Homogenization and the Neumann Poincaré operator

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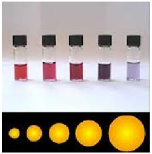
Outline:

1. Motivation : resonant frequencies in metallic nanoparticles
2. The NP operator/the Poincaré variational problem for a periodic collection of inclusions
3. The limiting spectra
4. Consequences concerning the homogenization of inclusions with non-positive conductivities
5. Conclusion

1. Resonant frequencies of metallic nanoparticles



Very small metallic particles exhibit interesting diffractive phenomena, related to resonances : localization and extremely large enhancement of the electromagentic fields in their vicinity

Many potential applications : nanophotonics, nanolithography, near field microscopy, biosensors, cancer therapy

2 main ingredients :

- The wavelength of the incident excitation should be larger than the particle diameter
- the real part of the electric permittivity $\varepsilon(\omega)$ inside the particle is negative

Typical model problem

Consider a particule that occupies a bounded C^2 domain $\delta D \subset \mathbf{R}^d$

δ is small, $|D| = 1$

$\omega \in \mathbf{C}$ is a resonant frequency of the nanoparticle D_δ if there exists a non-trivial solution U to the PDE (TE polarization):

$$\begin{cases} \Delta U + \omega^2 \varepsilon(x,\omega)\mu_0 U & = 0 \quad \text{in} \quad \mathbf{R}^d \setminus \overline{D_\delta} \cup D_\delta \\ [\varepsilon U] & = 0 \quad \text{on} \quad \partial D_\delta \\ \left[\frac{\partial U}{\partial \nu}\right] & = 0 \quad \text{on} \quad \partial D_\delta \\ \text{radiation condition} \end{cases}$$

The Drude model gives a good description of the electric permittivity ε of metals such as Au, Ag, Al, in the range of frequencies of interest

$$\varepsilon(x,\omega) = \begin{cases} \varepsilon_0 & \text{for } x \in \mathbf{R}^d \setminus \overline{D_\delta} \\ \varepsilon_0 \hat{\epsilon}(\omega) = \varepsilon_0 \left(\varepsilon_\infty - \frac{\omega_P^2}{\omega^2 + i\omega\Gamma} \right) & \text{for } x \in D_\delta \end{cases}$$

The change of variable $\tilde{x} = z + x/\delta$ transforms the original PDE into

$$\begin{cases} \Delta \tilde{U} + \delta^2 \omega^2 \varepsilon(x,\omega)\mu_0 \tilde{U} & = 0 \qquad \text{in } \mathbf{R}^2 \setminus \overline{D} \cup D \\ \left[\varepsilon \tilde{U}\right] & = 0 \qquad \text{on } \partial D \\ \left[\frac{\partial \tilde{U}}{\partial \nu}\right] & = 0 \qquad \text{on } \partial D \end{cases}$$

where $\tilde{U}(x) = U(\tilde{x})$ and one expects that $\varepsilon \tilde{U}$ converges to a solution of the quasistatic problem

$$\begin{cases} \operatorname{div}(1/\varepsilon(\omega)\nabla u) & = & 0 & \text{in } \mathbf{R}^d \\ u & \rightarrow & 0 & \text{as } |x| \rightarrow \infty \end{cases}$$

Electrostatic resonances: find the values of ε for which the above PDE has non trivial solutions

[Mayergoyz-Fredkin-Zhang, Grieser, Ammari-Millien-Ruiz-Zhang]

We may seek u in the form $u(x) = S_D\varphi(x)$ where S_D is the single layer potential on $\partial\Omega$

$$
\begin{aligned}
S_D\psi(x) &= \int_{\partial D} G(x,y)\psi(y)\,d\sigma(y), \quad x \in \mathbf{R}^d \\
G(x,y) &= \begin{cases} \dfrac{1}{2\pi}\ln|x-y| & \text{if } d=2 \\ \dfrac{|x-y|^{d-2}}{(2-d)\omega_d} & \text{if } d \geq 3 \end{cases}
\end{aligned}
$$

