Lecture 1: Gohberg-Sigal theory

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Gohberg-Sigal theory

- Gohberg-Sigal theory: Generalize the argument principle and Rouché's theorem to operator-valued functions.
- Argument principle and Rouché theorem.
- Generalization to matrix-valued functions.
- Generalization to infinite-dimensional spaces.

Gohberg-Sigal theory

- Argument principle:
  - f: holomorphic and has a zero of order n at z_0:

$$f(z) = (z - z_0)^n g(z)$$

g: holomorphic and nowhere vanishing in a neighborhood of z_0. $\Rightarrow$

$$\frac{f'(z)}{f(z)} = \frac{n}{z - z_0} + \frac{g'(z)}{g(z)}.$$

$\Rightarrow$ f'/f has a simple pole with residue n at z_0.

Gohberg-Sigal theory

- Argument principle:
  - f: has a pole of order n at z_0:

    $$f(z) = (z - z_0)^{-n} h(z)$$

    h: holomorphic and nowhere vanishing in a neighborhood of z_0. $\Rightarrow$

    $$\frac{f'(z)}{f(z)} = -\frac{n}{z - z_0} + \frac{h'(z)}{h(z)}.$$

    $\Rightarrow$ f'/f has a simple pole with residue $-n$ at z_0.
- f'/f has simple poles at the zeros and poles of f and the residue is simply the order of the zero of f or the negative of the order of the pole of f.

Gohberg-Sigal theory

- Argument principle: $V \subset \mathbb{C}$: bounded domain with smooth boundary ∂V positively oriented; $f(z)$: meromorphic function in a neighborhood of $\overline{V}$; P and N: the number of poles and zeros of f in V, counted with their orders. If f has no poles and never vanishes on ∂V, then

$$\frac{1}{2\pi i} \int_{\partial V} \frac{f'(z)}{f(z)} \, dz = N - P.$$

- Rouché's theorem [continuity result]: A holomorphic function can be perturbed slightly without changing the number of its zeros.
- Rouché's theorem: $f(z)$ and $g(z)$: holomorphic in a neighborhood of $\overline{V}$. If $|f(z)| > |g(z)|$ for all $z \in \partial V$, then f and $f + g$ have the same number of zeros in V.

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- Generalization to matrix-valued functions:
  - $A(z)$: matrix-valued function holomorphic in a neighborhood of $\overline{V}$ and is invertible in $\overline{V}$ except possibly at $z_0 \in V$.
  - Factorization (by Gauss-Jordan):

$$A(z) = E(z)D(z)F(z) \quad \text{in } V,$$

$E(z), F(z)$: holomorphic and invertible in V and $D(z)$:

$$D(z) = \begin{pmatrix} (z - z_0)^{k_1} & & 0 \\ & \ddots & \\ 0 & & (z - z_0)^{k_n} \end{pmatrix}.$$

$k_1, k_2, \ldots, k_n$: uniquely determined up to a permutation.

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- Generalization to matrix-valued functions:

$$\frac{1}{2\pi i}\,\mathrm{tr}\int_{\partial V} A(z)^{-1}\frac{d}{dz}A(z)\,dz$$
$$= \frac{1}{2\pi i}\,\mathrm{tr}\int_{\partial V}\left(E(z)^{-1}\frac{d}{dz}E(z) + D(z)^{-1}\frac{d}{dz}D(z) + F(z)^{-1}\frac{d}{dz}F(z)\right)\,dz$$
$$= \frac{1}{2\pi i}\,\mathrm{tr}\int_{\partial V} D(z)^{-1}\frac{d}{dz}D(z)\,dz$$
$$= \sum_{j=1}^{n} k_j.$$

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- Generalization to infinite-dimensional spaces:
  - Fredholm operators.
  - Characteristic value and its multiplicities.
  - Factorization of operators.

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- Compact operators:
  - $\mathcal{L}(\mathcal{B}, \mathcal{B}')$: linear bounded operators from $\mathcal{B}$ into $\mathcal{B}'$ (Banach spaces).
  - $K \in \mathcal{L}(\mathcal{B}, \mathcal{B}')$: compact iff K takes any bounded subset of $\mathcal{B}$ to a relatively compact subset of $\mathcal{B}'$ (a set with compact closure).
  - K: of finite rank if $\mathrm{Im}(K)$ (the range of K) is finite-dimensional.
  - Every operator of finite rank is compact.

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- Fredholm alternative:
  - K: compact operator on $\mathcal{B}$. For $\lambda \in \mathbb{C}, \lambda \neq 0$, $(\lambda I - K)$: surjective iff it is injective.
- Fredholm operators:
  - $A \in \mathcal{L}(\mathcal{B}, \mathcal{B}')$: Fredholm if ker A is finite-dimensional and $\mathrm{Im}\, A$ is closed in $\mathcal{B}'$ and of finite codimension $(\dim(\mathcal{B}'/\mathrm{Im}\, A)$.
  - $\mathrm{Fred}(\mathcal{B}, \mathcal{B}')$: collection of all Fredholm operators from $\mathcal{B}$ into $\mathcal{B}'$.
  - $\mathrm{Fred}(\mathcal{B}, \mathcal{B}')$: open in $\mathcal{L}(\mathcal{B}, \mathcal{B}')$.

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- Fredholm operators:
  - Index of $A \in \mathrm{Fred}(\mathcal{B}, \mathcal{B}')$:

$$\mathrm{ind}\, A = \dim \ker A - \mathrm{codim}\, \mathrm{Im}\, A.$$

  - ind: stable under compact perturbations.
  - If $A : \mathcal{B} \to \mathcal{B}'$: Fredholm and $K : \mathcal{B} \to \mathcal{B}'$: compact, then their sum $A + K$: Fredholm, and

$$\mathrm{ind}\,(A + K) = \mathrm{ind}\, A.$$

  - The mapping $A \mapsto \mathrm{ind}\, A$ is continuous in $\mathrm{Fred}(\mathcal{B}, \mathcal{B}')$; *i.e.*, ind: constant on each connected component of $\mathrm{Fred}(\mathcal{B}, \mathcal{B}')$.

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- $\mathfrak{U}(z_0)$: set of all operator-valued functions in $\mathcal{L}(\mathcal{B}, \mathcal{B}')$ which are holomorphic in some neighborhood of z_0, except possibly at z_0.
- z_0 characteristic value of $A(z) \in \mathfrak{U}(z_0)$ if there exists a vector-valued function $\phi(z)$ with values in $\mathcal{B}$ such that
    - $\phi(z)$: holomorphic at z_0 and $\phi(z_0) \neq 0$,
    - $A(z)\phi(z)$: holomorphic at z_0 and vanishes at this point.
    - $\phi(z)$: root function of $A(z)$ associated with the characteristic value z_0.

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- z_0: characteristic value of the function $A(z)$ and $\phi(z)$: an associated root.
- There exists a number $m(\phi) \geq 1$ and a vector-valued function $\psi(z)$ with values in $\mathcal{B}'$, holomorphic at z_0:

$$A(z)\phi(z) = (z - z_0)^{m(\phi)}\psi(z), \quad \psi(z_0) \neq 0.$$

- $m(\phi)$: multiplicity of the root function $\phi(z)$.
- For $\phi_0 \in \mathrm{Ker} A(z_0)$, $\mathrm{rank}(\phi_0)$ (the rank of ϕ_0) $=$ the maximum of the multiplicities of all root functions $\phi(z)$ with $\phi(z_0) = \phi_0$.

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- Suppose that $n = \dim \mathrm{Ker} A(z_0) < +\infty$ and that the ranks of all vectors in $\mathrm{Ker} A(z_0)$ are finite.
- Canonical system of eigenvectors:
  - A system of eigenvectors ϕ_0^j, $j = 1, \ldots, n$,: canonical system of eigenvectors of $A(z)$ associated to z_0 if for $j = 1, \ldots, n$, $\mathrm{rank}(\phi_0^j)$ is the maximum of the ranks of all eigenvectors in the direct complement in $\mathrm{Ker} A(z_0)$ of the linear span of the vectors $\phi_0^1, \ldots, \phi_0^{j-1}$.
- Null multiplicity of the characteristic value z_0 of $A(z)$:

$$N(A(z_0)) := \sum_{j=1}^{n} \mathrm{rank}(\phi_0^j).$$

- If z_0 is not a characteristic value of $A(z)$, we put $N(A(z_0)) = 0$.

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- Suppose that $A^{-1}(z)$ exists and is holomorphic in some neighborhood of z_0, except possibly at z_0.
- Multiplicity of z_0:

$$M(A(z_0)) = N(A(z_0)) - N(A^{-1}(z_0)).$$

- If z_0 is a characteristic value and not a pole of $A(z)$:

$$M(A(z_0)) = N(A(z_0)).$$

- If z_0 is a pole and not a characteristic value of $A(z)$:

$$M(A(z_0)) = -N(A^{-1}(z_0)).$$

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- Finitely meromorphic operator:
  - Suppose that z_0 is a pole of $A(z)$ and the Laurent series expansion of $A(z)$ at z_0:

$$A(z) = \sum_{j \geq -s} (z - z_0)^j A_j .$$

  - If A_{-j}, $j = 1, \ldots, s$, have finite-dimensional ranges, then $A(z)$ is finitely meromorphic at z_0.
- Operator of Fredholm type:
  - $A(z)$: of Fredholm type (of index zero) at the point z_0 if the operator A_0 in the Laurent series is Fredholm (of index zero).

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- Regular point: If $A(z)$ is holomorphic and invertible at z', then z' is a regular point of $A(z)$.
- Normal point: z_0: normal point of $A(z)$ if $A(z)$: finitely meromorphic, of Fredholm type at z_0, and regular in a neighborhood of z_0 except at z_0 itself.

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- Trace operator:
  - A: finite-rank operator acting from $\mathcal{B}$ into itself. Suppose that there exists a finite-dimensional invariant subspace $\mathcal{C}$ of A such that A annihilates some direct complement of $\mathcal{C}$ in $\mathcal{B}$.

$$\mathrm{tr}(A) = \mathrm{tr}(A|_{\mathcal{C}}).$$

  - $\mathrm{tr}\, A$ is independent of the choice of $\mathcal{C}$, so that it is well-defined.
  - tr is linear.
  - If B is a finite-rank operator from $\mathcal{B}$ to itself, then

$$\mathrm{tr}\, AB = \mathrm{tr}\, BA.$$

  - If M is a finite-rank operator from $\mathcal{B} \times \mathcal{B}'$ to itself:

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

  then $\mathrm{tr}\, M = \mathrm{tr}\, A + \mathrm{tr}\, D$.

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- $C(z)$: finitely meromorphic in the neighborhood $\overline{V}$ of z_0, which contains no poles of $C(z)$ except possibly z_0, then $\int_{\partial V} C(z)\, dz$ is a finite-rank operator.
- $A(z)$ and $B(z)$: two operator-valued functions which are finitely meromorphic in the neighborhood $\overline{V}$ of z_0, which contains no poles of $A(z)$ and $B(z)$ other than z_0. Then

$$\mathrm{tr} \int_{\partial V} A(z)B(z)\, dz = \mathrm{tr} \int_{\partial V} B(z)A(z)\, dz.$$

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- Factorization of operators:
  - $A(z) \in \mathfrak{U}(z_0)$ admits a factorization at z_0 if

    $$A(z) = E(z)D(z)F(z),$$

    $E(z), F(z)$: regular at z_0 and

    $$D(z) = P_0 + \sum_{j=1}^{n} (z - z_0)^{k_j} P_j.$$

    P_j's: mutually disjoint projections, $P_1, \ldots, P_n$ are rank-one operators, and $I - \sum_{j=0}^{n} P_j$ is a finite-rank operator.
  - $A(z) \in \mathfrak{U}(z_0)$ admits a factorization at z_0 iff $A(z)$ is finitely meromorphic and of Fredholm type of index zero at z_0.

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- Factorization of operators:
  - $A(z)$ is normal at z_0 iff $A(z)$ admits a factorization such that $I = \sum_{j=0}^{n} P_j$. Moreover,

$$M(A(z_0)) = k_1 + \cdots + k_n.$$

  - Every normal point of $A(z)$ is a normal point of $A^{-1}(z)$.

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- V: a simply connected bounded domain with rectifiable boundary ∂V.
- $A(z)$: finitely meromorphic and of Fredholm type in V and continuous on ∂V.
- $A(z)$ is normal with respect to ∂V if $A(z)$ is invertible in $\overline{V}$, except for a finite number of points of V which are normal points of $A(z)$.
- $A(z)$ is normal with respect to ∂V if it is finitely meromorphic and of Fredholm type in V, continuous on ∂V, and invertible for all $z \in \partial V$.

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- $A(z)$: normal with respect to the contour ∂V and z_i, $i = 1, \ldots, \sigma$, are all its characteristic values and poles lying in V.
- Full multiplicity of $A(z)$ in V:

$$\mathcal{M}(A(z); \partial V) = \sum_{j=1}^{\sigma} M(A(z_j)).$$

- $\mathcal{M}(A(z); \partial V)$= number of characteristic values of $A(z)$ in V, counted with their multiplicities, minus the number of poles of $A(z)$ in V, counted with their multiplicities.
- Generalized argument principle:

$$\mathcal{M}(A(z); \partial V) = \frac{1}{2\pi i} \mathrm{tr} \int_{\partial V} A^{-1}(z) \frac{d}{dz} A(z) dz.$$

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- General form of the argument principle:
  - $A(z)$: normal with respect to ∂V.
  - $f(z)$: a scalar function which is analytic in V and continuous in $\overline{V}$.
  - z_j, $j = 1, \ldots, \sigma$, all the points in V which are either poles or characteristic values of $A(z)$:

$$\frac{1}{2\pi i} \operatorname{tr} \int_{\partial V} f(z) A^{-1}(z) \frac{d}{dz} A(z) dz = \sum_{j=1}^{\sigma} M(A(z_j)) f(z_j).$$

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- Generalized Rouché's theorem:
  - $A(z)$: normal with respect to ∂V.
  - $S(z)$: finitely meromorphic in V and continuous on ∂V s.t.

$$\|A^{-1}(z)S(z)\|_{\mathcal{L}(\mathcal{B},\mathcal{B})} < 1, \quad z \in \partial V.$$

  - $\Rightarrow A(z) + S(z)$: also normal with respect to ∂V and

$$\mathcal{M}(A(z); \partial V) = \mathcal{M}(A(z) + S(z); \partial V).$$

Gohberg-Sigal theory

- Steinberg's theorem:
  - $K(z)$: compact operator on a Banach space, which is analytic in V.
  - $(I + K(z))^{-1}$: meromorphic in V.
- Generalized Steinberg's theorem:
  - $A(z)$: finitely meromorphic and of Fredholm type in the domain V.
  - If $A(z)$ is invertible at one point of V, then $A(z)$ has a bounded inverse for all $z \in V$, except possibly for certain isolated points.

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- Muller's method:
  - Compute the characteristic values of $A(z)$. item Discretization of $A(z)$.
  - Compute the zeros of functions on $\mathbb{C}$:

$$f : z \mapsto \frac{1}{(A^{-1}(z)\phi, \psi)}$$

  - ϕ and ψ: fixed random vectors.
  - Determine roots (simple or multiple) of a polynomial.

Lecture 2: Cavities and resonators

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Cavities and resonators

- Cavity: D bounded domain of class $\mathcal{C}^{1,\eta}, \eta > 0$
  - Helmholtz equation in D:

$$\Delta u + \omega^2 u = 0.$$

  - Dirichlet boundary conditions: $u = 0$ on ∂D;
  - Neumann boundary conditions: $\partial u / \partial \nu = 0$ on ∂D;
  - Robin boundary conditions: $\partial u / \partial \nu + \lambda u = 0$ on ∂D.
- Resonator:
  - Helmholtz equation in $\mathbb{R}^d$:

$$\begin{cases} \Delta u + \omega^2 n(x) u = 0 \quad \text{in } \mathbb{R}^d, \\ \left| \dfrac{\partial u}{\partial |x|} - i\omega u \right| = O\left(|x|^{-(d+1)/2} \right), \quad |x| \to +\infty, \text{ uniformly in } \dfrac{x}{|x|}; \end{cases}$$

  - $\text{supp}(n(x) - 1) = D$

Cavities and resonators

- Outgoing fundamental solution $\Gamma_\omega(x)$ to the Helmholtz operator $\Delta + \omega^2$ in $\mathbb{R}^d$, $d = 2, 3$: $(\Delta_x + \omega^2)\Gamma_\omega(x) = \delta_0(x)$

$$\Gamma_\omega(x) = \begin{cases} -\dfrac{i}{4} H_0^{(1)}(\omega|x|)\ , & d = 2, \\ -\dfrac{e^{i\omega|x|}}{4\pi|x|}\ , & d = 3, \end{cases}$$

- $H_0^{(1)}$: Hankel function of the first kind of order 0.
- Behavior of $H_0^{(1)}$ near 0:

$$-\frac{i}{4} H_0^{(1)}(\omega|x|) \sim \frac{1}{2\pi} \ln|x| \quad \big[\Delta_x(\frac{1}{2\pi} \ln|x|) = \delta_0(x)\big].$$

- Sommerfeld radiation condition:

$$\left| \frac{x}{|x|} \cdot \nabla\Gamma_\omega(x) - i\omega\Gamma_\omega(x) \right| = \begin{cases} O(|x|^{-3/2}), & d = 2, \\ O(|x|^{-2}), & d = 3. \end{cases}$$

Cavities and resonators

- Single- and double-layer potentials: For $\varphi \in L^2(\partial D)$,

$$\mathcal{S}_D^\omega[\varphi](x) = \int_{\partial D} \Gamma_\omega(x-y)\varphi(y)\, d\sigma(y), \quad x \in \mathbb{R}^d,$$
$$\mathcal{D}_D^\omega[\varphi](x) = \int_{\partial D} \frac{\partial \Gamma_\omega(x-y)}{\partial \nu(y)} \varphi(y)\, d\sigma(y)\,, \quad x \in \mathbb{R}^d \setminus \partial D,$$

- $\Gamma_\omega(x)$ outgoing fundamental solution to the Helmholtz operator $\Rightarrow$
  - $\mathcal{S}_D^\omega[\varphi]$ and $\mathcal{D}_D^\omega[\varphi]$ satisfy the Helmholtz equation

$$(\Delta + \omega^2)u = 0 \quad \text{in } D \text{ and in } \mathbb{R}^d \setminus \overline{D}.$$

  - $\mathcal{S}_D^\omega[\varphi]$ and $\mathcal{D}_D^\omega[\varphi]$ satisfy the Sommerfeld radiation condition.

