambda \in \mathbb{R}$ *belongs to* $\sigma_{\mathrm{ess}}(T)$ *if and only if there exists an associated singular Weyl sequence, i.e. a Weyl sequence* u_n *such that* $u_n \to 0$ *weakly in* H.

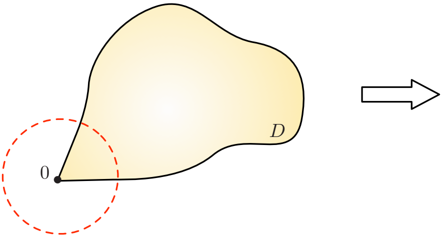
Theorem 9 ([BonZha, PerPu]).

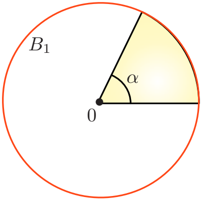
Let D be a piecewise smooth planar domain showing one corner at 0 with aperture α. The operator T_D has essential spectrum $\sigma_{\text{ess}}(T_D) = \left[\frac{\alpha}{2\pi}, 1 - \frac{\alpha}{2\pi}\right]$.

Sketch of the proof (from [BonZha]): Most of the proof relies on the analysis of truncated two-phase equation:

$$-\operatorname{div}(a(x)\nabla u) = f \text{ in } B_1, \text{ where } a(x) := \begin{cases} k & \text{in } D, \\ 1 & \text{otherwise} \end{cases} \qquad (\mathcal{C})$$

posed on the unit ball B_1 centered at 0, in which D coincides with the angular sector with aperture α (for simplicity, $0 < \alpha < \pi$).





Essential spectrum of T_D when D has a corner (II)

Proof of $\sigma_{\text{ess}}(T_D) \subset \left[\frac{\alpha}{2\pi}, 1 - \frac{\alpha}{2\pi}\right]$*:*

(i) By using the inf-sup condition ($\approx$ T-coercivity approach), we prove that, if $k \notin \left[-\frac{2\pi-\alpha}{\alpha}, -\frac{\alpha}{2\pi-\alpha}\right]$, the conductivity equation ($\mathcal{C}$) is well-posed on $H^1_0(B_1)$.

(ii) By the same token, the restriction of this equation near any other point $x_0 \in \partial D$ where ∂D is smooth is also well-posed.

Let $\lambda \in \sigma_{\text{ess}}(T_D)$ and $k = 1 - \frac{1}{\lambda}$; assume that $k \notin \left[-\frac{2\pi-\alpha}{\alpha}, -\frac{\alpha}{2\pi-\alpha}\right]$, and consider a singular Weyl sequence u_ε, i.e.

$$\sup_{\substack{v \in W^{1,-1}_0(\mathbb{R}^2) \\ ||v||_{W^{1,-1}_0(\mathbb{R}^2))=1}} \int_{\mathbb{R}^d} a(x) \nabla u_\varepsilon \cdot \nabla v \, dx \to 0,$$

$$\text{and } ||u_\varepsilon||_{W^{1,-1}_0(\mathbb{R}^2)} = 1, \quad u_\varepsilon \to 0 \text{ weakly in } W^{1,-1}_0(\mathbb{R}^2).$$

From (i) and (ii), for any $x_0 \in \partial D$, and $\rho > 0$ small enough:

$$\int_{B(x_0,\rho)} |\nabla u_\varepsilon|^2 \, dx \to 0.$$

Hence, $u_\varepsilon \to 0$ strongly in $W^{1,-1}_0(\mathbb{R}^2)$; a contradiction with $||u_\varepsilon||_{W^{1,-1}_0(\mathbb{R}^2)} = 1$.

Proof of $\sigma_{\text{ess}}(T_D) \supset \left[\frac{\alpha}{2\pi}, 1-\frac{\alpha}{2\pi}\right]$:

- Let $\lambda \in \left[\frac{\alpha}{2\pi}, 1-\frac{\alpha}{2\pi}\right]$, and $k = 1-\frac{1}{\lambda}$, so that $k \in \left[-\frac{2\pi-\alpha}{\alpha}, -\frac{\alpha}{2\pi-\alpha}\right]$.
- An explicit calculation using separation of variables shows that there exists a non trivial solution to $(\mathcal{C})$ of the form:

$$u(r,\theta) = r^{i\xi}\varphi(\theta),$$

where $\xi \equiv \xi(k)$ is real, and φ is smooth.
- This generalized eigenfunction u is not $W_0^{1,-1}(\mathbb{R}^2)$:

$$\begin{pmatrix} \frac{\partial u}{\partial r} \\ \frac{1}{r}\frac{\partial u}{\partial \theta} \end{pmatrix} = \begin{pmatrix} \frac{i\xi}{r} r^{i\xi}\varphi(\theta) \\ \frac{1}{r} r^{i\xi}\varphi'(\theta) \end{pmatrix} \Longrightarrow \int_{B_1\setminus B(0,\varepsilon)} |\nabla u|^2\, dx \xrightarrow{\varepsilon\to 0} +\infty.$$