For $\psi \in L^2(\partial D)$, the function $S_D\psi$ is harmonic in D and in $\mathbf{R}^d \setminus D$, continuous across ∂D and satisfies the Pelmelj jump relations

$$
\partial_\nu S_D\psi|_\pm = \pm 1/2\psi + K_D^*\psi
$$

The operator K_D^* (or its adjoint) is the Neumann-Poincaré operator

$$
K_D^*\psi(x) = \int_{\partial D} \frac{\nu(x)\cdot(x-y)}{|x-y|^2}\psi(y)\,d\sigma(y)
$$

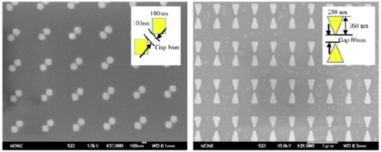
The layer potential φ yields a solution to the PDE provided

$$(\lambda(\omega)I - K_D^*)\varphi \quad = \quad 0$$

where $\lambda(\omega) = \dfrac{1/\hat{\epsilon}(\omega)+1}{2(1/\hat{\epsilon}(\omega)-1)}$ is thus an eigenvalue of K_D^*

- $\sigma(K_D^*) \subset [-1/2, 1/2]$
- When D is smooth ($\mathcal{C}^{1,\alpha}$), K_D^* is compact consisting of a countable sequence of eigenvalues accumulating at 0
- When D is Lipschitz, K_D^* may have continous spectrum

Goal in applications: tune the shape of D to trigger resonant frequencies at desired values of ω

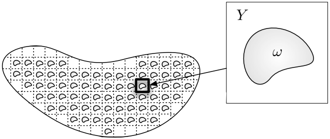


[Gang Bi et al, Optics Comm., 285 (2012) 2472]

The Neumann-Poincaré operator naturally appears also in other situations: cloaking, pointwise estimates on gradients of solutions to elliptic PDE's in composite media

[Ammari-Ciraolo-Kang-Lim, Perfekt-Putinar, Ola, Kang-Lim-Yu, EB-Triki]

2. The Neumann-Poincaré operator/ Poincaré variationnal problem for a periodic collection of inclusions



$\omega \subset\subset Y$

Consider $\Omega \subset \mathbf{R}^2$, smooth bounded domain, that contains a periodic collection of smooth inclusions

$$D \;=\; \omega_\varepsilon \;=\; \cup_{i\in N_\varepsilon}(\omega_{\varepsilon,i}) \qquad \omega_{\varepsilon,i} = z_{\varepsilon,i} + \varepsilon\omega, \quad i \in N_{\varepsilon,i}$$

Model PDE : given $f \in L^2(\Omega)$, seek $u \in H^1_0(\Omega)$ such that

$$-\mathrm{div}(A(x)\nabla u) \;=\; f \quad \text{in } \Omega, \qquad A(x) = \begin{cases} k & \text{in } \omega_\varepsilon \\ 1 & \text{otherwise} \end{cases}$$

What are the resonant frequencies of such a system ? Are there collective effects ?

What is $\lim_{\varepsilon\to 0} \sigma(K^*_\varepsilon)$?

As the definition of the Neumann-Poincaré depends on the number of inclusions, we work with the Poincaré variational operator

$$T_\varepsilon \ : H^1_0(\Omega) \to H^1_0(\Omega)$$

$$\forall\, v \in H^1_0(\Omega), \quad \int_\Omega \nabla T_\varepsilon u \cdot \nabla v \quad = \quad \int_{\omega_\varepsilon} \nabla u \cdot \nabla v$$

If $\quad T_\varepsilon u \;=\; \beta u \quad$ for some $u \in H^1_0(\Omega)$ and $\beta \in \mathbf{R}$, then for any $v \in H^1_0(\Omega)$

$$\begin{aligned} \int_\Omega \nabla T_\varepsilon u \cdot \nabla v \,-\, \int_{\omega_\varepsilon} \nabla u \cdot \nabla v \;&=\; \beta \int_\Omega \nabla u \cdot \nabla v \,-\, \int_{\omega_\varepsilon} \nabla u \cdot \nabla v \\ =\;\; \beta \int_{\Omega \setminus \omega_\varepsilon} \nabla u \cdot \nabla v + (\beta - 1) \int_{\omega_\varepsilon} \nabla u \cdot \nabla v \;&=\; 0 \end{aligned}$$