Cavities and resonators

- Jump relations: For $\varphi \in L^2(\partial D)$,

$$\frac{\partial(\mathcal{S}_D^\omega[\varphi])}{\partial \nu}\bigg|_{\pm}(x) = \left(\pm \frac{1}{2} I + (\mathcal{K}_D^\omega)^*\right)[\varphi](x) \quad \text{a.e. } x \in \partial D,$$

$$(\mathcal{D}_D^\omega[\varphi])\bigg|_{\pm}(x) = \left(\mp \frac{1}{2} I + \mathcal{K}_D^\omega\right)[\varphi](x) \quad \text{a.e. } x \in \partial D,$$

- $\mathcal{K}_D^\omega$ and $(\mathcal{K}_D^\omega)^*$:

$$\mathcal{K}_D^\omega[\varphi](x) = \int_{\partial D} \frac{\partial \Gamma_\omega(x-y)}{\partial \nu(y)} \varphi(y)\, d\sigma(y);$$

$$(\mathcal{K}_D^\omega)^*[\varphi](x) = \int_{\partial D} \frac{\partial \Gamma_\omega(x-y)}{\partial \nu(x)} \varphi(y)\, d\sigma(y).$$

- $(\mathcal{K}_D^\omega)^*$: L^2-adjoint of $\mathcal{K}_D^{-\omega}$ (complex inner product).
- $\mathcal{K}_D^\omega$ and $(\mathcal{K}_D^\omega)^*$: compact on $L^2(\partial D)$.

Cavities and resonators

- Three-dimensional case ($d = 3$): Holomorphic dependence of $\Gamma_\omega \Rightarrow \mathcal{K}_D^\omega$: operator-valued holomorphic function in $\mathbb{C}$.
- Two-dimensional case ($d = 2$): Holomorphic dependence of Γ_ω on $\mathbb{C} \setminus i\mathbb{R}^- \Rightarrow \mathcal{K}_D^\omega$: operator-valued holomorphic function on $\mathbb{C} \setminus i\mathbb{R}^-$.
- Neumann Eigenvalue characterization: Suppose that D is of class $\mathcal{C}^{1,\eta}$ for some $\eta > 0$. Let $\omega > 0$. Then ω^2: eigenvalue of $-\Delta$ on D with Neumann boundary condition iff ω: positive real characteristic value of $-(1/2)\, I + \mathcal{K}_D^\omega$.

Cavities and resonators

- Suppose ω^2: eigenvalue of

$$\begin{cases} \Delta u + \omega^2 u = 0 & \text{in } D, \\ \dfrac{\partial u}{\partial \nu} = 0 & \text{on } \partial D. \end{cases}$$

- Green's formula (multiply by Green's function and integrate by parts over D):

$$u(x) = \mathcal{D}_D^\omega[u|_{\partial D}](x), \quad x \in D.$$

- Jump formula: $(-I/2 + \mathcal{K}_D^\omega)[u|_{\partial D}] = 0$ and $u|_{\partial D} \neq 0$ since otherwise the unique continuation property for $\Delta + \omega^2$ would imply that $u \equiv 0$ in D.
- ω: characteristic value of $-(1/2)\, I + \mathcal{K}_D^\omega$.

Cavities and resonators

- ω: characteristic value of $-(1/2)\, I + \mathcal{K}_D^\omega$;
- There is a nonzero $\psi \in L^2(\partial D)$ s.t.

$$\left(-\frac{1}{2} I + \mathcal{K}_D^\omega\right)[\psi] = 0.$$

- $u = \mathcal{D}_D^\omega[\psi]$ on $\mathbb{R}^d \setminus \overline{D}$ is a solution to the Helmholtz equation with the boundary condition $u|_+ = 0$ on ∂D and satisfies the radiation condition.
- Uniqueness result (exterior Helmholtz equation + radiation condition + Dirichlet boundary condition) $\Rightarrow \mathcal{D}_D^\omega[\psi] = 0$ in $\mathbb{R}^d \setminus \overline{D}$.
- $\partial \mathcal{D}_D^\omega[\psi]/\partial \nu$ exists and has no jump across $\partial D \Rightarrow$

$$\frac{\partial \mathcal{D}_D^\omega[\psi]}{\partial \nu}\Big|_+ = \frac{\partial \mathcal{D}_D^\omega[\psi]}{\partial \nu}\Big|_- \quad \text{on } \partial D.$$

- $\mathcal{D}_D^\omega[\psi]$: a solution of the Helmholtz equation with Neumann boundary condition; $\mathcal{D}_D^\omega[\psi] \neq 0$ in D, since otherwise

$$\psi = \mathcal{D}_D^\omega[\psi]\big|_- - \mathcal{D}_D^\omega[\psi]\big|_+ = 0.$$

- ω^2: an eigenvalue of $-\Delta$ on D with Neumann condition.

Cavities and resonators

- Steinberg's theorem:
  - For $d = 3$: $-(1/2)\, I + \mathcal{K}_D^\omega$: invertible on $L^2(\partial D)$ for all $\omega \in \mathbb{C}$ except for a discrete set;
  - For $d = 3$: $(-(1/2)\, I + \mathcal{K}_D^\omega)^{-1}$: meromorphic function on $\mathbb{C}$.
  - For $d = 2$: $(-(1/2)\, I + \mathcal{K}_D^\omega)^{-1}$ has a continuation to an operator-valued meromorphic function on only $\mathbb{C} \setminus i\mathbb{R}^-$.

Cavities and resonators

- Eigenvalues of $-\Delta$ on D with Dirichlet boundary condition:
  - D of class $\mathcal{C}^{1,\eta}$ for some $\eta > 0$.
  - ω^2 ($\omega > 0$): eigenvalue of $-\Delta$ on D with Dirichlet boundary condition iff ω is a positive real characteristic value of $(1/2)\, I + (\mathcal{K}_D^\omega)^*$.
- Eigenvalues of $-\Delta$ on D with the Robin boundary condition:

$$\frac{\partial u}{\partial \nu} + \lambda u = 0 \quad \text{on } \partial D, \quad \lambda > 0.$$

  - D of class $\mathcal{C}^{1,\eta}$ for some $\eta > 0$.
  - ω^2 ($\omega > 0$): eigenvalue of $-\Delta$ on D with the Robin boundary condition iff if ω is a positive real characteristic value of $-(1/2)\, I + \mathcal{K}_D^\omega - \lambda \mathcal{S}_D^\omega$.

Cavities and resonators

- Zaremba eigenvalues of mixed boundary value problems:
  - D of class $\mathcal{C}^{1,\eta}$ for some $\eta > 0$.
  - Γ_D: subset of ∂D and let $\Gamma_N = \partial D \setminus \overline{\Gamma_D}$.
  - ω^2 $(\omega > 0)$: eigenvalue of $-\Delta$ on D with the mixed boundary conditions:

$$\begin{cases} \Delta u + \omega^2 u = 0 & \text{in } D, \\ u = 0 & \text{on } \Gamma_D, \\ \dfrac{\partial u}{\partial \nu} = 0 & \text{on } \Gamma_N, \end{cases}$$

iff ω is a positive real characteristic value of

$$\omega \mapsto \begin{bmatrix} (1/2)\, I + (\mathcal{K}^{\omega}_{\Gamma_D})^* & \frac{\partial}{\partial \nu} \mathcal{D}^{\omega}_{\Gamma_N}\Big|_{\Gamma_D} \\ -\mathcal{S}^{\omega}_{\Gamma_D}\Big|_{\Gamma_N} & -(1/2)\, I + \mathcal{K}^{\omega}_{\Gamma_N} \end{bmatrix}.$$

Cavities and resonators

- Neumann Function:
  - $0 = \mu_1 < \mu_2 \leq \mu_3 \leq \ldots$: the eigenvalues of $-\Delta$ on D with Neumann conditions on ∂D.
  - u_j: the normalized eigenfunction associated with μ_j ($\|u_j\|_{L^2(D)} = 1$).
  - $\omega \notin \{\sqrt{\mu_j}\}_{j\geq 1}$.
  - Neumann function N_D^ω for $\Delta + \omega^2$ in D corresponding to a Dirac mass at z:

$$\begin{cases} (\Delta_x + \omega^2) N_D^\omega(x, z) = -\delta_z & \text{in } D, \\ \left.\dfrac{\partial N_D^\omega}{\partial \nu}\right|_{\partial D} = 0 & \text{on } \partial D. \end{cases}$$

Cavities and resonators

- Pointwise spectral decomposition:

$$N_D^\omega(x,z) = \sum_{j=1}^{+\infty} \frac{u_j(x)u_j(z)}{\mu_j - \omega^2}, \quad x \neq z \in D.$$

  - Consider the function

$$f(x) := \sum_{j=1}^{+\infty} a_j u_j(x), \quad x \in D.$$

  - If $(\Delta_x + \omega^2) f(x) = -\delta_z(x)$, then

$$\sum_{j=1}^{+\infty} a_j(\omega^2 - \mu_j) u_j(x) = -\delta_z(x).$$

  - Integrate against u_k over D and use $\int_D u_j\, u_k = \delta_{jk}$:

$$a_k(\omega^2 - \mu_k) = -u_k(z).$$

Cavities and resonators

- Singularity of the Neumann function N_D^ω:
  - In two dimensions:

$$N_D^\omega(x,z) = -\frac{1}{2\pi} \ln |x-z| + R_D^\omega(x,z) \quad \text{for } x \neq z \in D;$$

  - In dimension $d \geq 3$:

$$N_D^\omega(x,z) = \frac{1}{(d-2)\omega_d} |x-z|^{2-d} + R_D^{\omega,d}(x,z) \quad \text{for } x \neq z \in D;$$

  - $R_D^\omega(\cdot,z) \in H^{3/2}(D)$ for any $z \in D$.

Cavities and resonators

- Dirichlet function:
  - $0 < \tau_1 < \tau_2 \leq \tau_3 \leq \ldots$: eigenvalues of $-\Delta$ on D with Dirichlet conditions on ∂D.
  - v_j: the normalized eigenfunction associated with τ_j.
  - Dirichlet function $G_D^\omega(x,z)$:

$$\begin{cases} (\Delta_x + \omega^2) G_D^\omega(x,z) = -\delta_z & \text{in } D, \\ G_D^\omega = 0 & \text{on } \partial D. \end{cases}$$

Cavities and resonators

- Pointwise spectral decomposition:

$$G_D^\omega(x,z) = \sum_{j=1}^{+\infty} \frac{v_j(x) v_j(z)}{\tau_j - \omega^2}, \quad x \neq z \in D.$$

- Singularity of G_D^ω:
    - $d = 2$,

$$G_D^\omega(x,z) = -\frac{1}{2\pi} \ln |x - z| + \widetilde{R}_D^{\omega,d}(x,z) \quad \text{for } x \neq z \in D;$$

    - $d \geq 3$

$$G_D^\omega(x,z) = \frac{1}{(d-2)\omega_d} |x - z|^{2-d} + \widetilde{R}_D^{\omega,d}(x,z) \quad \text{for } x \neq z \in D;$$

    - $\widetilde{R}_D^{\omega,d}(\cdot, z) \in H^{3/2}(D)$ for any $z \in D$.

Cavities and resonators

- Eigenvalues in circular domains:
  - κ_{nm}: positive zeros of $J_n(z)$ (Dirichlet), $J_n'(z)$ (Neumann), and $J_n'(z) + \lambda J_n(z)$ (Robin).
  - Index $n = 0, 1, 2, \ldots$ counts the order of Bessel functions of first kind J_n while $m = 1, 2, \ldots$ counts their positive zeros.
  - Rotational symmetry of $D = \{x : |x| < R\} \Rightarrow$ explicit representation of the eigenfunctions in polar coordinates:

$$u_{nml}(r, \theta) = J_n(\frac{\kappa_{nm} r}{R}) \times \begin{cases} \cos(n\theta), & l = 1, \\ \sin(n\theta), & l = 2 \quad (n \neq 0). \end{cases}$$

  - Eigenvalues of $-\Delta$ on D: κ_{nm}^2 / R^2.

Cavities and resonators

- Independent of l; Simple for $n = 0$ and twice degenerate for $n > 0$ (eigenfunction is any nontrivial linear combination of u_{nm1} and u_{nm2}).
- When the index n is fixed while m increases, the Bessel functions $J_n(\frac{\kappa_{nm} r}{R})$ rapidly oscillate, the amplitude of oscillations decreasing toward the boundary and the eigenfunctions u_{nml} are mainly localized at the origin, yielding focusing modes.
- When the index m is fixed while n increases, the Bessel functions $J_n(\frac{\kappa_{nm} r}{R})$ become strongly attenuated near the origin and essentially localized near the boundary: whispering gallery eigenmodes.

Cavities and resonators

- Shape derivative of the cavity modes:
    - D: bounded domain of class $\mathcal{C}^2$;
    - D_ε: ϵ-perturbation of D:

$$\partial D_\varepsilon = \left\{ \tilde{x} : \tilde{x} = x + \varepsilon h(x)\nu(x),\ x \in \partial D \right\}.$$

    - $h \in \mathcal{C}^2(\partial D)$.
- Asymptotic expansions of $\mathcal{S}_{D_\varepsilon}^{\omega}$ and $(\mathcal{K}_{D_\varepsilon}^{\omega})^*$ as $\varepsilon \to 0$.

Cavities and resonators

- $a, b \in \mathbb{R}$, $a < b$, $X(t) : [a, b] \to \mathbb{R}^2$ arclength parametrization of ∂D: X is a $\mathcal{C}^2$-function satisfying $|X'(t)| = 1$ for all $t \in [a, b]$ and

$$\partial D := \left\{ x = X(t), \ t \in [a, b] \right\}.$$

- Outward unit normal to ∂D:

$$\nu(x) = R_{-\pi/2} X'(t),$$

$R_{-\pi/2}$: rotation by $-\pi/2$, the tangential vector at x, $T(x) = X'(t)$, and $X'(t) \perp X''(t)$.

- Curvature $\tau(x)$:

$$X''(t) = \tau(x)\nu(x).$$

- Parametrization of ∂D_ε:

$$\tilde{X}(t) = X(t) + \epsilon h(t)\nu(x) = X(t) + \epsilon h(t) R_{-\pi/2} X'(t).$$

Cavities and resonators

- Outward unit normal to ∂D_ε at $\tilde{x}$, $\tilde{\nu}(\tilde{x})$,

$$\begin{aligned}\tilde{\nu}(\tilde{x}) &= \frac{R_{-\pi/2}\tilde{X}'(t)}{|\tilde{X}'(t)|}\\ &= \frac{\Big(1-\epsilon h(t)\tau(x)\Big)\nu(x)-\epsilon h'(t)X'(t)}{\sqrt{\epsilon^2 h'(t)^2+\Big(1-\epsilon h(t)\tau(x)\Big)^2}}\\ &= \frac{\Big(1-\epsilon h(t)\tau(x)\Big)\nu(x)-\epsilon h'(t)T(x)}{\sqrt{\epsilon^2 h'(t)^2+\Big(1-\epsilon h(t)\tau(x)\Big)^2}}.\end{aligned}$$

- Uniform expansion of $\tilde{\nu}(\tilde{x})$:

$$\tilde{\nu}(\tilde{x}) = \sum_{n=0}^{+\infty} \varepsilon^n \nu^{(n)}(x), \quad x \in \partial D,$$

$\nu^{(n)}$: bounded; The first two terms:

$$\nu^{(0)}(x) = \nu(x), \quad \nu^{(1)}(x) = -h'(t)T(x).$$

Cavities and resonators

- Uniformly convergent expansion for the length element $d\sigma_\epsilon(\tilde{y})$:

$$
\begin{aligned}
d\sigma_\epsilon(\tilde{y}) &= |\tilde{X}'(s)| ds \\
&= \sqrt{(1-\varepsilon\tau(s)h(s))^2 + \varepsilon^2 h'^2(s)} ds \\
&= \sum_{n=0}^{+\infty} \epsilon^n \sigma^{(n)}(y)\, d\sigma(y).
\end{aligned}
$$

- $\sigma^{(n)}$: bounded functions and

$$
\sigma^{(0)}(y) = 1, \quad \sigma^{(1)}(y) = -\tau(y)h(y).
$$

Cavities and resonators

- Expansion of the kernel $H_0^{(1)}(\omega|\tilde{x}-\tilde{y}|)$:

$$H_0^{(1)}(\omega|\tilde{x}-\tilde{y}|) = \sum_{n=0}^{+\infty} \varepsilon^n H_n^\omega(x,y);$$

- Series converges absolutely and uniformly;
- First two terms:

$$H_0^\omega(x,y) = H_0^{(1)}(\omega|x-y|)$$

and

$$H_1^\omega(x,y) = \omega (H_0^{(1)})'(\omega|x-y|) \frac{\langle x-y, h(t)\nu(x) - h(s)\nu(y)\rangle}{|x-y|}.$$

- $x = X(t), y = X(s), \tilde{x} = \tilde{X}(t), \tilde{y} = \tilde{X}(s)$.