Essential spectrum of T_D when D has a corner (IV)

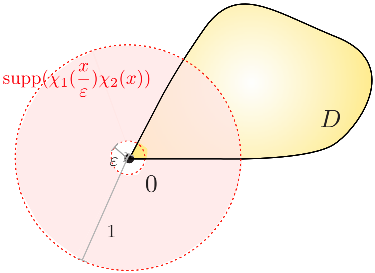
- However, u can be modified into a singular Weyl sequence for T_D and λ:

$$u_\varepsilon = s_\varepsilon \chi_1(\frac{x}{\varepsilon})\chi_2(x)u(x),$$

where

  - χ_1 is a smooth cutoff function with support in $\mathbb{R}^2 \setminus \overline{B_1}$,
  - χ_2 is a smooth cutoff function with support in B_1,
  - The constant s_ε is adjusted so that

$$||u_\varepsilon||_{W_0^{1,-1}(\mathbb{R}^2)} = 1.$$



- One proves indeed that:

$$||\lambda u_\varepsilon - T_D u_\varepsilon||_{H_0^1(\Omega)} \to 0, \ \ ||u_\varepsilon||_{H_0^1(\Omega)} = 1, \text{ and } ||u_\varepsilon||_{L^2(\Omega)} \to 0.$$

□

Final comments

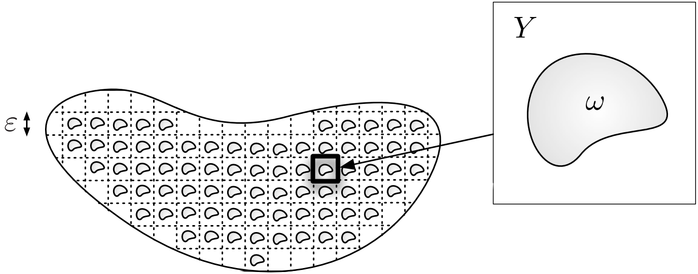
- The singular Weyl sequence constructed above gives a hint of the behavior 'generalized eigenfunctions' of T_D associated to $\lambda \in \sigma_{\mathrm{ess}}(T_D)$:

  $\Rightarrow$ Concentration of the energy in the neighborhood of the corner 0.

- The argument is readily generalized to the case of planar, piecewise smooth domains with several corners.

The homogenization setting

Microscopic inclusions with size ε and rescaled pattern $\omega \subset Y := (0,1)^d$ are periodically distributed in a 'hold-all' domain $\Omega \subset \mathbb{R}^d$.



Homogenized setting for a periodic distribution of inclusions.

Working assumptions:

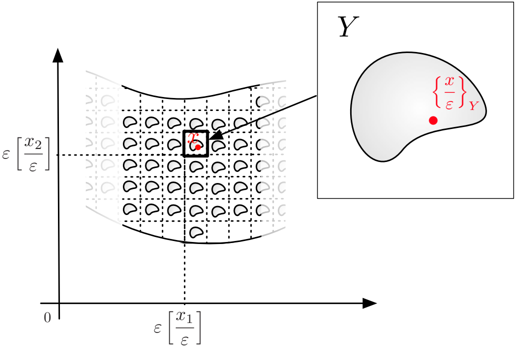
- ω is smooth and strongly included in Y: $\omega \Subset Y$;
- ω and $Y \setminus \overline{\omega}$ are connected.

The homogenization setting: notations

- For a point $x \in \mathbb{R}^d$:

$$x = \varepsilon \left[\frac{x}{\varepsilon}\right]_Y + \varepsilon \left\{\frac{x}{\varepsilon}\right\}_Y ;$$

- $\left[\frac{x}{\varepsilon}\right]_Y \in \mathbb{Z}^d$: macroscopic coordinate,
- $\left\{\frac{x}{\varepsilon}\right\}_Y \in Y$: microscopic coordinate.



- Indices of the cells strictly contained inside Ω:

$$\Xi_\varepsilon = \left\{\xi \in \mathbb{Z}^d,\ \varepsilon(\xi + Y) \Subset \Omega\right\}.$$

- The considered set of inclusions is:

$$\omega_\varepsilon = \bigcup_{\xi \in \Xi_\varepsilon} \omega_\varepsilon^\xi, \text{ where } \omega_\varepsilon^\xi := \varepsilon(\xi + \omega).$$

Goals of the study

The two concurrent goals pursued in this homogenization setting are:

1. Analyze the asymptotic behavior of the spectrum of $T_\varepsilon \equiv T_{\omega_\varepsilon}$ as a descriptor of the plasmonic resonances of the array of inclusions ω_ε

   $\Rightarrow$ study of the limiting spectrum:

$$\lim_{\varepsilon \to 0} \sigma(T_\varepsilon) = \left\{ \lambda \in [0,1], \text{ s.t. } \exists \varepsilon_j \downarrow 0, \; \lambda_{\varepsilon_j} \in \sigma(T_{\varepsilon_j}), \; \lambda_{\varepsilon_j} \to \lambda \right\}.$$

2. Explore the well-posedness of the conductivity equation for the voltage potential,

$$\left\{ \begin{array}{ll} -\mathrm{div}(a_\varepsilon \nabla u) = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{array} \right. , \text{ where } a_\varepsilon(x) := \left\{ \begin{array}{ll} k & \text{if } x \in \omega_\varepsilon, \\ 1 & \text{otherwise}, \end{array} \right.$$

   and the conductivity k inside the inclusions is negative, in the limit $\varepsilon \to 0$.