It follows that $\quad \mathrm{div}(a(\beta)\nabla u) = 0$

$$u = S_{\omega_\varepsilon}\varphi \quad \text{with} \quad (\lambda I - K^*_{\omega_\varepsilon})\varphi \;=\; 0, \qquad\qquad \lambda = 1/2 - \beta$$

We conclude that $\quad \sigma(T_\varepsilon) = 1/2 - \sigma(K^*_{\omega_\varepsilon})$

Theorem

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

• The first term is the Bloch spectrum and corresponds to bulk resonant modes of single cells or group of cells

$$\sigma_{\mathrm{Bloch}} \quad = \quad \cup_{i\geq 1}[\min_{\eta\in[0,1]^d} \lambda_i^-(\eta), \max_{\eta\in[0,1]^d} \lambda_i^-(\eta)] \cup [\min_{\eta\in[0,1]^d} \lambda_i^+(\eta), \max_{\eta\in[0,1]^d} \lambda_i^+(\eta)]$$

where the operators T_η are defined by

$$\forall\, v \in H^1_\#(Y), \quad \int_Y (\nabla T_\eta u + 2i\pi\eta T_\eta u)\cdot\overline{(\nabla v + 2i\pi\eta v)} \;= \int_\omega (\nabla u + 2i\pi\eta u)\cdot\overline{(\nabla v + 2i\pi\eta v)}, \quad \eta \neq 0$$

$$\forall\, v \in H^1_\#(Y)/\mathbf{R}, \quad \int_Y \nabla T_0 u\cdot\overline{\nabla v} \;=\; \int_\omega \nabla u\cdot\overline{\nabla v}, \quad \eta = 0$$

- The boundary layer spectrum $\sigma_{\partial\Omega}$ is defined as the set of $\lambda \in (0,1)$ such that

$$\exists\ (\lambda_\varepsilon) \subset \sigma(T_\varepsilon) \quad \text{such that } \lambda_\varepsilon \to \lambda$$

and for which the associated eigenvectors $u_\varepsilon \in H_0^1(\Omega)$ satisfy

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

where

$$\mathcal{U}_\varepsilon \quad = \quad \{x \in \Omega, d(x, \partial\Omega) < \varepsilon\}$$

Remarks :

- It is more convenient to work with T_ε (domains of definition easier to handle)

- Our work is largely inspired by the analysis of [Allaire-Conca] who studied the high frequency limit of spectra of diffusion equations using Bloch wave homogenization

- As $\varepsilon \longrightarrow 0$, the operators T_ε converge to a limiting operator T_∞ defined on $H_0^1(\Omega)$ by

$$\forall\, v \in H_0^1(\Omega) \quad \int_\Omega \nabla T_\infty u \cdot \nabla v \quad = \quad |\omega| \int_\Omega \nabla u \cdot \nabla v$$

  However, the convergence is only in a weak sense, and thus does not yield any information on $\lim_{\varepsilon\to 0} \sigma(T_\varepsilon)$

- To take into account the microscopic effects in the limit, we define a 2-scale version $\tilde{T}_\varepsilon$ of T_ε on the larger space $L^2(\Omega, H^1(\omega)/\mathbf{R})$, which has the same spectrum

- We show that the operators $\tilde{T}_\varepsilon$ converge strongly to a limiting operator $\tilde{T}_0$, and thus $\lim_{\varepsilon\to 0} \sigma(T_\varepsilon) \supset \sigma(\tilde{T}_0)$

Key ingredient :

2-scale convergence [Allaire, Nguetseng] and the associated compactness properties

Theorem : Let u_ε be a bounded sequence in $L^2(\Omega)$

1. Then there exists $u_0 \in L^2(\Omega \times L^2_\#(Y))$ such that u_ε 2-scale converges weakly to u_0, i.e.

$$\forall\, \phi \in L^2(\Omega, \mathcal{C}_\#(Y)), \quad \int_\Omega u_\varepsilon(x)\phi(x, x/\varepsilon)\, dx \quad \to \quad \int_{\Omega\times Y} u_0(x,y)\phi(x,y)\, dxdy$$