Cavities and resonators

- Ψ_ε: diffeomorphism from ∂D onto ∂D_ϵ

$$\Psi_\varepsilon(x) = x + \varepsilon h(t)\nu(x), \quad x = X(t).$$

- Asymptotic expansion of $\mathcal{K}_{D_\varepsilon}^\omega$ with respect to ε:

$$\mathcal{K}_{D_\varepsilon}^\omega[\cdot] \circ \Psi_\epsilon = \mathcal{K}_D^\omega[\cdot] + \varepsilon \mathcal{K}_{D,\omega}^{(1)}[\cdot] + \varepsilon^2 \mathcal{K}_{D,\omega}^{(2)}[\cdot] + \ldots;$$

- Each operator $\mathcal{K}_{D,\omega}^{(n)}$: bounded on $L^2(\partial D)$.

Cavities and resonators

- μ_j^ε eigenvalue of $-\Delta$ in D_ε with Neumann boundary conditions.
- $\mathcal{A}_\varepsilon(\omega) = -\frac{1}{2} I + \mathcal{K}_{D_\varepsilon}^\omega$;
- $\mathcal{A}_\varepsilon(\omega)$: Fredholm analytic with index 0 in $\mathbb{C} \setminus i\mathbb{R}^-$;
- $(\mathcal{A}_\varepsilon)^{-1}(\omega)$: meromorphic function.
- If ω: real characteristic value of $\mathcal{A}_\varepsilon$ (a real pole of $(\mathcal{A}_\varepsilon)^{-1}(\omega)$), then there exists j such that $\omega = \sqrt{\mu_j^\varepsilon}$.

Cavities and resonators

- Any $\sqrt{\mu_j}$ is a simple pole of $(\mathcal{A}_0)^{-1}(\omega)$.
- Let $\omega_0 = \sqrt{\mu_j}$ and suppose that μ_j is simple. Then there exists a positive constant δ_0 such that for $|\delta| < \delta_0$, $\omega \mapsto \mathcal{A}_\varepsilon(\omega)$ has exactly one characteristic value in $\overline{V_{\delta_0}}(\omega_0)$, where $V_{\delta_0}(\omega_0)$ is a disk of center ω_0 and radius $\delta_0 > 0$. This characteristic value is analytic with respect to ε in $]-\varepsilon_0, \varepsilon_0[$.
- $\mathcal{M}(\mathcal{A}_\varepsilon(\omega); \partial V_{\delta_0}) = 1$,
- $(\mathcal{A}_\varepsilon)^{-1}(\omega) = (\omega - \omega_\varepsilon)^{-1}\mathcal{L}_\varepsilon + \mathcal{R}_\varepsilon(\omega)$,
- $\mathcal{L}_\varepsilon : Ker((\mathcal{A}_\varepsilon(\omega_\varepsilon))^*) \to Ker(\mathcal{A}_\varepsilon(\omega_\varepsilon))$,
- $\mathcal{R}_\varepsilon(\omega)$: holomorphic function with respect to $(\varepsilon, \omega) \in]-\varepsilon_0, \varepsilon_0[\times V_{\delta_0}(\omega_0)$
- $\mathcal{L}_\varepsilon$: finite-dimensional operator.

Cavities and resonators

- Application of the generalized argument principle:
  - Let $\omega_0 = \sqrt{\mu_j}$ and suppose that μ_j is simple.
  - $\omega_\varepsilon = \sqrt{\mu_j^\varepsilon}$:

$$\omega_\varepsilon - \omega_0 = \frac{1}{2\pi i} \operatorname{tr} \int_{\partial V_{\delta_0}} (\omega - \omega_0) \mathcal{A}_\varepsilon(\omega)^{-1} \frac{d}{d\omega} \mathcal{A}_\varepsilon(\omega) d\omega.$$

- Asymptotic expansion of $\mathcal{A}_\varepsilon$:

$$\mathcal{A}_\varepsilon(\omega) = \mathcal{A}_0(\omega) + \varepsilon \mathcal{A}_1(\omega) + \ldots;$$

- Leading-order term in the asymptotic expansion of $\omega_\varepsilon - \omega_0$:

$$-\frac{1}{2i\pi} \operatorname{tr} \int_{\partial V_{\delta_0}} \mathcal{A}_0(\omega)^{-1} \mathcal{A}_1(\omega) \omega d\omega.$$

Cavities and resonators

- Neumann series converges uniformly with respect to ω in ∂V_{δ_0}:

$$\mathcal{A}_\varepsilon(\omega)^{-1} = \sum_{p=0}^{+\infty} \left[\mathcal{A}_0(\omega)^{-1}(\mathcal{A}_0(\omega) - \mathcal{A}_\varepsilon(\omega))\right]^p \mathcal{A}_0(\omega)^{-1},$$

- $\omega_\varepsilon - \omega_0 =$

$$\frac{1}{2\pi i}\sum_{p=0}^{+\infty} \mathrm{tr} \int_{\partial V_{\delta_0}} (\omega - \omega_0) \left[\mathcal{A}_0(\omega)^{-1}(\mathcal{A}_0(\omega) - \mathcal{A}_\varepsilon(\omega))\right]^p \mathcal{A}_0(\omega)^{-1} \frac{d}{d\omega}\mathcal{A}_\varepsilon(\omega) d\omega.$$

- Trace property: $A(z)$ and $B(z)$ finitely meromorphic in $\overline{V}$

$$\mathrm{tr} \int_{\partial V} A(z)B(z)\, dz = \mathrm{tr} \int_{\partial V} B(z)A(z)\, dz;$$

- Differentiation:

$$\frac{d}{d\omega}\mathcal{A}_0(\omega)^{-1} = -\mathcal{A}_0(\omega)^{-1}\frac{d\mathcal{A}_0}{d\omega}(\omega)\mathcal{A}_0(\omega)^{-1}.$$

Cavities and resonators

- $\Rightarrow$

$$\mathrm{tr}\int_{\partial V_{\delta_0}}(\omega-\omega_0)\frac{1}{p}\frac{d}{d\omega}\left[\mathcal{A}_0(\omega)^{-1}(\mathcal{A}_0(\omega)-\mathcal{A}_\varepsilon(\omega))\right]^p d\omega$$

$$=\mathrm{tr}\Bigg[\int_{\partial V_{\delta_0}}(\omega-\omega_0)\left[\mathcal{A}_0(\omega)^{-1}(\mathcal{A}_0(\omega)-\mathcal{A}_\varepsilon(\omega))\right]^{p-1}\mathcal{A}_0(\omega)^{-1}$$

$$\times\frac{d}{d\omega}(\mathcal{A}_0(\omega)-\mathcal{A}_\varepsilon(\omega))d\omega$$

$$-\int_{\partial V_{\delta_0}}(\omega-\omega_0)\left[\mathcal{A}_0(\omega)^{-1}(\mathcal{A}_0(\omega)-\mathcal{A}_\varepsilon(\omega))\right]^p\mathcal{A}_0(\omega)^{-1}\frac{d}{d\omega}\mathcal{A}_0(\omega)d\omega\Bigg].$$

- $\Rightarrow \omega_\varepsilon-\omega_0=$

$$-\frac{1}{2i\pi}\sum_{p=1}^{+\infty}\mathrm{tr}\int_{\partial V_{\delta_0}}(\omega-\omega_0)\frac{1}{p}\frac{d}{d\omega}\left[\mathcal{A}_0(\omega)^{-1}(\mathcal{A}_0(\omega)-\mathcal{A}_\varepsilon(\omega))\right]^p d\omega$$

$$+\frac{1}{2\pi i}\mathrm{tr}\int_{\partial V_{\delta_0}}(\omega-\omega_0)\mathcal{A}_0(\omega)^{-1}\frac{d}{d\omega}\mathcal{A}_0(\omega)d\omega.$$

Cavities and resonators

- ω_0: simple pole of $\mathcal{A}_0(\omega)^{-1}$ and $\mathcal{A}_0(\omega)$ is analytic $\Rightarrow$

$$\int_{\partial V_{\delta_0}} (\omega - \omega_0)\mathcal{A}_0(\omega)^{-1} \frac{d}{d\omega}\mathcal{A}_0(\omega) d\omega = 0.$$

- $\Rightarrow \omega_\varepsilon - \omega_0 =$

$$-\frac{1}{2\pi i}\sum_{p=1}^{+\infty} \mathrm{tr} \int_{\partial V_{\delta_0}} (\omega - \omega_0)\frac{1}{p}\frac{d}{d\omega}\left[\mathcal{A}_0^{-1}(\omega)(\mathcal{A}_0(\omega) - \mathcal{A}_\varepsilon(\omega))\right]^p d\omega.$$

- Integration by parts:

$$\omega_\varepsilon - \omega_0 = \frac{1}{2\pi i}\sum_{p=1}^{+\infty}\frac{1}{p}\,\mathrm{tr}\int_{\partial V_{\delta_0}} \left[\mathcal{A}_0(\omega)^{-1}(\mathcal{A}_0(\omega) - \mathcal{A}_\varepsilon(\omega))\right]^p d\omega.$$

Cavities and resonators

- $$\Big(\mathcal{A}_0(\omega)^{-1}(\mathcal{A}_0(\omega) - \mathcal{A}_\varepsilon(\omega))\Big)^p$$
$$= (-1)^p \sum_{n=p}^{+\infty} \varepsilon^n \sum_{\substack{n_1+\ldots+n_p=n \\ n_i \geq 1}} \mathcal{A}_0(\omega)^{-1}\mathcal{A}_{n_1}(\omega)\ldots\mathcal{A}_0(\omega)^{-1}\mathcal{A}_{n_p}(\omega)\omega^n.$$
- $$\mathcal{A}_\varepsilon(\omega) = \sum_{n=0}^{+\infty} \varepsilon^n \mathcal{A}_n(\omega).$$
- $\Rightarrow$ Leading-order term in the asymptotic expansion of $\omega_\varepsilon - \omega_0$:
$$-\frac{1}{2i\pi} \operatorname{tr} \int_{\partial V_{\delta_0}} \mathcal{A}_0(\omega)^{-1}\mathcal{A}_1(\omega)\omega d\omega.$$

Cavities and resonators

- Splitting of multiple eigenvalues:
  - Multiple eigenvalues may evolve, under perturbations, as separated, distinct eigenvalues, and the splitting may only become apparent at high orders in their Taylor expansions with respect to the perturbation parameter.
  - Splitting problem in the evaluation of the perturbations of the Neumann eigenvalues due to shape deformations.
  - Splitting problem: generalized argument principle.

Cavities and resonators

- Let $\omega_0 = \sqrt{\mu_j}$ and suppose that μ_j is a multiple Neumann eigenvalue of $-\Delta$ on D with geometric multiplicity m.
- There exists a positive constant δ_0 such that for $|\delta| < \delta_0$, $\omega \mapsto \mathcal{A}_\varepsilon(\omega)$ has exactly m characteristic values (counted according to their multiplicity) in $\overline{V_{\delta_0}}(\omega_0)$.
- $\mathcal{M}(\mathcal{A}_\varepsilon(\omega); \partial V_{\delta_0}) = \sum_{i=1}^{n} \mathcal{M}(\mathcal{A}_\varepsilon(\omega_\varepsilon^i); \partial V_{\delta_0}) = m,$
- $(\mathcal{A}_\varepsilon)^{-1}(\omega) = \sum_{i=1}^{n} (\omega - \omega_\varepsilon^i)^{-1} \mathcal{L}_\varepsilon^i + \mathcal{R}_\varepsilon(\omega);$
- $\mathcal{L}_\varepsilon^i : Ker((\mathcal{A}_\varepsilon(\omega_\varepsilon^i))^*) \to Ker(\mathcal{A}_\varepsilon(\omega_\varepsilon^i)),$
- $\mathcal{R}_\varepsilon(\omega)$: holomorphic function with respect to $\omega \in V_{\delta_0}(\omega_0)$;
- $\mathcal{L}_\varepsilon^i$ for $i = 1, \ldots, n$: finite-dimensional operator.

Cavities and resonators

- For $l \in \mathbb{N}$,

$$a_l(\varepsilon) = \frac{1}{2\pi i}\ \mathrm{tr} \int_{\partial V_{\delta_0}} (\omega - \omega_0)^l \mathcal{A}_\varepsilon(\omega)^{-1} \frac{d}{d\omega} \mathcal{A}_\varepsilon(\omega) d\omega.$$

- By the generalized argument principle:

$$a_l(\varepsilon) = \sum_{i=1}^{m} (\omega_\varepsilon^i - \omega_0)^l \quad \text{for } l \in \mathbb{N}.$$

- Asymptotic expansion as $\varepsilon \to 0$:

$$a_l(\varepsilon) = \frac{\varepsilon}{2i\pi}\ \mathrm{tr} \int_{\partial V_{\delta_0}} l(\omega - \omega_0)^{l-1} \mathcal{A}_0(\omega)^{-1} \mathcal{K}_D^{(1)}(\omega) d\omega + O(\varepsilon^2).$$

Cavities and resonators

- There exists a polynomial-valued function $\omega \mapsto Q_\varepsilon(\omega)$ of degree m and of the form

$$Q_\varepsilon(\omega) = \omega^m + c_1(\varepsilon)\omega^{m-1} + \ldots + c_i(\varepsilon)\omega^{m-i} + \ldots + c_m(\varepsilon)$$

  s.t. the perturbations $\omega_\varepsilon^i - \omega_0$ are precisely its zeros. The polynomial coefficients $(c_i)_{i=1}^m$ are given by the recurrence relation

$$a_{l+m} + c_1 a_{l+m-1} + \ldots + c_m a_l = 0 \quad \text{for } l = 0, 1, \ldots, m-1.$$

- Find a polynomial of degree m s.t. its zeros are precisely the perturbations $\omega_\varepsilon^i - \omega_0$.
- Computing the Taylor series of the polynomial coefficients $\Rightarrow$ complete asymptotic expansions of the perturbations in the eigenvalues.
- $m \in \{2, 3, 4\}$: explicitly have the expressions of the perturbed eigenvalues as functions of $(a_l)_{l=1}^m$.

Cavities and resonators

- Integral formulation of resonances:
- u: solution of

$$\begin{cases} \Delta u + \omega^2 n(x) u = 0, \\ u \ \text{satisfies the Sommerfeld radiation condition.} \end{cases}$$

- $n-1$: compactly supported in a bounded domain D.
- Integral representation formula:

$$u(x) + \omega^2 \int_D (n(y)-1)\Gamma_\omega(x-y)u(y)dy = 0, \quad x \in D.$$

- $\omega \in \mathbb{C}$: resonance if there is nontrivial solutions $u(x)$.

Cavities and resonators

- $\mathcal{A}_0(\omega)$:

$$\mathcal{A}_0(\omega)[u] = u(x) + \omega^2 \int_D (n(y) - 1)\Gamma_\omega(x - y)u(y)dy.$$

- Adjoint $\mathcal{A}_0^*(\omega)$:

$$\mathcal{A}_0^*(\omega)[v] = v(x) + (n(x) - 1)\omega^2 \int_D \Gamma_\omega(x - y)v(y)dy.$$

- ω_0: resonance iff it is a characteristic value of the meromorphic operator-valued function $\omega \mapsto \mathcal{A}_0(\omega)$.
- Given $n(x)$, by using Muller's method, solve the nonlinear eigenvalue problem $\mathcal{A}_0(\omega)[u] = 0$.

Cavities and resonators

- $\omega \in \mathbb{C}$: a resonance, quality factor Q:

$$Q = |\frac{\Re \omega}{\Im \omega}|.$$

- Quality factor: inversely proportional to the decay rate.
- Sensitivity of Q to changes in $n(x)$ by the generalized argument principle.
- $n_\epsilon(x) = n(x) + \epsilon\mu(x)$; μ: compactly supported in D; $\mathcal{A}_\varepsilon(\omega)$: associated with n_ε.

Cavities and resonators

- Then there exists a positive constant δ_0 such that for $|\delta| < \delta_0$, $\omega \mapsto \mathcal{A}_\varepsilon(\omega)$ has exactly one characteristic value in $\overline{V_{\delta_0}}(\omega_0)$.
- $$\omega_\varepsilon - \omega_0 = \frac{1}{2i\pi} \operatorname{tr} \int_{\partial V_{\delta_0}} (\omega - \omega_0) \mathcal{A}_\varepsilon(\omega)^{-1} \frac{d}{d\omega} \mathcal{A}_\varepsilon(\omega) d\omega,$$
- Leading-order of the expansion of $\omega_\varepsilon - \omega_0$:
$$-\frac{1}{2\pi i} \operatorname{tr} \int_{\partial V_{\delta_0}} \mathcal{A}_0(\omega)^{-1} \mathcal{A}_1^{(\mu)}(\omega) \omega d\omega,$$
- $\mathcal{A}_1^{(\mu)}$:
$$\mathcal{A}_1^{(\mu)}(\omega)[u] = \omega^2 \int_D \mu(y) \Gamma_\omega(x-y) u(y) dy.$$
- Fréchet derivative of the quality factor Q with respect to n.
- Given an admissible set of functions $n(x)$, optimal control can be used to maximize the quality factor of the resonator D.