One part of the following result was observed in [BuRam]:

Theorem 10.

For all $\varepsilon > 0$*, one has:*

$$\sigma(T_\varepsilon) \cap (0,1) \subset (m, M),$$

where $0 < m < M < 1$ *are explicit constants:*

$$m = \min_{\substack{u \in \widehat{\mathfrak{h}}_0 \\ u \neq 0}} \frac{\displaystyle\int_\omega |\nabla_y u|^2 \, dy}{\displaystyle\int_Y |\nabla_y u|^2 \, dy}, \ \text{and } M = \max_{\substack{u \in \widehat{\mathfrak{h}}_0 \\ u \neq 0}} \frac{\displaystyle\int_\omega |\nabla_y u|^2 \, dy}{\displaystyle\int_Y |\nabla_y u|^2 \, dy},$$

and $\widehat{\mathfrak{h}}_0 \subset H^1(Y)/\mathbb{R}$ *is the Hilbert space defined by:*

$$\widehat{\mathfrak{h}}_0 = \left\{ u \in H^1(Y)/\mathbb{R}, \ \Delta_y u = 0 \text{ in } \omega \cup (Y \setminus \overline{\omega}), \text{ and } \int_{\partial\omega} \frac{\partial u^+}{\partial n_y} \, ds = 0 \right\}.$$

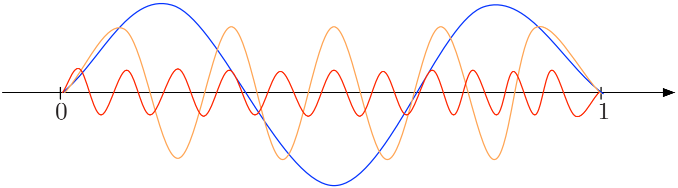
Hint of the proof: Use the min-max formulae for the eigenvalues of $T_\varepsilon : \mathfrak{h}_\varepsilon \to \mathfrak{h}_\varepsilon$.

How to study the limiting behavior of sequences $\lambda_\varepsilon \in \sigma(T_\varepsilon)$ (I)?

- T_ε converges weakly to the trivial operator $|\omega|\mathrm{Id}$:

$$\forall u \in H_0^1(\Omega), \quad T_\varepsilon u \xrightarrow{\varepsilon \to 0} |\omega| u, \text{ weakly in } H_0^1(\Omega).$$

- This poor convergence allows to infer nothing about the spectrum $\sigma(T_\varepsilon)$.
- As is well-known in homogenization theory, correctors are needed to obtain a stronger convergence, describing the oscillations of the $T_\varepsilon u$ at the ε-scale.
- These correctors can be used in the study of eigenvalues - see [SanVo, MosVo] - but this approach seems difficult in our context.



Typical behavior of a sequence $T_\varepsilon u$ converging weakly to 0 in $H_0^1(\Omega)$.

How to study the limiting behavior of sequences $\lambda_\varepsilon \in \sigma(T_\varepsilon)$ (II)?

- Our work is inspired by that of [AlCon] about Bloch wave homogenization. T_ε is rescaled into an operator
$$\mathbb{T}_\varepsilon : L^2(\Omega, H^1(\omega)/\mathbb{R}) \to L^2(\Omega, H^1(\omega)/\mathbb{R}),$$
which 'does the same' as T_ε, but acts on functions $\phi(x, y)$ depending on both macroscopic and microscopic variables x and y.

- We shall prove the pointwise convergence of the $\mathbb{T}_\varepsilon$, and rely on the result:

Proposition 11 ([Ka]).

Let H be a Hilbert space and let $S_\varepsilon : H \to H$ be a sequence of self-adjoint operators converging pointwise to $S : H \to H$, i.e.
$$\forall u \in H, \quad S_\varepsilon u \xrightarrow{\varepsilon \to 0} Su \text{ strongly}.$$
Then,
$$\lim_{\varepsilon \to 0} \sigma(S_\varepsilon) \supset \sigma(S).$$

The extension and projection operators E_ε and P_ε (I)

Definition 3 ([AlCon, CioDamGri]).