2. Assume that a sequence (u_ε) converges weakly in L^2 to some $u_0 \in H^1(\Omega)$. Then there exists $\hat{u} \in L^2(\Omega, H^1_\#(Y)/\mathbf{R})$ such that, up to a subsequence

- u_ε 2-scale converges to u
- ∇u_ε 2-scale converges to $\nabla u_0(x) + \nabla_y \hat{u}(x,y)$

3. Bloch wave homogenization

Following [Allaire-Conca] (see also [Cioranescu-Damlamian-Griso]) we define

- an extension operator $E_\varepsilon \ : L^2(\Omega) \longrightarrow L^2(\Omega \times Y)$

$$E_\varepsilon u(x,y) \quad = \quad \begin{cases} u(\varepsilon[x/\varepsilon] + \varepsilon y) & \text{if } x \in \omega_{\varepsilon,i} \subset \Omega \\ 0 & \text{otherwise} \end{cases}$$

- a projection operator $P_\varepsilon \ : L^2(\Omega \times Y) \longrightarrow L^2(\Omega)$

$$P_\varepsilon \phi(x) \quad = \quad \begin{cases} \displaystyle\int_Y \phi(\varepsilon[x/\varepsilon] + \varepsilon z, \{x/e\})\, dz & \text{if } x \in \omega_{\varepsilon,i} \subset \Omega \\ 0 & \text{otherwise} \end{cases}$$

Denoting Ω_ε the union of all the cells $\omega_{\varepsilon,i}$ that are fully contained in Ω

- E_ε and P_ε are bounded operators with norm 1
- $P_\varepsilon : L^2(\Omega \times Y) \to L^2(\Omega)$ and $E_\varepsilon : L^2(\Omega) \to L^2(\Omega \times Y)$ are adjoint operators
- P_ε and E_ε are almost inverse to one another

  for $u \in L^2(\Omega)$, $\quad P_\varepsilon E_\varepsilon u(x) = \begin{cases} u(x) & \text{if } x \in \Omega_\varepsilon \\ 0 & \text{otherwise} \end{cases}$

  for $\phi \in L^2(\Omega \times Y)$, $\quad E_\varepsilon P_\varepsilon \phi \to \phi$ strongly in $L^2(\Omega \times Y)$

In our setting, we should be cautious as the definition of T_ε involves derivatives, whereas the operators $E_\varepsilon, P_\varepsilon$ may not define functions in H^1

We set $\tilde{T}_\varepsilon := E_\varepsilon T_\varepsilon^\circ P_\varepsilon$ with

$$\begin{array}{rcl}
\tilde{T}_\varepsilon \ : L^2(\Omega, H^1(\omega)/\mathbf{R}) & \longrightarrow & L^2(\Omega, H^1(\omega)/\mathbf{R}) \\
P_\varepsilon \downarrow & & \uparrow \ E_\varepsilon \\
T_\varepsilon^\circ \ : H_\varepsilon := H^1(\omega_\varepsilon)/C(\omega_\varepsilon) & \longrightarrow & H_\varepsilon \\
\downarrow & & \uparrow \\
T_\varepsilon \ : H_0^1(\Omega) & \longrightarrow & H_0^1(\Omega)
\end{array}$$

where $C(\omega_\varepsilon) \ = \ \{u \in H_0^1(\Omega), \ \ u = (\mathrm{const})_i \text{ on } \omega_{\varepsilon,i}\}$

$$\begin{aligned}
&\phi \in L^2(\Omega \times H^1(\omega)/\mathbf{R}) \ \rightarrow \ P_\varepsilon\phi := u_\varepsilon \in H^1(\omega_\varepsilon)/C(\omega_\varepsilon) \\
&\rightarrow \ v_\varepsilon \in H_0^1(\Omega), \quad \text{such that} \quad \int_\Omega \nabla v_\varepsilon \cdot \nabla v \ = \int_{\omega_\varepsilon} \nabla u_\varepsilon \cdot \nabla v \\
&\rightarrow \ \tilde{T}_\varepsilon\phi = E_\varepsilon v_\varepsilon|_{\Omega\times\omega}
\end{aligned}$$