Lecture 3: Waves in the quasi-static regime

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Waves in the quasi-static regime

- Fundamental solution to the Laplacian:

$$\Gamma_0(x) = \begin{cases} \dfrac{1}{2\pi} \ln |x| \,, & d = 2, \\ \dfrac{1}{(2-d)\omega_d} |x|^{2-d} \,, & d \geq 3, \end{cases}$$

- ω_d: area of the unit sphere in $\mathbb{R}^d$.
- Ω: bounded domain in $\mathbb{R}^d$, $d \geq 2$, of class $\mathcal{C}^{1,\eta}$ for some $\eta > 0$.
- $\nu(y)$: outward unit normal to $\partial\Omega$ at y.

Waves in the quasi-static regime

- Single- and double-layer potentials of $\varphi \in L^2(\partial\Omega)$:

$$\mathcal{S}_\Omega^0[\varphi](x) := \int_{\partial\Omega} \Gamma_0(x-y)\varphi(y)\, d\sigma(y), \quad x \in \mathbb{R}^d,$$

$$\mathcal{D}_\Omega^0[\varphi](x) := \int_{\partial\Omega} \frac{\partial}{\partial\nu(y)}\Gamma_0(x-y)\varphi(y)\, d\sigma(y)\ , \quad x \in \mathbb{R}^d \setminus \partial\Omega.$$

- Neumann-Poincaré operator: $\mathcal{K}_\Omega^0 : L^2(\partial\Omega) \to L^2(\partial\Omega)$:

$$\mathcal{K}_\Omega^0[\varphi](x) := \frac{1}{\omega_d} \int_{\partial\Omega} \frac{\langle y-x, \nu(y)\rangle}{|x-y|^d} \varphi(y)\, d\sigma(y).$$

- $(\mathcal{K}_\Omega^0)^*$: L^2-adjoint of $\mathcal{K}_\Omega^0$.
- $\mathcal{K}_\Omega^0$ and $(\mathcal{K}_\Omega^0)^*$: compact in $L^2(\partial\Omega)$.

Waves in the quasi-static regime

- Jump relations: For $\varphi \in L^2(\partial\Omega)$,

$$(\mathcal{D}_\Omega^0[\varphi])\big|_\pm(x) = \left(\mp\frac{1}{2}I + \mathcal{K}_\Omega^0\right)[\varphi](x) \quad \text{a.e. } x \in \partial\Omega;$$

$$\mathcal{S}_\Omega^0[\varphi]\Big|_+(x) = \mathcal{S}_\Omega^0[\varphi]\Big|_-(x) \quad \text{a.e. } x \in \partial\Omega;$$

$$\frac{\partial}{\partial\nu}\mathcal{S}_\Omega^0[\varphi]\Big|_\pm(x) = \left(\pm\frac{1}{2}I + (\mathcal{K}_\Omega^0)^*\right)[\varphi](x) \quad \text{a.e. } x \in \partial\Omega,$$

- For $\varphi \in L^2(\partial\Omega)$, $\partial\mathcal{D}_\Omega^0[\varphi]/\partial\nu$ exists (in $H^{-1}(\partial\Omega)$) and has no jump across $\partial\Omega$:

$$\frac{\partial}{\partial\nu}\mathcal{D}_\Omega^0[\varphi]\Big|_+ = \frac{\partial}{\partial\nu}\mathcal{D}_\Omega^0[\varphi]\Big|_- .$$

- For $\varphi \in L^2(\partial\Omega)$,

$$\frac{\partial}{\partial\nu}\mathcal{S}_\Omega^0[\varphi]\Big|_+(x) - \frac{\partial}{\partial\nu}\mathcal{S}_\Omega^0[\varphi]\Big|_-(x) = \varphi(x) \quad \text{a.e. } x \in \partial\Omega.$$

Waves in the quasi-static regime

- Dirichlet-to-Neumann operator $\mathcal{N} : L^2(\partial\Omega) \to H^{-1}(\partial\Omega)$:

$$\mathcal{N}[\varphi] = \frac{\partial u}{\partial \nu}\bigg|_{\partial\Omega};$$

- u: solution to

$$\begin{cases} \Delta u = 0 & \text{in } \Omega, \\ u = \varphi & \text{on } \partial\Omega, \end{cases}$$

- Identity:

$$\frac{\partial}{\partial \nu} \mathcal{D}_\Omega^0[\varphi]\bigg|_{\pm} = (\frac{1}{2} + (\mathcal{K}_\Omega^0)^*)\mathcal{N}[\varphi].$$

Waves in the quasi-static regime

- Capacity:
  - $d = 2$; $(\varphi_e, a) \in L^2(\partial\Omega) \times \mathbb{R}$:

$$\begin{cases} \displaystyle \frac{1}{2\pi} \int_{\partial\Omega} \ln|x-y| \varphi_e(y) d\sigma(y) + a = 0 \quad \text{on } \partial\Omega, \\ \displaystyle \int_{\partial\Omega} \varphi_e(y) d\sigma(y) = 1. \end{cases}$$

  - Logarithmic capacity of $\partial\Omega$: $\mathrm{cap}(\partial\Omega) := e^{2\pi a}$.
  - $d = 3$; $\varphi_e \in L^2(\partial\Omega)$:

$$\begin{cases} \displaystyle \int_{\partial\Omega} \frac{\varphi_e(y)}{|x-y|} d\sigma(y) = \text{constant} \quad \text{on } \partial\Omega, \\ \displaystyle \int_{\partial\Omega} \varphi_e(y) d\sigma(y) = 1. \end{cases}$$

  - Capacity of $\partial\Omega$: $\displaystyle \frac{1}{\mathrm{cap}(\partial\Omega)} := -\mathcal{S}_\Omega^0[\varphi_e]$.

Waves in the quasi-static regime

- Spectrum of the Neumann–Poincaré Operator:
  - $(\mathcal{K}_\Omega^0)^* : L^2(\partial\Omega) \to L^2(\partial\Omega)$.
  - Spectrum of $(\mathcal{K}_\Omega^0)^*$:

$$\sigma(\mathcal{K}_\Omega^0)^*) \subset (-1/2, 1/2].$$

  - $(1/2)\, I + \mathcal{K}_\Omega^0$: invertible on $L^2(\partial\Omega)$.
  - $-(1/2)\, I + \mathcal{K}_\Omega^0$: invertible on $L^2_0(\partial\Omega)$.
  - $L^2_0(\partial\Omega) := \left\{ \varphi \in L^2(\partial\Omega) : \int_{\partial\Omega} \varphi \, d\sigma = 0 \right\}$.

Waves in the quasi-static regime

- Proof by contradiction:
  - $\lambda \in (-\infty, -1/2] \cup (1/2, +\infty)$; $\varphi \in L^2(\partial\Omega)$ satisfies $(\lambda I - (\mathcal{K}_\Omega^0)^*)[\varphi] = 0$ and $\varphi \neq 0$.
  - $\mathcal{K}_\Omega^0[1] = 1/2 \Rightarrow$

$$0 = \int_{\partial\Omega} (\lambda I - (\mathcal{K}_\Omega^0)^*)[\varphi] \, d\sigma = \int_{\partial\Omega} \varphi(\lambda - \frac{1}{2}) \, d\sigma.$$

  - $\Rightarrow \int_{\partial\Omega} \varphi d\sigma = 0$.
  - $\Rightarrow \mathcal{S}_\Omega^0[\varphi](x) = O(|x|^{1-d})$ and $\nabla \mathcal{S}_\Omega^0[\varphi](x) = O(|x|^{-d})$, $|x| \to +\infty$ for $d \geq 2$.
  - $\varphi \neq 0 \Rightarrow (A, B)$ cannot be zero:

$$A = \int_\Omega |\nabla \mathcal{S}_\Omega^0[\varphi]|^2 \, dx \text{ and } B = \int_{\mathbb{R}^d \setminus \overline{\Omega}} |\nabla \mathcal{S}_\Omega^0[\varphi]|^2 \, dx.$$

  - By contradiction: if A and B are zero, then $\mathcal{S}_\Omega^0[\varphi] =$ constant in Ω and in $\mathbb{R}^d \setminus \overline{\Omega} \Rightarrow \varphi = 0$.

Waves in the quasi-static regime

- Divergence theorem $\Rightarrow$
$$A = \int_{\partial\Omega} (-\frac{1}{2}I + (\mathcal{K}_\Omega^0)^*)[\varphi]\, \mathcal{S}_\Omega^0[\varphi]\, d\sigma \text{ and } B = -\int_{\partial\Omega} (\frac{1}{2}I + (\mathcal{K}_\Omega^0)^*)[\varphi]\, \mathcal{S}_\Omega^0[\varphi]\, d\sigma.$$
- $(\lambda I - (\mathcal{K}_\Omega^0)^*)[\varphi] = 0 \Rightarrow$
$$\lambda = \frac{1}{2}\frac{B-A}{B+A} \Rightarrow |\lambda| < 1/2 \Rightarrow \text{ contradiction.}$$
- For $\lambda \in (-\infty, -\frac{1}{2}] \cup (\frac{1}{2}, +\infty)$, $\lambda I - (\mathcal{K}_\Omega^0)^*$: one to one on $L^2(\partial\Omega)$.
- If $\lambda = 1/2$, then $A = 0 \Rightarrow \mathcal{S}_\Omega^0[\varphi] =$ constant in Ω.
- $\Rightarrow$
  - $\mathcal{S}_\Omega^0[\varphi]$: harmonic in $\mathbb{R}^d \setminus \partial\Omega$;
  - $\mathcal{S}_\Omega^0[\varphi](x) = O(|x|^{1-d})$, $|x| \to +\infty$ (since $\varphi \in L_0^2(\partial\Omega)$);
  - $\mathcal{S}_\Omega^0[\varphi]$: constant on $\partial\Omega$.
- $(\mathcal{K}_\Omega^0)^*[\varphi] = (1/2)\,\varphi \Rightarrow$
$$B = -\int_{\partial\Omega} \varphi\, \mathcal{S}_\Omega^0[\varphi]\, d\sigma = C\int_{\partial\Omega} \varphi\, d\sigma = 0,$$
- $\Rightarrow \varphi = 0 \Rightarrow (1/2)\, I - (\mathcal{K}_\Omega^0)^*$: one to one on $L_0^2(\partial\Omega)$.

Waves in the quasi-static regime

- Symmetrization of $(\mathcal{K}_\Omega^0)^*$:
    - Non-self-adjoint operator $(\mathcal{K}_\Omega^0)^*$: can be realized as a self-adjoint operator on $H^{-1/2}(\partial\Omega)$ by introducing a new inner product.
    - $\mathcal{S}_\Omega^0$ in $H^{-1/2}(\partial\Omega)$: self-adjoint and $-\mathcal{S}_\Omega^0 \geq 0$ on $H^{-1/2}(\partial\Omega)$.
    - $(\mathcal{K}_\Omega^0)^* : H^{-1/2}(\partial\Omega) \rightarrow H^{-1/2}(\partial\Omega)$: compact.
    - Calderón identity $\Rightarrow$

$$\mathcal{S}_\Omega^0(\mathcal{K}_\Omega^0)^* = \mathcal{K}_\Omega^0\mathcal{S}_\Omega^0 \quad \text{on } H^{-1/2}(\partial\Omega)\,.$$

Waves in the quasi-static regime

- Kernel of $\mathcal{S}_\Omega^0$:
  - $d \geq 3$; $\mathcal{S}_\Omega^0 : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega)$ has a bounded inverse.
  - $d = 2$; If $\phi_0 \in \mathrm{Ker}(\mathcal{S}_\Omega^0)$, then u:

$$u(x) := \mathcal{S}_\Omega^0[\phi_0](x), \quad x \in \mathbb{R}^2$$

    satisfies $u = 0$ on $\partial\Omega \Rightarrow u(x) = 0$ for all $x \in \Omega$.
  - Jump condition $\Rightarrow$

$$(\mathcal{K}_\Omega^0)^*[\phi_0] = \frac{1}{2}\phi_0 \quad \text{on } \partial\Omega\,.$$

  - If $\langle \chi(\partial\Omega), \phi_0 \rangle_{1/2,-1/2} = 0$, then $u(x) \to 0$ as $|x| \to \infty \Rightarrow u(x) = 0$ for $x \in \mathbb{R}^2 \setminus \Omega \Rightarrow \phi_0 = 0$.
  - Eigenfunctions: one dimensional subspace of $H^{-1/2}(\partial\Omega)$.
  - $\Rightarrow \mathrm{Ker}(\mathcal{S}_\Omega^0)$: of at most one dimension.
  - $\mathcal{S}_\Omega^0 : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega)$ has a bounded inverse iff $\log \mathrm{cap}(\partial\Omega) \neq 0$.

Waves in the quasi-static regime

- $d = 3$; inner product:

$$\langle u, v\rangle_{\mathcal{H}^*} = -\langle \mathcal{S}_\Omega^0[v], u\rangle_{\frac{1}{2},-\frac{1}{2}} ,$$

- Equivalent: $H^{-1/2}(\partial\Omega)$.
- $(\mathcal{K}_\Omega^0)^*$: self-adjoint in $\mathcal{H}^*(\partial\Omega)$;
- (λ_j, φ_j), $j = 0, 1, 2, \ldots$: eigenvalue and normalized eigenfunction pair of $(\mathcal{K}_\Omega^0)^*$ in $\mathcal{H}^*(\partial\Omega)$ with $\lambda_0 = 1/2$.
- $\lambda_j \in (-\frac{1}{2}, \frac{1}{2})$ for $j \geq 1$ with $|\lambda_1| \geq |\lambda_2| \geq \ldots \to 0$ as $j \to \infty$;
- Spectral representation formula: for any $\psi \in H^{-1/2}(\partial\Omega)$,

$$(\mathcal{K}_\Omega^0)^*[\psi] = \sum_{j=0}^{\infty} \lambda_j \langle \varphi_j, \psi\rangle_{\mathcal{H}^*} \varphi_j .$$

- $\mathcal{H}(\partial\Omega)$: $H^{1/2}(\partial\Omega)$ equipped with the equivalent inner product

$$\langle u, v\rangle_{\mathcal{H}} = \langle v, (-\mathcal{S}_\Omega^0)^{-1}[u]\rangle_{\frac{1}{2},-\frac{1}{2}} .$$

- $\mathcal{S}_\Omega^0$: isometry between $\mathcal{H}^*(\partial\Omega)$ and $\mathcal{H}(\partial\Omega)$.

Waves in the quasi-static regime

- $d = 2$; $\mathcal{S}_\Omega^0 : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega)$: not injective (in general).
- Substitute:

$$\widetilde{\mathcal{S}}_\Omega[\psi] := \begin{cases} \mathcal{S}_\Omega^0[\psi] & \text{if } \langle \chi(\partial\Omega), \psi \rangle_{\frac{1}{2},-\frac{1}{2}} = 0\,, \\ -\chi(\partial\Omega) & \text{if } \psi = \varphi_0\,, \end{cases}$$

- φ_0: unique eigenfunction of $(\mathcal{K}_\Omega^0)^*$ associated with eigenvalue $1/2$ s.t. $\langle \chi(\partial\Omega), \varphi_0 \rangle_{\frac{1}{2},-\frac{1}{2}} = 1$.
- $\widetilde{\mathcal{S}}_\Omega : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega)$: invertible.
- Calderón identity:

$$\mathcal{K}_\Omega^0 \widetilde{\mathcal{S}}_\Omega = \widetilde{\mathcal{S}}_\Omega (\mathcal{K}_\Omega^0)^*.$$

Waves in the quasi-static regime

- $(\mathcal{K}_\Omega^0)^*$: compact self-adjoint in $\mathcal{H}^*(\partial\Omega)$ equipped with

$$\langle u, v\rangle_{\mathcal{H}^*} = -\langle \widetilde{\mathcal{S}}_\Omega[v], u\rangle_{\frac{1}{2},-\frac{1}{2}} .$$

- (λ_j, φ_j), $j = 0, 1, 2, \ldots,$: eigenvalue and normalized eigenfunction pair of $(\mathcal{K}_\Omega^0)^*$ with $\lambda_0 = \frac{1}{2}$. $\lambda_j \in (-\frac{1}{2}, \frac{1}{2})$ with $|\lambda_1| \geq |\lambda_2| \geq \ldots \to 0$ as $j \to \infty$;
- Twin property: For any $j \geq 1$, $\pm\lambda_j$: eigenvalues of $(\mathcal{K}_\Omega^0)^*$;
- $\mathcal{H}^*(\partial\Omega) = \mathcal{H}_0^*(\partial\Omega) \oplus \{\mu\varphi_0,\ \mu \in \mathbb{C}\}$, where $\mathcal{H}_0^*(\partial\Omega)$: zero mean subspace of $\mathcal{H}^*(\partial\Omega)$;
- For any $\psi \in H^{-1/2}(\partial\Omega)$,

$$(\mathcal{K}_\Omega^0)^*[\psi] = \sum_{j=0}^{\infty} \lambda_j \langle \varphi_j, \psi\rangle_{\mathcal{H}^*}\, \varphi_j .$$

- $\mathcal{H}(\partial\Omega)$: $H^{1/2}(\partial\Omega)$ equipped with the equivalent inner product:

$$\langle u, v\rangle_{\mathcal{H}} = \langle v, -\widetilde{\mathcal{S}}_\Omega^{-1}[u]\rangle_{\frac{1}{2},-\frac{1}{2}} .$$

- $\widetilde{\mathcal{S}}_\Omega$: isometry between $\mathcal{H}^*(\partial\Omega)$ and $\mathcal{H}(\partial\Omega)$.