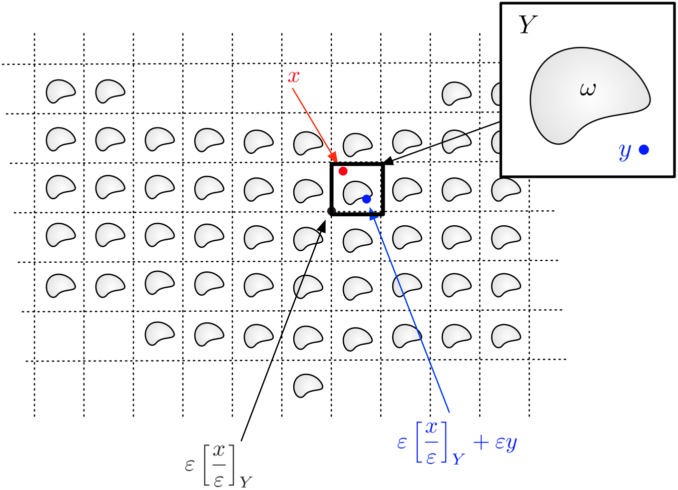
- *The* extension *operator* $E_\varepsilon : L^2(\Omega) \to L^2(\Omega \times Y)$ *is defined by:*

$$E_\varepsilon u(x,y) = \begin{cases} u(\varepsilon \left[\frac{x}{\varepsilon}\right]_Y + \varepsilon y) & \text{if } x \in \mathcal{O}_\varepsilon, \\ 0 & \text{otherwise.} \end{cases}$$

- *The* projection *operator* $P_\varepsilon : L^2(\Omega \times Y) \to L^2(\Omega)$ *is defined by:*

$$P_\varepsilon \phi(x) = \begin{cases} \displaystyle\int_Y \phi(\varepsilon \left[\frac{x}{\varepsilon}\right]_Y + \varepsilon z, \left\{\frac{x}{\varepsilon}\right\}_Y)\, dz & \text{if } x \in \mathcal{O}_\varepsilon, \\ 0 & \text{otherwise.} \end{cases}$$

The extension and projection operators E_ε and P_ε (II)



The operator E_ε rescales the content of each cell to size 1.

The rescaled operator $\mathbb{T}_\varepsilon$

The rescaled operator $\mathbb{T}_\varepsilon$ is defined by:

$$\boxed{\mathbb{T}_\varepsilon = E_\varepsilon T_\varepsilon P_\varepsilon : L^2(\Omega, H^1(\omega)/\mathbb{R}) \to L^2(\Omega, H^1(\omega)/\mathbb{R}).}$$

Proposition 12.

The rescaled operator $\mathbb{T}_\varepsilon$ has the following properties:

- $\mathbb{T}_\varepsilon$ *is self-adjoint.*
- $\sigma(\mathbb{T}_\varepsilon) = \sigma(T_\varepsilon) \setminus \{0\}$.

Single cell resonances.

- It follows from the two-scale convergence technology [Al, Ngue] that $\mathbb{T}_\varepsilon$ converges pointwise to a limit $\mathbb{T}_0$.
- This strong convergence of sequence $\mathbb{T}_\varepsilon u$ shows that $\mathbb{T}_0 u$ 'keeps track' of the ε-oscillations of the $\mathbb{T}_\varepsilon u$.
- This result allows to identify one part $\sigma(T_0) \subset \sigma(\mathbb{T}_0)$ of $\lim_{\varepsilon\to 0} \sigma(T_\varepsilon)$, corresponding to the resonance modes of a single inclusion $\omega \subset Y$.

Theorem 13.

The limit spectrum $\lim_{\varepsilon\to 0} \sigma(T_\varepsilon)$ *contains the cell spectrum, i.e. the spectrum of the operator* $T_0 : H^1_\#(Y)/\mathbb{R} \to H^1_\#(Y)/\mathbb{R}$ *defined by: for* $u \in H^1_\#(Y)/\mathbb{R}$,

$$\forall v \in H^1_\#(Y)/\mathbb{R}, \quad \int_Y \nabla_y (T_0 u) \cdot \nabla_y v \, dy = \int_\omega \nabla_y u \cdot \nabla_y v \, dy.$$

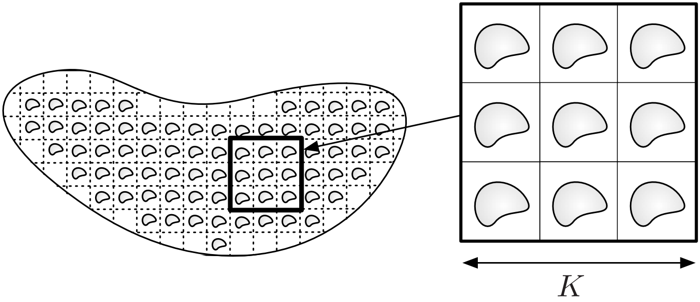
Rescaling T_ε over packs of cells (I)

Following [AlCon, Plan], the previous rescaling procedure can be performed over packs KY of K^d cells, containing a set ω^K of K^d copies of ω $(K > 1)$.

We define new extension and projection operators over K^d cells:

$$E_\varepsilon^K : L^2(\Omega) \to L^2(\Omega \times KY), \text{ and } P_\varepsilon^K : L^2(\Omega \times KY) \to L^2(\Omega),$$

which satisfy analogous properties to those of their single-cell counterparts.



Rescaling over a pack of K^d cells.