Proposition

- $\tilde{T}_\varepsilon$ is self-adjoint and $\quad \sigma(\tilde{T}_\varepsilon) \;=\; \sigma(T_\varepsilon) \setminus \{0\}$

- For any $\phi \in L^2(\Omega, H^1(\omega)/\mathbf{R})$, $\tilde{T}_\varepsilon \phi$ converges strongly in $L^2(\Omega, H^1(\omega)/\mathbf{R})$ to some $\tilde{T}_0 \phi$

  $\tilde{T}_0 \phi = Q\hat{v}$ where $Q \; : L^2(\Omega, H^1_\#(Y)/\mathbf{R}) \longrightarrow L^2(\Omega, H^1(\omega)/\mathbf{R})$ is the restriction operator and $\hat{v}$ is the unique solution in $L^2(\Omega, H^1_\#(Y)/\mathbf{R})$ of

  $$-\Delta_y \hat{v}(x,y) \;=\; -\mathrm{div}_y(1_\omega(y) \nabla_y \phi)(x,y) \qquad \text{in } Y,\ a.e.\ x \in \Omega$$

- It follows that $\quad \lim_{\varepsilon \to 0} \sigma(T_\varepsilon) \supset \sigma(\tilde{T}_0)$

- Actually, $\sigma(\tilde{T}_0) = \sigma(T_0) \setminus \{0\}$, where $T_0 \; : H^1_\#(Y)/\mathbf{R} \longrightarrow H^1_\#(Y/\mathbf{R})$ is defined by

  $$\forall\, v \in H^1_\#(Y), \quad \int_Y \nabla T_0 u \cdot \nabla v \;=\; \int_\omega \nabla u \cdot \nabla v$$

The values in $\sigma(T_0)$ can be interpreted as eigenvalues of single-cell resonant modes

This follows from the compactness induced by 2-scale convergence :

$$\phi \in L^2(\Omega \times H^1(\omega)/\mathbf{R}) \;\rightarrow\; P_\varepsilon \phi := u_\varepsilon \in H^1(\omega_\varepsilon)/C(\omega_\varepsilon)$$
$$\rightarrow\; v_\varepsilon \in H_0^1(\Omega), \quad \text{such that} \quad \int_\Omega \nabla v_\varepsilon \cdot \nabla v \;=\; \int_{\omega_\varepsilon} \nabla u_\varepsilon \cdot \nabla v$$
$$\rightarrow\; \tilde{T}_\varepsilon \phi = E_\varepsilon v_\varepsilon|_{\Omega\times\omega}$$

then

$$\begin{cases} \varepsilon v_\varepsilon & \rightharpoonup \quad v_0 & \text{weakly in } H_0^1(\Omega) \\ \varepsilon E_\varepsilon(\nabla v_\varepsilon) & \rightharpoonup \quad \nabla v_0 + \nabla_y \hat{v} & \text{weakly in } L^2(\Omega \times Y) \end{cases}$$

$$\int_{\Omega\times Y} (\nabla v_0 + \nabla_y \hat{v}) \cdot (\nabla\phi + \nabla_y \psi) \quad = \quad \int_{\Omega\times\omega} \nabla_y \phi(x,y) \cdot (\nabla\phi + \nabla_y\psi)$$

Collective resonances of the inclusions

The rescaling procedure can also be performed on a pack of cells (i.e. over K^d copies of the unit cell Y)

- define corresponding projection and extension operators $E_\varepsilon^K, P_\varepsilon^K$
- define $\tilde{T}_\varepsilon^K$
- show that $\tilde{T}_\varepsilon^K$ converges strongly to a limiting operator $\tilde{T}_0^K$
- whose spectrum coincides with that of $T_0^K \; : H^1_\#(KY)/\mathbf{R} \longrightarrow H^1_\#(KY)/\mathbf{R}$ defined by

$$\forall\, v \in H^1_\#(KY), \quad \int_{KY} \nabla T_0 u \cdot \nabla v \quad = \quad \int_{\omega^K} \nabla u \cdot \nabla v$$

- and in fact $\quad \sigma(T_0^K) \; = \; \cup_{0 \le j \le K-1} \sigma(T_\eta) \qquad \eta = j/K$