Waves in the quasi-static regime

- Conductivity problem in free space
  - B: bounded smooth domain in $\mathbb{R}^d$; $O \in B$.
  - $0 < k \neq 1 < +\infty$ and $\lambda(k) := (k+1)/(2(k-1))$.
  - h: harmonic function in $\mathbb{R}^d$; u:

$$\begin{cases} \nabla \cdot ((1 + (k-1)\chi(B))\nabla u_k) = 0 & \text{in } \mathbb{R}^d, \\ u_k(x) - h(x) = O(|x|^{1-d}) & \text{as } |x| \to +\infty. \end{cases}$$

  - Integral representation formula:

$$u_k(x) = h(x) + \mathcal{S}_B^0 (\lambda(k) I - (\mathcal{K}_B^0)^*)^{-1} [\frac{\partial h}{\partial \nu}|_{\partial B}](x) \quad \text{for } x \in \mathbb{R}^d.$$

Waves in the quasi-static regime

- Taylor's formula expansion:

$$\Gamma_0(x-y) = \sum_{\alpha, |\alpha|=0}^{+\infty} \frac{(-1)^{|\alpha|}}{\alpha!} \partial_x^\alpha \Gamma_0(x) y^\alpha, \quad y \text{ in a compact set}, \quad |x| \to +\infty.$$

- Far-field expansion of $(u_k - h)(x)$ as $|x| \to +\infty$:

$$\sum_{|\alpha|,|\beta|=1}^{+\infty} \frac{(-1)^{|\alpha|}}{\alpha!\beta!} \partial_x^\alpha \Gamma_0(x) \partial^\beta h(0) \int_{\partial B} (\lambda(k) I - (\mathcal{K}_B^0)^*)^{-1} \left[\nu(x) \cdot \nabla x^\alpha\right](y) y^\beta \, d\sigma(y).$$

- For a multi-index $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}^d$: $\partial^\alpha f = \partial_1^{\alpha_1} \ldots \partial_d^{\alpha_d} f$ and $x^\alpha := x_1^{\alpha_1} \ldots x_d^{\alpha_d}$.

Waves in the quasi-static regime

- Generalized polarization tensor $M_{\alpha\beta}$, $\alpha, \beta \in \mathbb{N}^d$:

$$M_{\alpha\beta}(\lambda(k), B) := \int_{\partial B} y^\beta \phi_\alpha(y)\, d\sigma(y);$$

- ϕ_α:

$$\phi_\alpha(y) := (\lambda(k)I - (\mathcal{K}_B^0)^*)^{-1}\big[\nu(x) \cdot \nabla x^\alpha\big](y), \quad y \in \partial B.$$

- For $|\alpha| = |\beta| = 1$, $M = (m_{pq})_{p,q=1}^d$ polarization tensor

$$m_{pq} := \int_{\partial B} y_q (\lambda(k)I - (\mathcal{K}_B^0)^*)^{-1}\big[\nu_p\big](y)\, d\sigma(y),$$

- $\nu = (\nu_1, \ldots, \nu_d)$.
- Generalized polarization tensors $\Rightarrow$ complete information about the far-field expansion of u.

Waves in the quasi-static regime

- From

$$(\lambda(k)I - (\mathcal{K}_B^0)^*)^{-1}[\psi] = \sum_{j=0}^{\infty} \frac{\langle \psi, \varphi_j \rangle_{\mathcal{H}^*} \varphi_j}{\lambda(k) - \lambda_j},$$

- (λ_j, φ_j): eigenvalues and eigenvectors of $(\mathcal{K}_B^0)^*$ in $\mathcal{H}^*$.
- Decomposition of the entries of the polarization tensor:

$$m_{pq}(\lambda(k), B) = \sum_{j=1}^{\infty} \frac{\langle \nu_p, \varphi_j \rangle_{\mathcal{H}^*} \langle \varphi_j, x_q \rangle_{-\frac{1}{2},\frac{1}{2}}}{\lambda(k) - \lambda_j}.$$

- $\langle \nu_p, \chi(\partial B) \rangle_{-\frac{1}{2},\frac{1}{2}} = 0$. $\lambda_0 = 1/2 \Rightarrow \langle \nu_p, \varphi_0 \rangle_{\mathcal{H}^*} = 0$.

Waves in the quasi-static regime

- From:

$$\langle \varphi_j, x_q \rangle_{-\frac{1}{2},\frac{1}{2}} = \left\langle \left(\tfrac{1}{2} - \lambda_j\right)^{-1} \left(\tfrac{1}{2} I - (\mathcal{K}_B^0)^*\right)[\varphi_j], x_q \right\rangle_{-\frac{1}{2},\frac{1}{2}}$$

$$= \frac{-1}{1/2 - \lambda_j} \left\langle \frac{\partial \mathcal{S}_B^0[\varphi_j]}{\partial \nu}\Big|_{-}, x_q \right\rangle_{-\frac{1}{2},\frac{1}{2}}$$

$$= \frac{-1}{1/2 - \lambda_j} \left[\int_{\partial B} \frac{\partial x_q}{\partial \nu} \mathcal{S}_B^0[\varphi_j] d\sigma - \int_B \left(\Delta x_q \mathcal{S}_B^0[\varphi_j] - x_q \Delta \mathcal{S}_B^0[\varphi_j] \right) dx \right]$$

$$= \frac{\langle \nu_q, \varphi_j \rangle_{\mathcal{H}^*}}{1/2 - \lambda_j}$$

- $\Rightarrow$

$$m_{pq}(\lambda(k), B) = \sum_{j=1}^{\infty} \frac{\langle \nu_p, \varphi_j \rangle_{\mathcal{H}^*} \langle \nu_q, \varphi_j \rangle_{\mathcal{H}^*}}{(1/2 - \lambda_j)(\lambda(k) - \lambda_j)}.$$

Waves in the quasi-static regime

- Properties of the polarization tensor:
  - $M(\lambda(k), B)$: symmetric;
  - $M(\lambda(k), B)$: positive definite if $k > 1$;
  - $M(\lambda(k), B)$: negative definite if $0 < k < 1$.
  - Optimal bounds:

$$\frac{1}{k-1}\,\mathrm{tr}(M(\lambda(k), B)) < (1 + \frac{1}{k})|B|$$

and

$$(k-1)\,\mathrm{tr}(M(\lambda(k), B)^{-1}) \leq \frac{(1+k)}{|B|}.$$

Waves in the quasi-static regime

- Conductivity equation with complex coefficients: $k \in \mathbb{C}$; $\lambda(k) \notin \sigma((\mathcal{K}_B^0)^*)$,
  - There exists C independent of k s.t. for any harmonic function h in $\mathbb{R}^d$, the unique solution u_k satisfies

$$\|\nabla(u_k - h)\|_{L^2(\mathbb{R}^d)} \leq \frac{C}{\mathrm{dist}\big(\lambda(k), \sigma((\mathcal{K}_B^0)^*)\big)} \|\frac{\partial h}{\partial \nu}\|_{H^{-1/2}(\partial B)}.$$

  - There exists C independent of k s.t. for $|k' - k|$ small enough, such that for any harmonic functions h in $\mathbb{R}^d$

$$\|\nabla(u_k - u_{k'})\|_{L^2(\mathbb{R}^d)} \leq \frac{C|k' - k|}{\mathrm{dist}\big(\lambda(k), \sigma((\mathcal{K}_B^0)^*)\big)} \|\frac{\partial h}{\partial \nu}\|_{H^{-1/2}(\partial B)}.$$

Lecture 4: Periodic and quasi-periodic Green's functions

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Periodic and quasi-periodic Green's functions

- Periodic and quasi-periodic Green's functions:
  - Periodic Green's functions for gratings;
  - Periodic, and quasi-periodic Green's functions;
  - Periodic and quasi-periodic layer potentials for the Laplacian and the Helmholtz operator.
- Applications:
  - Diffractive gratings;
  - Photonic and phononic crystals;
  - Metasurfaces;
  - Metamaterials.

Periodic and quasi-periodic Green's functions

- $G_\sharp$: Periodic Green's function for the one-dimensional grating in $\mathbb{R}^2$:
  - $G_\sharp : \mathbb{R}^2 \to \mathbb{C}$:

$$\Delta G_\sharp(x) = \sum_{n\in\mathbb{Z}} \delta_0(x + (n, 0)).$$

  - Explicit formula: $x = (x_1, x_2)$,

$$G_\sharp(x) = \frac{1}{4\pi} \ln \left(\sinh^2(\pi x_2) + \sin^2(\pi x_1) \right).$$

Periodic and quasi-periodic Green's functions

- Poisson summation formula:

$$\sum_{n\in\mathbb{Z}} \delta_0(x_1+n) = \sum_{n\in\mathbb{Z}} e^{i2\pi n x_1}.$$

- $\Rightarrow$

$$\begin{aligned} \Delta G_\sharp(x) &= \sum_{n\in\mathbb{Z}} \delta_0(x+(n,0)) \\ &= \sum_{n\in\mathbb{Z}} \delta_0(x_2)\delta_0(x_1+n) \\ &= \sum_{n\in\mathbb{Z}} \delta_0(x_2) e^{i2\pi n x_1}. \end{aligned}$$

- $G_\sharp$: periodic in x_1 of period 1 $\Rightarrow$

$$G_\sharp(x) = \sum_{n\in\mathbb{Z}} \beta_n(x_2) e^{i2\pi n x_1}.$$

$$\Delta G_\sharp(x) = \sum_{n\in\mathbb{Z}} (\beta_n^{''}(x_2) + (i2\pi n)^2 \beta_n(x_2)) e^{i2\pi n x_1}.$$

Periodic and quasi-periodic Green's functions

- ODE:
$$\beta_n''(x_2) + (i2\pi n)^2 \beta_n(x_2) = \delta_0(x_2).$$
- Solution:
$$\begin{aligned} \beta_0(x_2) &= \frac{1}{2}|x_2| + c, \\ \beta_n(x_2) &= \frac{-1}{4\pi|n|} e^{-2\pi|n||x_2|}, \quad n \neq 0; \end{aligned}$$
c: constant.
- Define $c := -\frac{\ln(2)}{2\pi}$ and use the summation identity:
$$\sum_{n\in\mathbb{N}\setminus\{0\}} \frac{1}{2\pi n} e^{-2\pi n|x_2|} \cos(2\pi n x_1) = \frac{1}{2}|x_2| - \frac{\ln(2)}{2\pi} - \frac{1}{4\pi} \ln\left(\sinh^2(\pi x_2) + \sin^2(\pi x_1)\right).$$

Periodic and quasi-periodic Green's functions

- $$\begin{aligned} G_\sharp(x) &= \frac{1}{2}|x_2| + c - \sum_{n\in\mathbb{Z}\setminus\{0\}} \frac{1}{4\pi|n|} e^{-2\pi|n||x_2|} e^{i2\pi n x_1} \\ &= \frac{1}{2}|x_2| + c - \sum_{n\in\mathbb{N}\setminus\{0\}} \frac{1}{2\pi n} e^{-2\pi n|x_2|} \cos(2\pi n x_1) \\ &= \frac{1}{4\pi} \ln\left(\sinh^2(\pi x_2) + \sin^2(\pi x_1)\right). \end{aligned}$$

- Taylor expansion of $G_\sharp$:

$$G_\sharp(x) = \frac{\ln|x|}{2\pi} + R(x);$$

- R: smooth function s.t.

$$R(x) = \frac{1}{4\pi}\ln(1 + O(x_2^2 - x_1^2)).$$

Periodic and quasi-periodic Green's functions

- $G_\sharp(x,y) := G_\sharp(x-y)$; $\Omega \Subset \big(-\frac{1}{2},\frac{1}{2}\big)\times\mathbb{R}$: bounded smooth domain;
- One-dimensional periodic single-layer potential and periodic Neumann–Poincaré operator:

$$\begin{aligned} \mathcal{S}_{\Omega,\sharp} : H^{-\frac{1}{2}}(\partial\Omega) &\longrightarrow H^1_{\mathrm{loc}}(\mathbb{R}^2), H^{\frac{1}{2}}(\partial\Omega) \\ \varphi &\longmapsto \mathcal{S}_{\Omega,\sharp}[\varphi](x) = \int_{\partial\Omega} G_\sharp(x,y)\varphi(y)d\sigma(y) \end{aligned}$$

for $x \in \mathbb{R}^2$ (or $x \in \partial\Omega$);

$$\begin{aligned} \mathcal{K}^*_{\Omega,\sharp} : H^{-\frac{1}{2}}(\partial\Omega) &\longrightarrow H^{-\frac{1}{2}}(\partial\Omega) \\ \varphi &\longmapsto \mathcal{K}^*_{\Omega,\sharp}[\varphi](x) = \int_{\partial\Omega} \frac{\partial G_\sharp(x,y)}{\partial\nu(x)}\varphi(y)d\sigma(y) \end{aligned}$$

for $x \in \partial\Omega$.

Periodic and quasi-periodic Green's functions

- Symmetrization of the periodic Neumann–Poincaré operator $\mathcal{K}^*_{\Omega,\sharp}$:
  - For any $\varphi \in H^{-\frac{1}{2}}(\partial\Omega)$, $\mathcal{S}_{\Omega,\sharp}[\varphi]$: harmonic in Ω and in $\left(-\dfrac{1}{2}, \dfrac{1}{2}\right) \times \mathbb{R} \setminus \overline{\Omega}$;
  - Trace formula: For any $\varphi \in H^{-\frac{1}{2}}(\partial\Omega)$,
  $$(-\frac{1}{2} I + \mathcal{K}^*_{\Omega,\sharp})[\varphi] = \frac{\partial \mathcal{S}_{\Omega,\sharp}[\varphi]}{\partial \nu}\Big|_- ;$$
  - Calderón identity: $\mathcal{K}_{\Omega,\sharp}\mathcal{S}_{\Omega,\sharp} = \mathcal{S}_{\Omega,\sharp}\mathcal{K}^*_{\Omega,\sharp}$; $\mathcal{K}_{\Omega,\sharp}$: L^2-adjoint of $\mathcal{K}^*_{\Omega,\sharp}$;
  - $\mathcal{K}^*_{\Omega,\sharp} : H_0^{-\frac{1}{2}}(\partial\Omega) \to H_0^{-\frac{1}{2}}(\partial\Omega)$: compact self-adjoint equipped with the inner product:
  $$\langle u, v \rangle_{\mathcal{H}^*_0} = -\langle \mathcal{S}_{\Omega,\sharp}[v], u \rangle_{\frac{1}{2},-\frac{1}{2}}$$
  - (λ_j, φ_j), $j = 1, 2, \ldots$: eigenvalue and normalized eigenfunction pair of $\mathcal{K}^*_{\Omega,\sharp}$ in $\mathcal{H}^*_0(\partial\Omega)$; $\lambda_j \in (-\frac{1}{2}, \frac{1}{2})$ and $\lambda_j \to 0$ as $j \to \infty$.

Periodic and quasi-periodic Green's functions

- Periodic Green's function:
  - Effective medium properties of subwavelength resonators;
  - Periodic transmission problem for the Laplace operator.
- $Y = (-1/2, 1/2)^d$: unit cell; $\overline{D} \subset Y$.
- Periodic transmission problem: for $p = 1, \ldots, d$,

$$\begin{cases} \nabla \cdot \Big(1 + (k-1)\chi(D)\Big) \nabla u_p = 0 \quad \text{in } Y \,, \\ u_p - x_p \;\; \text{periodic (in each direction) with period } 1 \,, \\ \displaystyle\int_Y u_p \, dx = 0 \,. \end{cases}$$

- Representation formula for u_p.

Periodic and quasi-periodic Green's functions

- Lattice sum representation of the periodic Green's function:

$$G_\sharp(x) = -\sum_{n\in\mathbb{Z}^d\setminus\{0\}} \frac{e^{i2\pi n\cdot x}}{4\pi^2|n|^2}.$$

- In the sense of distributions:

$$\Delta G_\sharp(x) = \sum_{n\in\mathbb{Z}^d\setminus\{0\}} e^{i2\pi n\cdot x} = \sum_{n\in\mathbb{Z}^d} e^{i2\pi n\cdot x} - 1\,;$$

- $G_\sharp$ has mean zero: $\displaystyle\int_Y G_\sharp = 0$.
- Poisson's summation formula:

$$\sum_{n\in\mathbb{Z}^d} e^{i2\pi n\cdot x} = \sum_{n\in\mathbb{Z}^d} \delta_0(x-n)\,,$$

- $\Rightarrow$

$$\Delta G_\sharp(x) = \sum_{n\in\mathbb{Z}^d} \delta_0(x-n) - 1\,.$$

Periodic and quasi-periodic Green's functions

- There exists a smooth function $R_d(x)$ in the unit cell Y s.t.

$$G_\sharp(x) = \begin{cases} \dfrac{1}{2\pi} \ln |x| + R_2(x), & d = 2\,, \\ \dfrac{1}{(2-d)\omega_d} \dfrac{1}{|x|^{d-2}} + R_d(x), & d \geq 3\,. \end{cases}$$

- Taylor's formula expansion of $R_d(x)$ at 0 for $d \geq 2$:

$$R_d(x) = R_d(0) - \frac{1}{2d}(x_1^2 + \ldots + x_d^2) + O(|x|^4)\,.$$

Periodic and quasi-periodic Green's functions

- Periodic single-layer potential of $\phi \in L^2_0(\partial\Omega)$:

$$\mathcal{S}^0_{\Omega,\sharp}[\phi](x) := \int_{\partial\Omega} G_\sharp(x-y)\phi(y)\, d\sigma(y), \quad x \in \mathbb{R}^2 .$$

- Behaviors at the boundary: $\phi \in L^2_0(\partial\Omega)$,

$$\frac{\partial}{\partial\nu}\mathcal{S}^0_{\Omega,\sharp}[\phi]\Big|_\pm(x) = (\pm\frac{1}{2}I + (\mathcal{K}^0_{\Omega,\sharp})^*)[\phi](x) \text{ on } \partial\Omega\, ;$$

- $(\mathcal{K}^0_{\Omega,\sharp})^* : L^2_0(\partial\Omega) \to L^2_0(\partial\Omega)$:

$$(\mathcal{K}^0_{\Omega,\sharp})^*[\phi](x) = \text{p.v. } \int_{\partial\Omega} \frac{\partial}{\partial\nu(x)} G_\sharp(x-y)\phi(y)\, d\sigma(y), \quad x \in \partial D\, .$$

- If $\phi \in L^2_0(\partial\Omega)$, then $\mathcal{S}^0_{\Omega,\sharp}[\phi]$: harmonic in Ω and $Y \setminus \overline{\Omega}$.
- If $|\lambda| \geq \frac{1}{2}$, then $\lambda I - (\mathcal{K}^0_{\Omega,\sharp})^*$: invertible on $L^2_0(\partial\Omega)$.