Rescaling T_ε over packs of cells (II)

$\lim_{\varepsilon\to 0}\sigma(T_\varepsilon)$ contains the spectrum of $T_0^K : H^1_\#(KY)/\mathbb{R} \to H^1_\#(KY)/\mathbb{R}$, defined by:

$$\forall v \in H^K, \int_{KY} \nabla_y(T_0^K u)\cdot\nabla_y v\, dy = \int_{\omega^K} \nabla_y u \cdot \nabla_y v\, dy.$$

The spectrum $\sigma(T_0^K)$ is analyzed using a discrete Bloch decomposition [AguiCon]:

Theorem 14.

Let u in $L^2_\#(KY)$. Then, there exist a unique set of K^d complex-valued functions $u_j(y) \in L^2_\#(Y)$, $j = (j_1, ..., j_d)$, $j_1, ..., j_d = 0, ..., K-1$, such that:

$$u(z) = \sum_{0\le j\le K-1} u_j(z)\, e^{\frac{2i\pi j}{K}\cdot z}, \text{ a.e. } z \in KY;$$

Furthermore, the Parseval identity holds:

$$\forall u, v \in L^2_\#(KY), \ \frac{1}{K^d}\int_{KY} u(z)\overline{v(z)}\, dx = \sum_{0\le j\le K-1}\int_Y u_j(y)\overline{v_j(y)}\, dy.$$

The Bloch spectrum.

Bloch decomposition behaves well with functions $u \in H^1(\omega^K)$, and diagonalizes operators with Y-periodic coefficients. Hence,

$$\sigma(T_0^K) = \bigcup_{0 \leq j \leq K-1} \sigma(T_{\eta_j}), \text{ for } \eta_j = \frac{j}{K},$$

and where the operators T_η are defined by:

- For $\eta \neq 0$, $T_\eta : H^1_\#(Y) \to H^1_\#(Y)$ is given by:

$$\forall v \in H^1_\#(Y), \int_Y (\nabla_y(T_\eta u) + 2i\pi\eta(T_\eta u)) \cdot \overline{(\nabla_y v + 2i\pi\eta v)}\, dy = \int_\omega (\nabla_y(T_\eta u) + 2i\pi\eta u) \cdot \overline{(\nabla_y v + 2i\pi\eta v)}\, dy.$$

- $T_0 : H^1_\#(Y)/\mathbb{R} \to H^1_\#(Y)/\mathbb{R}$ is the the same as in the case of a single cell:

$$\forall v \in H^1_\#(Y)/\mathbb{R}, \int_Y \nabla_y(T_0 u) \cdot \overline{\nabla_y v}\, dy = \int_\omega \nabla_y u \cdot \overline{\nabla_y v}\, dy.$$

The Bloch spectrum.

Theorem 15.

The spectrum $\sigma(T_\eta)$ *is composed of a discrete sequence of real eigenvalues:*

$$0 < \lambda_1^-(\eta) \leq \lambda_2^-(\eta) \leq \ldots \leq \frac{1}{2} \leq \ldots \leq \lambda_2^+(\eta) \leq \lambda_1^+(\eta) \leq 1.$$

Moreover, for any $i = 1, \ldots,$ *the mapping* $\overline{Y} \ni \eta \mapsto \lambda_i^\pm(\eta)$ *is Lipschitz continuous.*

Since the previous analysis can be performed for packs made from an arbitrary number K of cells, this implies:

Theorem 16.

The limit spectrum $\lim_{\varepsilon\to 0} \sigma(T_\varepsilon)$ *contains the Bloch spectrum* σ_{Bloch} *defined by*

$$\sigma_{\mathrm{Bloch}} = \bigcup_{i=1}^{\infty} \left[\min_{\eta\in[0,1]^d} \lambda_i^-(\eta), \max_{\eta\in[0,1]^d} \lambda_i^-(\eta) \right] \cup \bigcup_{i=1}^{\infty} \left[\min_{\eta\in[0,1]^d} \lambda_i^+(\eta), \max_{\eta\in[0,1]^d} \lambda_i^+(\eta) \right].$$

The completeness result

The remainder of $\lim_{\varepsilon\to 0}\sigma(T_\varepsilon)$ gathers the limit behaviors of the eigenvectors of T_ε which spend a 'not too small' part of their energy near the macroscopic boundary $\partial\Omega$.

Theorem 17.

The limit spectrum is decomposed as:

$$\lim_{\varepsilon\to 0}\sigma(T_\varepsilon) = \{0,1\}\cup\sigma_{\text{Bloch}}\cup\sigma_{\partial\Omega},$$

where the boundary layer spectrum $\sigma_{\partial\Omega}$ is the set of the $\lambda\in(0,1)$ such that, for any sequence $\lambda_\varepsilon\in\sigma(T_\varepsilon)$ with $\lambda_\varepsilon\to\lambda$, and any corresponding (normalized) eigenvector sequence $u_\varepsilon\in H^1_0(\Omega)$:

$$\forall s>0,\ \lim_{\varepsilon\to 0}\varepsilon^{-(1-1/d+s)}||\nabla u_\varepsilon||_{L^2(\mathcal{U}_\varepsilon)} = \infty,$$

where $\mathcal{U}_\varepsilon := \{x\in\Omega,\ d(x,\partial\Omega)<\varepsilon\}$ is the tubular neighborhood of $\partial\Omega$ with width ε.