4. Homogenization with NIM's

Let $f \in L^2(\Omega)$ and consider $u_\varepsilon \in H_0^1(\Omega)$ solution to

$$(P_\varepsilon) \qquad -\operatorname{div}(A_\varepsilon(x)\nabla u_\varepsilon(x)) = f \qquad \text{in } \Omega$$

where $A_\varepsilon(x) = \begin{cases} a > 0 & x \in \omega_\varepsilon \\ 1 & \text{otherwise} \end{cases}$

Then $u_\varepsilon \rightharpoonup u_*$ weakly in $H_0^1(\Omega)$, with

$$(P_*) \qquad -\operatorname{div}(A_*\nabla u_*(x)) = f \qquad \text{in } \Omega$$

A_* is a (constant) matrix, whose entries are given in terms of the solutions to the cell problems : find $\chi_j \in H^1_\#(Y)/\mathbf{R}$ such that

$$-\operatorname{div}(A(y)\nabla(\chi_j(x) + y_j)) = 0 \qquad \text{in } Y$$

What happens in the more general case when $a \in \mathbb{C}$?

[Bouchitté-Bourel-Feldbacq, Hoai-Minh Nguyen, Bunoiu-Ramdani,...]

Note that if $\lambda = 1/(1-a)$ is not in the spectrum of $T_0 \; : H^1_\#(y) \to H^1_\#(Y)$

$$\forall\, v \in H^1_\#(Y) \quad \int_Y \nabla T_0 u \cdot \nabla v \quad = \quad \int_\omega \nabla u \cdot \nabla v$$

the homogenized tensor is formally well defined

Prop.

Let $f \in H^{-1}(\Omega)$. Assume that $\lambda = 1/(1-a) \notin \sigma(T_0)$ so that A^* is well defined

- If u_ε is a sequence of solutions to (P_ε) such that $u_\varepsilon \to u$ weakly in H^1, then u is a solution to (P_*)
- If u is a solution to (P_*) (if any), then there exists a sequence $(f_\varepsilon) \subset H^{-1}(\Omega), f_\varepsilon \to f$ such that the solutions $u_\varepsilon \in H_0^1(\Omega)$ to

$$-\mathrm{div}(A_\varepsilon \nabla u_\varepsilon) \quad = \quad f_\varepsilon \quad \text{in } \Omega$$

  satisfy $u_\varepsilon \rightharpoonup u$ weakly in $H^1(\Omega)$

In particular, homogenization cannot discriminate among solutions to the homogenized equation, if they are not unique

We can then relate (partially) the limiting spectrum with the homogenization tensor

Prop.

Let $a \in \mathbb{C} \setminus \sigma(T_0)$ and let A_* denote the associated homogenized matrix

Assume that there exists $f \in H^{-1}(\Omega)$ such that the PDE

$$-\mathrm{div}(A^* \nabla u) \quad = \quad f \qquad \text{in } \Omega$$

does not have a solution in $H_0^1(\Omega)$

Then $\quad 1/(1-a) \in \lim_{\varepsilon \to 0} \sigma(T_\varepsilon)$

The converse is false: the case of rank-one laminates shows that the above system can be well-posed when a is in the limiting spectrum

High contrast ($a \to \pm\infty$ or $a \to 0$)

Recall that we assumed that $\omega \subset\subset Y$

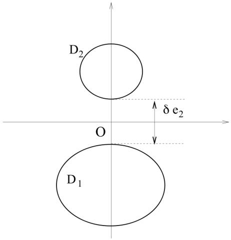
Prop.
There exists $-\infty < c < C < 0$ such that if $\quad -\infty < a < c \quad$ or if $\quad C < a < 0$

- (P_ε) is well posed and its solution u_ε depends continuously on f
- The homogenized tensor A^* is elliptic (uniform bounds wrt a)

  In particular the homogenized problem (P_*) is well-posed.

5. Conclusion/perspectives

- Does the Bloch spectrum really play a role wrt resonance ?
- How to better characterize the boundary spectrum
- What if the inclusions are not smooth ?
- The hypothesis $\omega \subset\subset Y$ plays an important role. Laminates provide counter-examples to some of the properties we derived
- Is it possible to construct hyperbolic media under the hypothesis that $\omega \subset\subset Y$?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