Periodic and quasi-periodic Green's functions

- Representation formula for the solution of the periodic transmission problem: u_p, $p = 1, \ldots, d$,

$$u_p(x) = x_p + C_p + \mathcal{S}^0_{\Omega,\sharp}\Big(\frac{k+1}{2(k-1)} I - (\mathcal{K}^0_{\Omega,\sharp})^*\Big)^{-1}[\nu_p](x) \quad \text{in } Y\,;$$

- C_p: constant and ν_p: p-component of the outward unit normal ν to $\partial\Omega$.

Periodic and quasi-periodic Green's functions

- $u_p, p = 1, \ldots, d$, satisfies

$$\begin{cases} \Delta u_p = 0 \quad \text{in } \Omega \cup (Y \setminus \overline{\Omega}), \\ u_p|_+ - u_p|_- = 0 \quad \text{on } \partial\Omega, \\ \dfrac{\partial u_p}{\partial \nu}\Big|_+ - k \dfrac{\partial u_p}{\partial \nu}\Big|_- = 0 \quad \text{on } \partial\Omega, \\ u_p - x_p \ \text{ periodic with period } 1, \\ \displaystyle\int_Y u_p \, dx = 0. \end{cases}$$

- Define $V_p(x) = \mathcal{S}^0_{\Omega,\sharp}((\frac{k+1}{2(k-1)} I - (\mathcal{K}^0_{\Omega,\sharp})^*)^{-1}[\nu_p](x) \quad \text{in } Y.$

$$\begin{cases} \Delta V_p = 0 \ \text{ in } \ \Omega \cup (Y \setminus \overline{D}), \\ V_p|_+ - V_p|_- = 0 \ \text{ on } \ \partial\Omega, \\ \dfrac{\partial V_p}{\partial \nu}|_+ - k \dfrac{\partial V_p}{\partial \nu}|_- = (k-1)\nu_p \ \text{ on } \partial\Omega, \\ V_p \text{ periodic with period } 1. \end{cases}$$

Periodic and quasi-periodic Green's functions

- Choose C_p s.t. $\int_Y u_p \, dx = 0$.
- General periodic lattice in two dimensions:
  - $r_n = n_1 a^{(1)} + n_2 a^{(2)}, n = (n_1, n_2) \in \mathbb{Z}^2$.
  - $a^{(1)}$ and $a^{(2)}$ determine the unit cell $Y := \{sa^{(1)} + ta^{(2)}, s, t \in (-1/2, 1/2)\}$ of the array.
  - Reciprocal vector of r_n: $k_n \cdot a^{(i)} = n_i, i = 1, 2$.
  - Periodic Green's function of the Laplacian:

$$\begin{cases} \Delta G_\sharp^a = \displaystyle\sum_{n \in \mathbb{Z}^2} \delta_0(x - r_n) - \frac{1}{|Y|}, \\ G_\sharp^a(x + r_n) = G_\sharp^a(x), \quad \forall\, n \in \mathbb{Z}^2. \end{cases}$$

Periodic and quasi-periodic Green's functions

- Rotate and scale the given lattice in order to satisfy $a^{(1)} = (1,0)$ and $a^{(2)} = (a, b)$ with $b > 0 \Rightarrow$

$$r_n = n_1(1,0) + n_2(a,b), \quad k_n = n_1(1, -\frac{a}{b}) + n_2(0, \frac{1}{b}), \quad n = (n_1, n_2) \in \mathbb{Z}^2.$$

- Lattice sum representation of $G_\sharp^a$:

$$G_\sharp^a(x) = -\sum_{n \in \mathbb{Z}^2 \setminus \{0\}} \frac{e^{i2\pi(n_1 x_1 + (-\frac{a}{b}n_1 + \frac{1}{b}n_2)x_2)}}{4\pi^2\big(n_1^2 + (-\frac{a}{b}n_1 + \frac{1}{b}n_2)^2\big)^2}.$$

Periodic and quasi-periodic Green's functions

- Quasi-periodic Green's functions:
  - For $\alpha \in (0, 2\pi)^d$, a function u: α-quasi-periodic if $e^{-i\alpha\cdot x}u$: periodic.
  - Lattice sum representation of quasi-periodic Green's function:

$$G_\alpha(x) = -\sum_{n\in\mathbb{Z}^d} \frac{e^{i(2\pi n+\alpha)\cdot x}}{|2\pi n + \alpha|^2}, \quad \alpha \in (0, 2\pi)^d.$$

  - $e^{-i\alpha\cdot x}G_\alpha(x)$: periodic in $\mathbb{R}^d$.

$$\Delta G_\alpha(x) = \sum_{n\in\mathbb{Z}^d} \delta_0(x-n)e^{i\alpha\cdot n} \quad \text{in } \mathbb{R}^d,$$

$$\Big(\Delta + i\alpha\cdot\nabla - |\alpha|^2\Big)\big(e^{-i\alpha\cdot x}G_\alpha(x)\big) = \sum_{n\in\mathbb{Z}^d} \delta_0(x-n) \quad \text{in } \mathbb{R}^d.$$

Periodic and quasi-periodic Green's functions

- $\mathcal{S}^0_{\Omega,\alpha}, \mathcal{D}^0_{\Omega,\alpha}$, and $(\mathcal{K}^0_{\Omega,\alpha})^*$: α-quasi-periodic single- and double-layer potentials and the α-quasi-periodic Neumann–Poincaré operator associated with G_α.
- $\alpha \in (0, 2\pi)^2$; $(\mathcal{K}^0_{\Omega,\alpha})^* : H_0^{-\frac{1}{2}}(\partial\Omega) \to H_0^{-\frac{1}{2}}(\partial\Omega)$: compact self-adjoint equipped with the following inner product

$$\langle u, v \rangle_{\mathcal{H}_0^*} = -\langle \mathcal{S}^0_{\Omega,\alpha}[v], u \rangle_{\frac{1}{2},-\frac{1}{2}}$$

- $(\lambda_{j,\alpha}, \varphi_{j,\alpha})$, $j = 1, 2, \ldots$: eigenvalue and normalized eigenfunction pair of $(\mathcal{K}^0_{\Omega,\alpha})^*$ in $\mathcal{H}_0^*(\partial\Omega)$, then $\lambda_{j,\alpha} \in (-\frac{1}{2}, \frac{1}{2})$ and $\lambda_{j,\alpha} \to 0$ as $j \to \infty$.
- Ewald's method: computing periodic and quasi-periodic Green's functions (series slowly converge).

Periodic and quasi-periodic Green's functions

- Quasi-periodic layer potentials for the Helmholtz equation:
  - α: quasi-momentum variable in the Brillouin zone $B = [0, 2\pi)^2$.
  - Two-dimensional quasi-periodic Green's function $G^{\alpha,\omega}$:

$$(\Delta + \omega^2) G^{\alpha,\omega}(x, y) = \sum_{n \in \mathbb{Z}^2} \delta_0(x - y - n) e^{in\cdot\alpha}.$$

  - If $\omega \neq |2\pi n + \alpha|, \forall\, n \in \mathbb{Z}^2$, Poisson's summation formula:

$$\sum_{n \in \mathbb{Z}^2} e^{i(2\pi n + \alpha)\cdot x} = \sum_{n \in \mathbb{Z}^2} \delta_0(x - n) e^{in\cdot\alpha}.$$

  - $\Rightarrow$ $G^{\alpha,\omega}$ can be represented as a sum of augmented plane waves over the reciprocal lattice:

$$G^{\alpha,\omega}(x, y) = \sum_{n \in \mathbb{Z}^2} \frac{e^{i(2\pi n + \alpha)\cdot(x-y)}}{\omega^2 - |2\pi n + \alpha|^2}.$$

Periodic and quasi-periodic Green's functions

- Representation of $G^{\alpha,\omega}$ as a sum of images:

$$G^{\alpha,\omega}(x,y) = -\frac{i}{4}\sum_{n\in\mathbb{Z}^2} H_0^{(1)}(\omega|x-n-y|)e^{in\cdot\alpha};$$

- $H_0^{(1)}$: Hankel function of the first kind of order 0.
- Series in the spatial representation of $G^{\alpha,\omega}$ converges uniformly for x, y in compact sets of $\mathbb{R}^2$ and $\omega \neq |2\pi n + \alpha|$ for all $n \in \mathbb{Z}^2$.
- $H_0^{(1)}(z) = (2i/\pi)\ln z + O(1)$ as $z \to 0 \Rightarrow G^{\alpha,\omega}(x,y) - (1/2\pi)\ln|x-y|$: smooth for all $x, y \in Y$.
- Disadvantage of the spectral representation of the Green's function: singularity as $|x-y| \to 0$ is not explicit.

Periodic and quasi-periodic Green's functions

- Assumption: $\omega \neq |2\pi n + \alpha|$ for all $n \in \mathbb{Z}^2$.
- D: bounded smooth domain in $\mathbb{R}^2$; ν: unit outward normal to ∂D.
- For $\omega > 0$; $\mathcal{S}^{\alpha,\omega}$ and $\mathcal{D}^{\alpha,\omega}$: quasi-periodic single- and double-layer potentials. associated with $G^{\alpha,\omega}$ on D;
- Given density $\varphi \in L^2(\partial D)$,

$$\mathcal{S}^{\alpha,\omega}[\varphi](x) = \int_{\partial D} G^{\alpha}_{\omega}(x,y)\varphi(y)\, d\sigma(y), \quad x \in \mathbb{R}^2,$$

$$\mathcal{D}^{\alpha,\omega}[\varphi](x) = \int_{\partial D} \frac{\partial G^{\alpha}_{\omega}(x,y)}{\partial \nu(y)}\varphi(y)\, d\sigma(y), \quad x \in \mathbb{R}^2 \setminus \partial D.$$

- $\mathcal{S}^{\alpha,\omega}[\varphi]$ and $\mathcal{D}^{\alpha,\omega}[\varphi]$ satisfy $(\Delta + \omega^2)\mathcal{S}^{\alpha,\omega}[\varphi] = (\Delta + \omega^2)\mathcal{D}^{\alpha,\omega}[\varphi] = 0$ in D and $Y \setminus \overline{D}$.
- $\mathcal{S}^{\alpha,\omega}[\varphi]$ and $\mathcal{D}^{\alpha,\omega}[\varphi]$: α-quasi-periodic.

Periodic and quasi-periodic Green's functions

- Jump relations: $\varphi \in L^2(\partial D)$,

$$\frac{\partial(\mathcal{S}^{\alpha,\omega}[\varphi])}{\partial \nu}\Big|_{\pm}(x) = \left(\pm \frac{1}{2} I + (\mathcal{K}^{-\alpha,\omega})^* \right)[\varphi](x) \quad \text{a.e. } x \in \partial D,$$

$$(\mathcal{D}^{\alpha,\omega}[\varphi])\Big|_{\pm}(x) = \left(\mp \frac{1}{2} I + \mathcal{K}^{\alpha,\omega} \right)[\varphi](x) \quad \text{a.e. } x \in \partial D,$$

- $\mathcal{K}^{\alpha,\omega}$:

$$\mathcal{K}^{\alpha,\omega}[\varphi](x) = \text{p.v.} \int_{\partial D} \frac{\partial G^{\alpha,\omega}(x,y)}{\partial \nu(y)} \varphi(y)\, d\sigma(y)$$

- $(\mathcal{K}^{-\alpha,\omega})^*$: L^2-adjoint operator of $\mathcal{K}^{-\alpha,\omega}$,

$$(\mathcal{K}^{-\alpha,\omega})^*[\varphi](x) = \text{p.v.} \int_{\partial D} \frac{\partial G^{\alpha,\omega}(x,y)}{\partial \nu(x)} \varphi(y)\, d\sigma(y).$$

- $\mathcal{K}^{\alpha,\omega}$ and $(\mathcal{K}^{-\alpha,\omega})^*$: compact on $L^2(\partial D)$;
- $G^{\alpha,\omega}(x,y) - (1/2\pi) \ln|x-y|$: smooth for all x, y.

Periodic and quasi-periodic Green's functions

- Assumption: $\alpha \neq 0$ and ω^2: neither an eigenvalue of $-\Delta$ in D with the Dirichlet boundary condition on ∂D nor in $Y \setminus \overline{D}$ with the Dirichlet boundary condition on ∂D and the α-quasi-periodic condition on ∂Y.
- $\mathcal{S}^{\alpha,\omega} : L^2(\partial D) \to H^1(\partial D)$: invertible.

Periodic and quasi-periodic Green's functions

- Suppose that $\phi \in L^2(\partial D)$ satisfies $\mathcal{S}^{\alpha,\omega}[\phi] = 0$ on ∂D.
- Then $u = \mathcal{S}^{\alpha,\omega}[\phi]$ satisfies $(\Delta + \omega^2)u = 0$ in D and in $Y \setminus \overline{D}$.
- ω^2: neither an eigenvalue of $-\Delta$ in D with the Dirichlet boundary condition nor in $Y \setminus \overline{D}$ with the Dirichlet boundary condition on ∂D and the quasi-periodic condition on $\partial Y \Rightarrow u = 0$ in Y.
- $\phi = \partial u/\partial \nu|_+ - \partial u/\partial \nu|_- = 0$.

Periodic and quasi-periodic Green's functions

- Define

$$G^{\alpha,0}(x,y) := G_\alpha(x-y) = -\sum_{n\in\mathbb{Z}^2} \frac{e^{i(2\pi n+\alpha)\cdot(x-y)}}{|2\pi n+\alpha|^2} \quad \text{for } \alpha \neq 0.$$

- For $\alpha = 0$:

$$G^{0,0}(x,y) := G_\sharp(x-y) = -\sum_{n\in\mathbb{Z}^2\setminus\{0\}} \frac{e^{i2\pi n\cdot(x-y)}}{4\pi^2|n|^2},$$

- $G^{0,0}(x,y)$ satisfies

$$\Delta_x G^{0,0}(x,y) = \delta_y - 1 \quad \text{in } Y$$

with periodic Dirichlet boundary conditions on ∂Y.

Periodic and quasi-periodic Green's functions

- As $\omega \to 0$, $G^{\alpha,\omega}$ can be decomposed as

$$G^{\alpha,\omega}(x,y) = G^{\alpha,0}(x,y) - \sum_{l=1}^{+\infty} \underbrace{\omega^{2l} \sum_{n\in\mathbb{Z}^2} \frac{e^{i(2\pi n+\alpha)\cdot(x-y)}}{|2\pi n+\alpha|^{2(l+1)}}}_{:=-G_l^{\alpha,\omega}(x,y)},$$

  for $\alpha \neq 0$;

- For $\alpha = 0$:

$$G^{0,\omega}(x,y) = \frac{1}{\omega^2} + G^{0,0}(x,y) - \sum_{l=1}^{+\infty} \underbrace{\omega^{2l} \sum_{n\in\mathbb{Z}^2\setminus\{0\}} \frac{e^{i2\pi n\cdot(x-y)}}{(4\pi^2)^{l+1}|n|^{2(l+1)}}}_{:=-G_l^{0,\omega}(x,y)}.$$

Periodic and quasi-periodic Green's functions

- $\mathcal{S}_l^{\alpha,\omega}$ and $(\mathcal{K}_l^{-\alpha,\omega})^*$, for $l \geq 0$ and $\alpha \in [0, 2\pi)^2$, layer potentials associated with the kernel $G_l^{\alpha,\omega}(x, y)$:

$$\mathcal{S}^{\alpha,\omega} = \mathcal{S}^{\alpha,0} + \sum_{l=1}^{+\infty} \mathcal{S}_l^{\alpha,\omega} \quad \text{and} \quad (\mathcal{K}^{\alpha,\omega})^* = (\mathcal{K}^{\alpha,0})^* + \sum_{l=1}^{+\infty} (\mathcal{K}_l^{-\alpha,\omega})^*.$$

- $(1/2)\, I + (\mathcal{K}^{-\alpha,0})^* : L^2(\partial D) \to L^2(\partial D)$: invertible.