The difficulty to characterize more precisely $\sigma_{\partial\Omega}$ reveals very strong interactions between the macroscopic boundary Ω and the inclusions; see [CasZua, MosVo].

General setting for the conductivity equation

- We now study the well-posedness and limit behavior of the conductivity equation:

$$\begin{cases} -\mathrm{div}(a_\varepsilon \nabla u_\varepsilon) = f & \text{in } \Omega, \\ u_\varepsilon = 0 & \text{on } \partial\Omega, \end{cases} \quad \text{where } a_\varepsilon(x) = \begin{cases} k & \text{if } x \in \omega_\varepsilon, \\ 1 & \text{otherwise.} \end{cases} \qquad (\mathcal{P}_\varepsilon)$$

  The conductivity k is in $\mathbb{C}$ and the source f is in $H^{-1}(\Omega)$.

- When $\mathcal{I}m(k) \neq 0$ or $k > 0$, the classical homogenization theory states that u_ε converges weakly in $H_0^1(\Omega)$ to the unique solution u_* of

$$\begin{cases} -\mathrm{div}(a^* \nabla u_*) = f & \text{in } \Omega, \\ u_* = 0 & \text{on } \partial\Omega, \end{cases} \qquad (\mathcal{P}^*)$$

  where the positive definite homogenized tensor is defined by:

$$a^*_{ij} = \int_Y a(y)(\nabla_y w_i + e_i) \cdot (\nabla_y w_j + e_j)\, dy, \ \text{where } a(y) = \begin{cases} k & \text{if } y \in \omega, \\ 1 & \text{if } y \in Y \setminus \overline{\omega}. \end{cases}$$

  and the cell functions $w_i \in H^1_\#(Y)/\mathbb{R}$ solve

$$-\mathrm{div}(a(y)(\nabla w_i + e_i)) = 0 \text{ in } Y, \quad i = 1, ..., d.$$

- What happens when $k < 0$?

The formal, homogenized tensor in the case $a < 0$

The cell problems

$$-\mathrm{div}(a(y)(\nabla_y w_i + e_i)) = 0 \text{ in } Y, \quad i = 1, ..., d.$$

are well-posed provided $\lambda := \frac{1}{1-k}$ does not belong to the spectrum $\sigma(T_0)$ of the cell operator $T_0 : H^1_\#(Y)/\mathbb{R} \to H^1_\#(Y)/\mathbb{R}$:

$$\forall v \in H^1_\#(Y)/\mathbb{R}, \int_Y \nabla_y(T_0 u) \cdot \nabla_y v \, dy = \int_\omega \nabla_y u \cdot \nabla_y v \, dy.$$

It then makes sense to define the (formal) homogenized tensor

$$a^*_{ij} = \int_Y a(y)(\nabla_y w_i + e_i) \cdot (\nabla_y w_j + e_j) \, dy$$

as soon as $k \notin \Sigma_\omega := \left\{ k \in \mathbb{C}, \frac{1}{1-k} \in \sigma(T_0) \right\}$.

Theorem 18.

Let $k \in \mathbb{C} \setminus \Sigma_\omega$; *then,*

- *If* $u_\varepsilon \in H_0^1(\Omega)$ *is a sequence of solutions to* $(\mathcal{P}_\varepsilon)$ *such that*

$$||\nabla u_\varepsilon||_{L^2(\Omega)} \leq C,$$

  then up to a subsequence, u_ε *converges weakly in* $H_0^1(\Omega)$ *to a solution of* $(\mathcal{P}^*)$.

- *Conversely, if* $u \in H_0^1(\Omega)$ *is one solution to* $(\mathcal{P}^*)$ *(if any), then for any sequence* $k_\varepsilon \to k$, $k_\varepsilon \notin \Sigma_\omega$, *there exists a sequence* $f_\varepsilon \in H^{-1}(\Omega)$ *converging pointwise to* f *and a sequence* u_ε *of associated voltage potentials, i.e.:*

$$\begin{cases} -\mathrm{div}(a_\varepsilon \nabla u_\varepsilon) = f_\varepsilon & \text{in } \Omega, \\ u_\varepsilon = 0 & \text{on } \partial\Omega \end{cases}, \text{ where } a_\varepsilon(x) = \begin{cases} k_\varepsilon & \text{if } x \in \omega_\varepsilon, \\ 1 & \text{otherwise,} \end{cases}$$

  such that $u_\varepsilon \to u$ *weakly in* $H_0^1(\Omega)$.

This indicates that no 'good' solution to $(\mathcal{P}^*)$ can be singled out via such a limiting process.

The particular case of high-contrast

The previous material reveals that the conductivity equation $(\mathcal{P}_\varepsilon)$ is uniformly well-posed as $\varepsilon \to 0$ when $k < 0$ is either 'very small' or 'very large'.

Theorem 19.