Periodic and quasi-periodic Green's functions

- u and v: α-quasi-periodic smooth functions $\Rightarrow$

$$\int_{\partial Y} \frac{\partial u}{\partial \nu} \overline{v} \, d\sigma = 0.$$

$\Leftarrow$

$$\int_{\partial Y} \frac{\partial u}{\partial \nu} \overline{v} = \int_{\partial Y} \left[\frac{\partial (u e^{-i\alpha \cdot x})}{\partial \nu} + i\alpha \cdot \nu u e^{-i\alpha \cdot x} \right] \overline{e^{-i\alpha \cdot x} v}.$$

Periodic and quasi-periodic Green's functions

- $\phi \in L^2(\partial D)$ satisfy $((1/2)\, I + (\mathcal{K}^{-\alpha,0})^*)[\phi] = 0$ on ∂D.
- If $\alpha = 0$, then $\int_{\partial D} \phi = 0$.
- For $x \in D$

$$\mathcal{D}^{0,0}[1](x) = -\int_{Y\setminus\overline{D}} \Delta_y G^{0,0}(x,y)dy = |Y \setminus \overline{D}|,$$

- $|\ |$: volume.
-

$$(\frac{1}{2} I + \mathcal{K}^{0,0})[1] = |Y \setminus \overline{D}| \quad \text{on } \partial D.$$

$$|Y\setminus\overline{D}| \int_{\partial D} \phi\, d\sigma = \int_{\partial D} (\frac{1}{2} I + \mathcal{K}^{0,0})[1]\, \phi\, d\sigma = \int_{\partial D} (\frac{1}{2} I + (\mathcal{K}^{0,0})^*)[\phi]\, d\sigma = 0.$$

Periodic and quasi-periodic Green's functions

- For any $\alpha \in [0, 2\pi)^2$, $u = \mathcal{S}^{\alpha,0}[\phi]$ is α-quasi-periodic and satisfies $\Delta u = 0$ in $Y \setminus \overline{D}$ with

$$\frac{\partial u}{\partial \nu}\bigg|_+ = (\frac{1}{2}I + (\mathcal{K}^{-\alpha,0})^*)[\phi] = 0 \quad \text{on } \partial D.$$

- $$\int_{Y\setminus\overline{D}} |\nabla u|^2 = \int_{\partial Y} \frac{\partial u}{\partial \nu}\overline{u} - \int_{\partial D} \frac{\partial u}{\partial \nu}\bigg|_+ \overline{u} = 0.$$

- u: constant in $Y \setminus \overline{D}$ and hence in $D \Rightarrow$

$$\phi = \frac{\partial u}{\partial \nu}\bigg|_+ - \frac{\partial u}{\partial \nu}\bigg|_- = 0.$$

Lecture 5: Fundamental results in wave propagation

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Fundamental results in wave propagation

- Reciprocity;
- Lippman-Schwinger representation formula (filtering effect);
- Helmholtz-Kirchhoff Identity (resolution limit);
- Optical theorem (energy conservation);
- Scattering amplitude and scattering coefficients.

Fundamental results in wave propagation

- Reciprocity: Important property satisfied by the outgoing fundamental solution of the Helmholtz equation.
- μ and ε: two piecewise smooth functions s.t. $\mu(x) = \mu_m$ and $\varepsilon(x) = \varepsilon_m$ for $|x| \geq R_0$ for some positive R_0.
- $k_m = \omega\sqrt{\varepsilon_m \mu_m}$; $y \in \mathbb{R}^d$; Fundamental solution $\Phi_{k_m}(x, y)$:

$$(\nabla_x \cdot \frac{1}{\mu(x)} \nabla_x + \omega^2 \varepsilon(x)) \Phi_{k_m}(x, y) = \frac{1}{\mu_m} \delta_y(x),$$

  subject to the Sommerfeld radiation condition:

$$\left| \frac{\partial \Phi_{k_m}}{\partial r} - i k_m \Phi_{k_m} \right| = O\left(r^{-(d+1)/2} \right) \quad \text{as } r = |x| \to +\infty \quad \text{uniformly in } \frac{x}{|x|}.$$

- For $x \neq y$,

$$\Phi_{k_m}(x, y) = \Phi_{k_m}(y, x) \,.$$

Fundamental results in wave propagation

- Reciprocity identity: the wave recorded at x when there is a time-harmonic source at y is equal to the wave recorded at y when there is a time-harmonic source at x.
- Consider the equations satisfied by the fundamental solution with the source at y_2 and with the source at y_1 (with $y_1 \neq y_2$):

$$(\nabla_x \cdot \frac{1}{\mu}\nabla_x + \omega^2 \varepsilon)\Phi_{k_m}(x, y_2) = \frac{1}{\mu_m}\delta_{y_2} \, ,$$
$$(\nabla_x \cdot \frac{1}{\mu}\nabla_x + \omega^2 \varepsilon)\Phi_{k_m}(x, y_1) = \frac{1}{\mu_m}\delta_{y_1} \, .$$

- Multiply the first equation by $\Phi_{k_m}(x, y_1)$ and subtract the second equation multiplied by $\Phi_{k_m}(x, y_2)$:

$$\nabla_x \cdot \frac{\mu_m}{\mu}\Big[\Phi_{k_m}(x, y_1)\nabla_x \Phi_{k_m}(x, y_2) - \Phi_{k_m}(x, y_2)\nabla_x \Phi_{k_m}(x, y_1)\Big]$$
$$= -\Phi_{k_m}(x, y_2)\delta_{y_1} + \Phi_{k_m}(x, y_1)\delta_{y_2}$$
$$= -\Phi_{k_m}(y_1, y_2)\delta_{y_1} + \Phi_{k_m}(y_2, y_1)\delta_{y_2} \, .$$

Fundamental results in wave propagation

- Integrate over the ball B_R of center 0 and radius R which contains both y_1 and y_2 and use the divergence theorem:

$$\int_{\partial B_R} \nu \cdot \Big[\Phi_{k_m}(x, y_1) \nabla_x \Phi_{k_m}(x, y_2) - \Phi_{k_m}(x, y_2) \nabla_x \Phi_{k_m}(x, y_1) \Big] d\sigma(x)$$
$$= -\Phi_{k_m}(y_1, y_2) + \Phi_{k_m}(y_2, y_1)\,;$$

- $\nu = x/|x|$: unit outward normal to the ball B_R.
- If $x \in \partial B_R$ and $R \to \infty$, then by the Sommerfeld radiation condition:

$$\nu \cdot \nabla_x \Phi_{k_m}(x, y) = i k_m \Phi_{k_m}(x, y) + O\Big(\frac{1}{R^{(d+1)/2}} \Big)\,.$$

- $R \to \infty$,

$$-\Phi_{k_m}(y_1, y_2) + \Phi_{k_m}(y_2, y_1)$$
$$= i k_m \int_{\partial B_R} \Big[\Phi_{k_m}(x, y_1) \Phi_{k_m}(x, y_2) - \Phi_{k_m}(x, y_2) \Phi_{k_m}(x, y_1) \Big] d\sigma(x)$$
$$= 0\,.$$

Fundamental results in wave propagation

- Lippmann-Schwinger representation formula for Φ_{k_m}: For any $x \neq y$,

$$\begin{aligned}\Phi_{k_m}(x,y) &= \Gamma_{k_m}(x,y) + \int (\frac{\mu_m}{\mu(z)} - 1)\nabla\Phi_{k_m}(z,x)\cdot\nabla\Gamma_{k_m}(z,y)\,dz \\ &\quad + k_m^2 \int (1 - \frac{\varepsilon(z)}{\varepsilon_m})\Phi_{k_m}(z,x)\Gamma_{k_m}(z,y)\,dz\,.\end{aligned}$$

- $\Gamma_{k_m}(x,y) := \Gamma_{k_m}(x-y)$: fundamental outgoing solution to the Helmholtz operator $\Delta + k_m^2$ in $\mathbb{R}^d$; for $x \neq 0$,

$$\Gamma_{k_m}(x) = \begin{cases} -\dfrac{i}{4} H_0^{(1)}(k_m|x|)\,, & d = 2, \\ -\dfrac{e^{ik_m|x|}}{4\pi|x|}\,, & d = 3, \end{cases}$$

- $H_0^{(1)}$: Hankel function of the first kind of order 0.

Fundamental results in wave propagation

- Multiply
$$(\nabla_x \cdot \frac{1}{\mu(x)} \nabla_x + \omega^2 \varepsilon(x)) \Phi_{k_m}(x,y) = \frac{1}{\mu_m} \delta_y(x),$$
by Γ_{k_m} and subtract the equation satisfied by Γ_{k_m} multiplied by $\frac{1}{\mu_m}\Phi_{k_m}$:
$$\nabla_z \cdot \left[\frac{1}{\mu(z)} \Gamma_{k_m}(z,y) \nabla_z \Phi_{k_m}(z,x) - \frac{1}{\mu_m} \Phi_{k_m}(z,x) \nabla_z \Gamma_{k_m}(z,y) \right]$$
$$= (\frac{1}{\mu(z)} - \frac{1}{\mu_m}) \nabla_z \Phi_{k_m}(z,x) \cdot \nabla_z \Gamma_{k_m}(z,y)$$
$$+ \omega^2 \varepsilon_m (1 - \frac{\varepsilon(z)}{\varepsilon_m}) \Phi_{k_m}(z,x) \Gamma_{k_m}(z,y)$$
$$+ \frac{1}{\mu_m} (\Gamma_{k_m}(x,y) \delta_x(z) - \Phi_{k_m}(x,y) \delta_y(z)) .$$
- Integrate over B_R (with R large enough so that it encloses the support of $\mu - \mu_m$ and $\varepsilon - \varepsilon_m$) and send $R \to +\infty$.
- Divergence theorem + Sommerfeld radiation condition $\Rightarrow$ Lipmann-Schwinger representation formula.

Fundamental results in wave propagation

- Lippmann-Schwinger representation representation formula: basis for expanding the fundamental solution Φ_{k_m} when $\mu \approx \mu_m$ and $\varepsilon \approx \varepsilon_m$.
- Replace Φ_{k_m} in the right-hand side by Γ_{k_m}:

$$\begin{aligned}\Phi_{k_m}(x,y) \quad &\approx \quad \Gamma_{k_m}(x,y) + \int (\frac{\mu_m}{\mu(z)} - 1)\nabla\Gamma_{k_m}(z,y)\cdot\nabla\Gamma_{k_m}(z,x)\,dz \\ &\quad + k_m^2 \int (1 - \frac{\varepsilon(z)}{\varepsilon_m})\Gamma_{k_m}(z,y)\Gamma_{k_m}(z,x)\,dz\,.\end{aligned}$$

- First-order Born approximation for Φ_{k_m}.

Fundamental results in wave propagation

- Helmholtz-Kirchhoff theorem: resolution limit in imaging with waves.
- ∂B_R: sphere of radius R and center 0;

$$\int_{\partial B_R} \left(\frac{\partial \overline{\Gamma_{k_m}}}{\partial \nu}(x,y)\Gamma_{k_m}(z,y) - \overline{\Gamma_{k_m}}(x,y)\frac{\partial \Gamma_{k_m}}{\partial \nu}(z,y) \right) d\sigma(y) = 2i\Im\Gamma_{k_m}(x,z)\,;$$

- Multiply by $\overline{\Gamma_{k_m}}$ the equation satisfied by Γ_{k_m} and integrate by parts.
- Sommerfeld radiation condition $\Rightarrow$

$$\lim_{R\to+\infty}\int_{\partial B_R} \overline{\Gamma_{k_m}}(x,y)\Gamma_{k_m}(z,y)\,d\sigma(y) = -\frac{1}{k_m}\Im\Gamma_{k_m}(x,z)\,.$$

Fundamental results in wave propagation

- Helmholtz-Kirchhoff theorem: valid in inhomogeneous media.
- Outgoing fundamental solution Φ_{k_m}:

$$(\nabla_x \cdot \frac{1}{\mu(x)} \nabla_x + \omega^2 \varepsilon(x)) \Phi_{k_m}(x, y) = \frac{1}{\mu_m} \delta_y(x),$$

  subject to the Sommerfeld radiation condition.
- Helmholtz-Kirchhoff theorem for Φ_{k_m}:

$$\lim_{R \to +\infty} \int_{|y|=R} \overline{\Phi_{k_m}}(x, y) \Phi_{k_m}(z, y)\, d\sigma(y) = -\frac{1}{k_m} \Im\, \Phi_{k_m}(x, z)\,.$$

Fundamental results in wave propagation

- Second Green's identity and Sommerfeld radiation condition.
- Consider

$$
\begin{aligned}
(\nabla_y \cdot \tfrac{1}{\mu} \nabla_y + \omega^2 \varepsilon) \Phi_{k_m}(y, x_2) &= \frac{1}{\mu_m} \delta_{x_2} , \\
(\nabla_y \cdot \tfrac{1}{\mu} \nabla_y + \omega^2 \varepsilon) \Phi_{k_m}(y, x_1) &= \frac{1}{\mu_m} \delta_{x_1} .
\end{aligned}
$$

- Multiply the first equation by $\overline{\Phi_{k_m}}(y, x_1)$ and subtract the second equation multiplied by $\Phi_{k_m}(y, x_2)$:

$$
\begin{aligned}
& \nabla_y \frac{\mu_m}{\mu} \cdot \left[\overline{\Phi_{k_m}}(y, x_1) \nabla_y \Phi_{k_m}(y, x_2) - \Phi_{k_m}(y, x_2) \nabla_y \overline{\Phi_{k_m}}(y, x_1) \right] \\
&\quad = -\Phi_{k_m}(y, x_2) \delta_{x_1} + \overline{\Phi_{k_m}}(y, x_1) \delta_{x_2} \\
&\quad = -\Phi_{k_m}(x_1, x_2) \delta_{x_1} + \overline{\Phi_{k_m}}(x_1, x_2) \delta_{x_2} .
\end{aligned}
$$

Fundamental results in wave propagation

- Use reciprocity property: $\Phi_{k_m}(x_1, x_2) = \Phi_{k_m}(x_2, x_1)$.
- Integrate over the ball B_R and we the divergence theorem:

$$\int_{\partial B_R} \nu \cdot \left[\overline{\Phi_{k_m}}(y, x_1) \nabla_y \Phi_{k_m}(y, x_2) - \Phi_{k_m}(y, x_2) \nabla_y \overline{\Phi_{k_m}}(y, x_1) \right] d\sigma(y)$$
$$= -\Phi_{k_m}(x_1, x_2) + \overline{\Phi_{k_m}}(x_1, x_2) \,.$$

- Green's function also satisfies the Sommerfeld radiation condition:

$$\lim_{|y| \to \infty} |y| \left(\frac{y}{|y|} \cdot \nabla_y - \; ik_m \right) \Phi_{k_m}(y, x_1) = 0 \,,$$

  uniformly in all directions $y/|y|$.
- Substitute $ik_m \Phi_{k_m}(y, x_2)$ for $\nu \cdot \nabla_y \Phi_{k_m}(y, x_2)$ in the surface integral over ∂B_R, and $-ik_m \overline{\Phi_{k_m}}(y, x_1)$ for $\nu \cdot \nabla_y \overline{\Phi_{k_m}}(y, x_1)$ $\Rightarrow$ Helmholtz-Kirchhoff theorem.

Fundamental results in wave propagation

- Resolution: determined by the behavior of the imaginary part of the Green function. Helmholtz-Kirchhoff identity:

$$\Im m\, \Phi_{k_m}(x,z) = k_m \int_{|y|=R} \overline{\Phi_{k_m}(y,z)} \Phi_{k_m}(x,y) d\sigma(y), \quad R \to +\infty.$$

- The sharper is $\Im m\, \Phi_{k_m}$, the better is the resolution.
- Local resonant media used to make sharp peaks of $\Im m\, \Phi_{k_m}$.
  resolution.

Fundamental results in wave propagation

- D: bounded domain in $\mathbb{R}^d$ with smooth boundary ∂D;
- (ε_m, μ_m): pair of electromagnetic parameters (permittivity and permeability) of $\mathbb{R}^2 \setminus \overline{D}$ and (ε_c, μ_c): of D.
- Permittivity and permeability distributions:

$$\varepsilon = \varepsilon_m \chi(\mathbb{R}^d \setminus \overline{D}) + \varepsilon_c \chi(D) \quad \text{and} \quad \mu = \mu_m \chi(\mathbb{R}^d \setminus \overline{D}) + \mu_c \chi(D) \, .$$

- ω: given operating frequency; $k_c = \omega\sqrt{\varepsilon_c \mu_c}$ and $k_m = \omega\sqrt{\varepsilon_m \mu_m}$.
- Incident plane wave $u^{\mathrm{in}}(x) = e^{ik_m \xi \cdot x}$; ξ: unit vector.

Fundamental results in wave propagation

- Transmission problem for the Helmholtz equation:

$$\begin{cases} \nabla \cdot \frac{1}{\mu} \nabla u + \omega^2 \varepsilon u = 0 \quad \text{in } \mathbb{R}^d, \\ u^s := u - u^{\text{in}} \text{ satisfies the Sommerfeld radiation condition,} \end{cases}$$

- Sommerfeld radiation condition:

$$\left| \frac{\partial u^s}{\partial r} - i k_m u^s \right| = O\left(r^{-(d+1)/2} \right) \quad \text{as } r = |x| \to +\infty \quad \text{uniformly in } \frac{x}{|x|}.$$

-

$$\begin{cases} (\Delta + k_m^2) u = 0 \quad \text{in } \mathbb{R}^d \setminus \overline{D}, \\ (\Delta + k_c^2) u = 0 \quad \text{in } D, \\ u|_+ = u|_- \quad \text{on } \partial D, \\ \frac{1}{\mu_m} \frac{\partial u}{\partial \nu}\Big|_+ = \frac{1}{\mu_c} \frac{\partial u}{\partial \nu}\Big|_- \text{on } \partial D, \\ u^s := u - u^{\text{in}} \text{ satisfies the Sommerfeld radiation condition.} \end{cases}$$

Fundamental results in wave propagation

- Integral representation.
- Existence and uniqueness of a solution.
- Scattering coefficients.
- Scattering amplitude.
- Link between the scattering amplitude and scattering coefficients.
- Optical theorem.