There exists a constant $0 < \alpha$ *such that, if the conductivity* k *belongs to* $(-\infty, -1/\alpha) \cup (-\alpha, 0)$, *then:*

(i) *For* $0 < \varepsilon$, *the system* $(\mathcal{P}_\varepsilon)$ *for* u_ε *is well-posed, i.e. it has a unique solution for any source* $f \in H^{-1}(\Omega)$, *and* u_ε *depends continuously on* f.

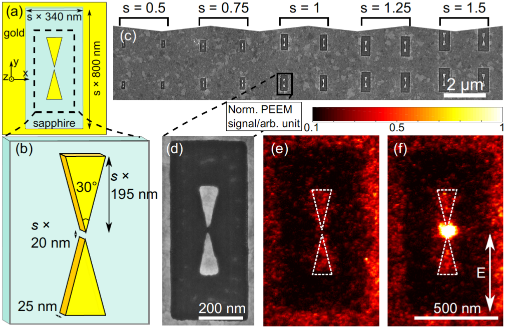
(ii) *The homogenized tensor* a^* *is elliptic; in particular,* $(\mathcal{P}^*)$ *is well-posed.*

(iii) *For any source* $f \in H^{-1}(\Omega)$, *the unique solution* $u_\varepsilon \in H^1_0(\Omega)$ *to* $(\mathcal{P}_\varepsilon)$ *converges, weakly in* $H^1_0(\Omega)$, *to the unique solution* u_* *of* $(\mathcal{P}^*)$.

Why bowtie-shaped antennas?

Physical experiments report that:

- Bowtie-shaped antennas support multiple surface plasmon modes, and can therefore operate under a large bandwidth.
- Some of the surface plasmon modes show highly localized energy near the tips.

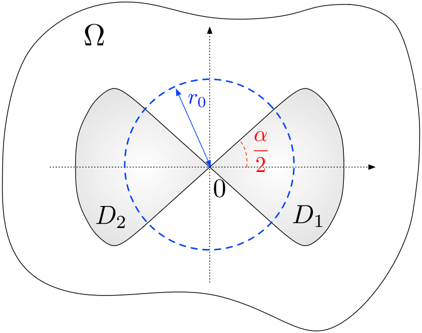


Depending on the incident illumination, the electric field is enhanced at the level of the whole bowtie device, or it is concentrated near the tips; excerpted from [LorMarLos].

The bowtie-shaped antenna

- The situation takes place In the plane $\mathbb{R}^2$, inside a bounded 'hold-all' domain Ω.
- The domain $D \Subset \Omega$ is bowtie-shaped (and not Lipschitz): $D = D_1 \cup D_2$, where,

$$D_1 \cap B_{r_0} = \left\{(r\cos\theta, r\sin\theta),\ \ r \in (0, r_0),\ \ \theta \in \left(-\frac{\alpha}{2}, \frac{\alpha}{2}\right)\right\},$$
$$D_2 \cap B_{r_0} = \left\{(r\cos\theta, r\sin\theta),\ \ r \in (0, r_0),\ \ \theta \in \left(\pi - \frac{\alpha}{2}, \pi + \frac{\alpha}{2}\right)\right\}.$$



Program of the study

For simplicity (and w.l.o.g.), we consider the version of the Poincaré variational operator featuring Ω and homogeneous Dirichlet boundary conditions on $\partial\Omega$.

For $u \in H^1_0(\Omega)$, $T_D u$ is the unique element in $H^1_0(\Omega)$ such that:

$$\forall v \in H^1_0(\Omega), \quad \int_\Omega \nabla(T_D u) \cdot \nabla v \, dx = \int_D \nabla u \cdot \nabla v \, dx.$$

Questions:

- What is the spectrum of T_D when D is a bowtie?
- What do the generalized eigenfunctions look like?
- How can we relate this spectrum to that of a more realistic 'near bowtie antenna'?

Plasmonic resonances of the bowtie antenna (I)

Theorem 20 (Essential spectrum of T_D).

The operator T_D has only essential spectrum and $\sigma(T_D) = [0,1]$.

Hint of proof: The proof is very close in spirit to that of Theorem 9.

- Let $\lambda \in [0, \frac{1}{2}) \cup (\frac{1}{2}, 1]$ and $k = 1 - \frac{1}{\lambda} \in (-\infty, -1) \cup (-1, 0)$; we consider the two-phase conductivity equation:

$$-\operatorname{div}(a(x)\nabla u) = f \text{ in } B_1, \text{ where } a(x) := \begin{cases} k & \text{in } D \cap B_1, \\ 1 & \text{otherwise} \end{cases} \qquad (\mathcal{C})$$

- A calculation using separation of variables shows that there exists
  - A real number $\xi \equiv \xi(k) \neq 0$,
  - a smooth, 2π-periodic function $\varphi(\theta)$,

  such that

$$u(r,\theta) := r^{i\xi}\varphi(\theta)$$

  is one solution to $(\mathcal{C})$ in the sense of distributions.

- The function u does not belong to $H^1_0(\Omega)$ since its gradient blows up at 0.

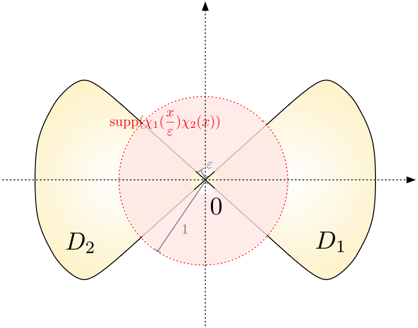
Plasmonic resonances of the bowtie antenna (II)

- However, u may be modified into a singular Weyl sequence u_ε for T_D and λ:

$$u_\varepsilon(x) = s_\varepsilon \chi_1\left(\frac{x}{\varepsilon}\right)\chi_2(x)u(x),$$

where:

  - χ_1 is a smooth cutoff function with support in $\mathbb{R}^2 \setminus B_1$,
  - χ_2 is a smooth cutoff function with support in B_1,
  - The normalization constant s_ε is adjusted so that $||u_\varepsilon||_{H_0^1(\Omega)} = 1$.



- One indeed proves that:

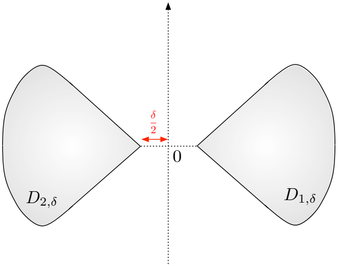
$$||\lambda u_\varepsilon - T_D u_\varepsilon||_{H_0^1(\Omega)} = \sup_{\substack{v\in H_0^1(\Omega)\\ ||v||_{H_0^1(\Omega)}=1}} \int_\Omega a(x)\nabla u_\varepsilon \cdot \nabla v \, dx \xrightarrow{\varepsilon\to 0} 0.$$

The near bowtie antenna, with close-to-touching wings (I)

Let $D_\delta = D_{1,\delta} \cup D_{2,\delta}$ be a piecewise smooth version of the bowtie antenna, with only close-to-touching wings:

$$D_{1,\delta} = \left(\frac{\delta}{2}, 0\right) + D_1, \text{ and } D_{2,\delta} = \left(-\frac{\delta}{2}, 0\right) + D_2,$$

for small enough $\delta > 0$.



We are interested in the limiting spectrum of $\sigma(T_{D_\delta})$ as $\delta \to 0$:

$$\lim_{\delta \to 0} \sigma(T_{D_\delta}) := \left\{\lambda \in \mathbb{R}, \ \exists \delta_n \downarrow 0, \ \lambda_n \in \sigma(T_{D_{\delta_n}}), \ \lambda_n \to \lambda\right\}.$$

The near bowtie antenna, with close-to-touching wings (II)

Theorem 21 (Limiting spectrum for a near-bowtie antenna).

The limiting spectrum of T_{D_δ} is exactly that of the Poincaré variational operator of the bowtie antenna D:

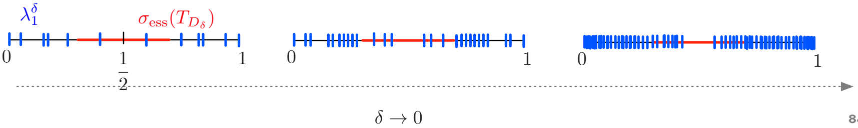
$$\lim_{\delta \to 0} \sigma(T_{D_\delta}) = \sigma(T_D) = [0, 1].$$

Remark:

- For fixed $\delta > 0$, D_δ is piecewise smooth with corners of aperture α, so that Theorem 9 applies: $\sigma(T_{D_\delta})$ is the reunion of a set of discrete eigenvalues $\{\lambda_i^\delta\}_{i=0,\ldots}$ and the interval of essential spectrum:

$$\sigma_{\mathrm{ess}}(T_{D_\delta}) = \left[\frac{\alpha}{2\pi}, 1 - \frac{\alpha}{2\pi}\right] \Subset [0, 1].$$

- Theorem 21 implies that as $\delta \to 0$, the eigenvalues $\{\lambda_i^\delta\}_{i=0,\ldots}$ densify to eventually fill the whole gaps $[0, 1] \setminus \sigma_{\mathrm{ess}}(T_{D_\delta})$.



Hint of the proof: From the 'convergence of domains'

$$\mathbb{1}_{D_\delta} \xrightarrow{\delta \to 0} \mathbb{1}_D \text{ in } L^1(\Omega),$$

the pointwise convergence of associated operators follows easily:

$$\text{For all } u \in H_0^1(\Omega), \quad T_{D_\delta} u \xrightarrow{\delta \to 0} T_D u \text{ strongly in } H_0^1(\Omega).$$

The result is then directly implied by the abstract fact:

Proposition 22 ([Ka]).

Let H be a Hilbert space and let $S_\varepsilon : H \to H$ be a sequence of self-adjoint operators converging pointwise to $S : H \to H$. Then,

$$\lim_{\varepsilon \to 0} \sigma(S_\varepsilon) \supset \sigma(S).$$

□

Remark: A more constructive proof is possible, involving surgery of the generalized eigenfunctions for T_D to produce 'quasi-eigenfunctions' for T_{D_δ}.

Thank you for your attention!

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