Fundamental results in wave propagation

- Integral representation of u:

$$u(x) = \begin{cases} u^{\mathrm{in}}(x) + \mathcal{S}_D^{k_m}[\psi](x), & x \in \mathbb{R}^d \setminus \overline{D}, \\ \mathcal{S}_D^{k_c}[\varphi](x), & x \in D. \end{cases}$$

- Assume that k_m^2 is not a Dirichlet eigenvalue for $-\Delta$ on D.
- Unique solution $(\varphi, \psi) \in L^2(\partial D) \times L^2(\partial D)$:

$$\begin{cases} \mathcal{S}_D^{k_c}[\varphi] - \mathcal{S}_D^{k_m}[\psi] = u^{\mathrm{in}} \\ \displaystyle \frac{1}{\mu_c} \frac{\partial(\mathcal{S}_D^{k_c}[\varphi])}{\partial \nu}\bigg|_- - \frac{1}{\mu_m} \frac{\partial(\mathcal{S}_D^{k_m}[\psi])}{\partial \nu}\bigg|_+ = \frac{1}{\mu_m} \frac{\partial u^{\mathrm{in}}}{\partial \nu} \end{cases} \quad \text{on } \partial D.$$

- There exists a constant $C = C(k_c, k_m, D)$ s.t.

$$\|\varphi\|_{L^2(\partial D)} + \|\psi\|_{L^2(\partial D)} \leq C(\|u^{\mathrm{in}}\|_{L^2(\partial D)} + \|\nabla u^{\mathrm{in}}\|_{L^2(\partial D)}).$$

- C can be chosen scale independent: There exists δ_0 s.t. if one denotes by $(\varphi_\delta, \psi_\delta)$ the solution of the system of integral equations with k_c and k_m respectively replaced by δk_c and δk_m, then

$$\|\varphi_\delta\|_{L^2(\partial D)} + \|\psi_\delta\|_{L^2(\partial D)} \leq C(\|u^{\mathrm{in}}\|_{L^2(\partial D)} + \|\nabla u^{\mathrm{in}}\|_{L^2(\partial D)}).$$

Fundamental results in wave propagation

- Suppose: k_m^2 is not a Dirichlet eigenvalue for $-\Delta$ on D. For each $(F, G) \in H^1(\partial D) \times L^2(\partial D)$, there exists a unique solution $(f, g) \in L^2(\partial D) \times L^2(\partial D)$ to the system of integral equations:

$$\begin{cases} \mathcal{S}_D^{k_c}[f] - \mathcal{S}_D^{k_m}[g] = F \\ \dfrac{1}{\mu_c} \dfrac{\partial(\mathcal{S}_D^{k_c}[f])}{\partial \nu}\Big|_{-} - \dfrac{1}{\mu_m} \dfrac{\partial(\mathcal{S}_D^{k_m}[g])}{\partial \nu}\Big|_{+} = G \end{cases} \quad \text{on } \partial D.$$

  Furthermore, there exists a constant C independent of F and G s.t.

$$\|f\|_{L^2(\partial D)} + \|g\|_{L^2(\partial D)} \leq C\Big(\|F\|_{H^1(\partial D)} + \|G\|_{L^2(\partial D)} \Big).$$

- Proof for $d = 3$ and $\mu_m \neq \mu_c$.

Fundamental results in wave propagation

- Rellich's lemma:
  - $R_0 > 0$ and $B_R = \{|x| < R\}$.
  - v: satisfy the Helmholtz equation $\Delta v + \omega^2 v = 0$ for $|x| > R_0$.
  - $$\lim_{R \to +\infty} \int_{\partial B_R} |v(x)|^2 \, d\sigma(x) = 0.$$
  - Then, $v \equiv 0$ for $|x| > R_0$.
- Rellich's lemma does not hold if ω is imaginary or $\omega = 0$.

Fundamental results in wave propagation

- Uniqueness of a solution to the transmission problem: If u satisfies

$$\begin{cases} \nabla \cdot \dfrac{1}{\mu} \nabla u + \omega^2 \varepsilon u = 0 \quad \text{in } \mathbb{R}^d, \\ u \text{ satisfies the Sommerfeld radiation condition,} \end{cases}$$

  then $u \equiv 0$ in $\mathbb{R}^d$.

- Proof based on Rellich's lemma:
  - $B_R = \{|x| < R\}$; R s.t. $D \subset B_R$.
  - Multiply $\Delta u + \omega^2 u = 0$ by $\overline{u}$ and integrate by parts over $B_R \setminus \overline{D}$,

$$\Im \int_{\partial B_R} \overline{u} \frac{\partial u}{\partial \nu} \, d\sigma = 0.$$

  - $\Rightarrow$

$$\Im \int_{\partial B_R} \overline{u} \left(\frac{\partial u}{\partial \nu} - i\omega u \right) d\sigma = -\omega \int_{\partial B_R} |u|^2.$$

Fundamental results in wave propagation

- Apply the Cauchy–Schwarz inequality,

$$\left| \Im \int_{\partial B_R} \overline{u} \left(\frac{\partial u}{\partial \nu} - i\omega u \right) d\sigma \right| \leq \left(\int_{\partial B_R} |u|^2 \right)^{1/2} \left(\int_{\partial B_R} \left| \frac{\partial u}{\partial \nu} - i\omega u \right|^2 d\sigma \right)^{1/2}.$$

- Use the radiation condition,

$$\left| \Im \int_{\partial B_R} \overline{u} \left(\frac{\partial u}{\partial \nu} - i\omega u \right) d\sigma \right| \leq \frac{C}{R} \left(\int_{\partial B_R} |u|^2 \right)^{1/2},$$

  for some positive constant C independent of R.

- Estimate

$$\left(\int_{\partial B_R} |u|^2 \right)^{1/2} \leq \frac{C}{R},$$

  and Rellich's lemma $\Rightarrow u \equiv 0$ in $\mathbb{R}^d \setminus \overline{B_R}$.

- Unique continuation property for $\Delta + \omega^2 \Rightarrow u \equiv 0$.

Fundamental results in wave propagation

- $X := L^2(\partial D) \times L^2(\partial D)$ and $Y := H^1(\partial D) \times L^2(\partial D)$;
- Define $T : X \to Y$ by

$$T(f,g) := \left(\mathcal{S}_D^{k_c}[f] - \mathcal{S}_D^{k_m}[g], \frac{1}{\mu_c} \frac{\partial(\mathcal{S}_D^{k_c}[f])}{\partial \nu}\bigg|_- - \frac{1}{\mu_m} \frac{\partial(\mathcal{S}_D^{k_m}[g])}{\partial \nu}\bigg|_+ \right).$$

- Define T_0 by

$$T_0(f,g) := \left(\mathcal{S}_D^{0}[f] - \mathcal{S}_D^{0}[g], \frac{1}{\mu} \frac{\partial(\mathcal{S}_D^{0}[f])}{\partial \nu}\bigg|_- - \frac{1}{\mu_m} \frac{\partial(\mathcal{S}_D^{0}[g])}{\partial \nu}\bigg|_+ \right).$$

- $\mathcal{S}_D^{k_0} - \mathcal{S}_D^0 : L^2(\partial D) \to H^1(\partial D)$ and $\frac{\partial}{\partial \nu}\mathcal{S}_D^{k_m}|_\pm - \frac{\partial}{\partial \nu}\mathcal{S}_D^{0}|_\pm : L^2(\partial D) \to L^2(\partial D)$: compact operators.
- $T - T_0$: compact operator from X into Y.
- $T_0 : X \to Y$: invertible: $T_0(f,g) = (F,G)$

$$f = g + (\mathcal{S}_D^0)^{-1}(F)$$

$$g = \frac{\mu_m \mu_c}{\mu_m - \mu_c}(\lambda I + (\mathcal{K}_D^0)^*)^{-1}\left(G + \frac{1}{\mu_c}(\frac{1}{2}I - (\mathcal{K}_D^0)^*)((\mathcal{S}_D^0)^{-1}[F]) \right).$$

- $\lambda = (\mu_c + \mu_m)/(2(\mu_c - \mu_m))$.

Fundamental results in wave propagation

- Invertibility of $\mathcal{S}_D^0$ and $\lambda I + (\mathcal{K}_D^0)^*$ + Fredholm alternative $\Rightarrow$ it is enough to prove that T: injective.
- Suppose that $T(f,g) = 0$. Define u by

$$u(x) := \begin{cases} \mathcal{S}_D^{k_m}[g](x) & \text{if } x \in \mathbb{R}^d \setminus \overline{D}, \\ \mathcal{S}_D^{k_c}[f](x) & \text{if } x \in D. \end{cases}$$

- u satisfies the transmission problem with $u^{\mathrm{in}} = 0 \Rightarrow u \equiv 0$ in $\mathbb{R}^d$.
- $\mathcal{S}_D^{k_m}[g] = 0$ on ∂D.
- $(\Delta + k_m^2)\mathcal{S}_D^{k_m}[g] = 0$ in D and k_m^2 is not a Dirichlet eigenvalue for $-\Delta$ on $D \Rightarrow \mathcal{S}_D^{k_m}[g] = 0$ in D, and hence in $\mathbb{R}^d$.
- Jump relation $\Rightarrow$

$$g = \frac{\partial(\mathcal{S}_D^{k_m}[g])}{\partial \nu}\bigg|_+ - \frac{\partial(\mathcal{S}_D^{k_m}[g])}{\partial \nu}\bigg|_- = 0 \quad \text{on } \partial D.$$

- On the other hand, $\mathcal{S}_D^{k_c} f$ satisfies $(\Delta + k_c^2)\mathcal{S}_D^{k_c}[f] = 0$ in $\mathbb{R}^d \setminus \overline{D}$ and $\mathcal{S}_D^{k_c}[f] = 0$ on ∂D.
- $\mathcal{S}_D^{k_c}[f] = 0 \Rightarrow f = 0$.

Fundamental results in wave propagation

- Graf's addition formula:

$$H_0^{(1)}(k|x-y|) = \sum_{l\in\mathbb{Z}} H_l^{(1)}(k|x|)e^{il\theta_x} J_l(k|y|)e^{-il\theta_y} \quad \text{for } |x| > |y|;$$

- $x = (|x|, \theta_x)$ and $y = (|y|, \theta_y)$ in polar coordinates;
- $H_l^{(1)}$: Hankel function of the first kind of order l and J_l: Bessel function of order l.
- Asymptotic formula as $|x| \to \infty$:

$$u(x) - u^{\mathrm{in}}(x) = -\frac{i}{4} \sum_{l\in\mathbb{Z}} H_l^{(1)}(k_m|x|)e^{il\theta_x} \int_{\partial D} J_l(k_m|y|)e^{-il\theta_y} \psi(y) d\sigma(y) \,.$$

Fundamental results in wave propagation

- $(\varphi_{l'}, \psi_{l'}) \in L^2(\partial D) \times L^2(\partial D)$: solution of the system of integral equations on ∂D:

$$\begin{cases} \mathcal{S}_D^{k_c}[\varphi_{l'}] - \mathcal{S}_D^{k_m}[\psi_{l'}] = J_{l'}(k_m|x|)e^{il'\theta_x}, \\ \dfrac{1}{\mu_c}\dfrac{\partial(\mathcal{S}_D^{k_c}[\varphi_{l'}])}{\partial \nu}\Big|_- - \dfrac{1}{\mu_m}\dfrac{\partial(\mathcal{S}_D^{k_m}[\psi_{l'}])}{\partial \nu}\Big|_+ = \dfrac{1}{\mu_m}\dfrac{\partial(J_{l'}(k_m|x|)e^{il'\theta_x})}{\partial \nu}. \end{cases}$$

- Scattering coefficients $W_{ll'}$, $l, l' \in \mathbb{Z}$:

$$W_{ll'} = W_{ll'}[\varepsilon, \mu, \omega] := \int_{\partial D} J_l(k_m|y|)e^{-il\theta_y}\psi_{l'}(y)d\sigma(y).$$

Fundamental results in wave propagation

- Exponential decay of the scattering coefficients: There is a constant C depending on $(\varepsilon, \mu, \omega)$ s.t.

$$|W_{ll'}[\varepsilon, \mu, \omega]| \leq \frac{C^{|l|+|l'|}}{|l|^{|l|}|l'|^{|l'|}} \quad \text{for all } l, l' \in \mathbb{Z} \setminus \{0\}\,.$$

- As $l' \to \infty$,

$$J_{l'}(t) \sim \frac{(-1)^{l'}}{\sqrt{2\pi|l'|}}\left(\frac{et}{2|l'|}\right)^{|l'|}.$$

- From

$$\|u^{\mathrm{in}}\|_{L^2(\partial D)} + \|\nabla u^{\mathrm{in}}\|_{L^2(\partial D)} \leq \frac{C^{|l'|}}{|l'|^{|l'|}}$$

for some constant C $\Rightarrow$

$$\|\psi_{l'}\|_{L^2(\partial D)} \leq \frac{C^{|l'|}}{|l'|^{|l'|}}$$

for another constant C.

Fundamental results in wave propagation

- Completeness relation for cylindrical waves $\{J_n(k_m|y|)e^{-in\theta_y}\}_n$:

$$\frac{\delta_0(r-r_0)\delta_0(\theta-\theta_0)}{r} = \sum_{l'\in\mathbb{Z}} \frac{1}{2\pi} \int_0^{+\infty} t J_{l'}(tr) J_{l'}(tr_0)\, dt\; e^{il'(\theta-\theta_0)}.$$

- Jacobi-Anger expansion of plane waves: $x = (|x|, \theta_x)$ and $\xi = (|\xi|, \theta_\xi)$ in the polar coordinates,

$$e^{ik_m \xi\cdot x} = \sum_{l'\in\mathbb{Z}} e^{il'(\frac{\pi}{2}-\theta_\xi)} J_{l'}(k_m|x|) e^{il'\theta_x}.$$

- $|x| \to \infty$,

$$u(x) - e^{ik_m\xi\cdot x} = -\frac{i}{4} \sum_{l\in\mathbb{Z}} H_l^{(1)}(k_m|x|) e^{il\theta_x} \sum_{l'\in\mathbb{Z}} W_{ll'} e^{il'(\frac{\pi}{2}-\theta_\xi)}.$$

Fundamental results in wave propagation

- $W_{ll'}$: scattering coefficients, $\xi = (\cos\theta_\xi, \sin\theta_\xi)$, and $x = (|x|, \theta_x)$, $|x| \to \infty$,

$$u(x) - e^{ik_m \xi\cdot x} = -\frac{i}{4}\sum_{l\in\mathbb{Z}} H_l^{(1)}(k_m|x|)e^{il\theta_x}\sum_{l'\in\mathbb{Z}} W_{ll'}\, e^{il'(\frac{\pi}{2}-\theta_\xi)} .$$

- Far-field pattern $A_\infty[\varepsilon,\mu,\omega]$: $|x| \to \infty$,

$$u(x) - e^{ik_m\xi\cdot x} = -ie^{-\frac{\pi i}{4}}\frac{e^{ik_m|x|}}{\sqrt{|x|}} A_\infty[\varepsilon,\mu,\omega](\theta_\xi,\theta_x) + o(|x|^{-\frac{1}{2}}) .$$

- θ and θ': respectively the incident and scattered direction,

$$A_\infty[\varepsilon,\mu,\omega](\theta,\theta') = \sum_{l,l'\in\mathbb{Z}} i^{(l'-l)} e^{il\theta'} W_{ll'}[\varepsilon,\mu,\omega]e^{-il'\theta} .$$

- Scattering coefficients: basically the Fourier coefficients of the far-field pattern.

Fundamental results in wave propagation

- As $t \to \infty$,

$$H_0^{(1)}(t) \sim \sqrt{\frac{2}{\pi t}} e^{i(t-\frac{\pi}{4})}.$$

- $|x|$: large while $|y|$: bounded,

$$|x-y| = |x| - |y|\cos(\theta_x - \theta_y) + O(\frac{1}{|x|}).$$

- $|x| \to \infty$,

$$H_0^{(1)}(k_m|x-y|) \sim e^{-\frac{\pi i}{4}} \sqrt{\frac{2}{\pi k_m |x|}} e^{ik_m(|x|-|y|\cos(\theta_x-\theta_y))}.$$

- $|x| \to \infty$,

$$u(x) - e^{ik_m \xi\cdot x} \sim -ie^{-\frac{\pi i}{4}} \frac{e^{ik_m|x|}}{\sqrt{8\pi k_m |x|}} \int_{\partial D} e^{-ik_m|y|\cos(\theta_x-\theta_y)} \psi(y)\, d\sigma(y)$$

- $$A_\infty[\varepsilon,\mu,\omega](\theta_\xi,\theta_x) = \frac{1}{\sqrt{8\pi k_m}} \int_{\partial D} e^{-ik_m|y|\cos(\theta_x-\theta_y)} \psi(y)\, d\sigma(y),$$

Fundamental results in wave propagation

- Fourier series of $A_\infty[\varepsilon, \mu, \omega](\theta_\xi, \cdot)$:

$$A_\infty[\varepsilon, \mu, \omega](\theta_\xi, \theta_x) = \sum_{l \in \mathbb{Z}} b_l(\theta_\xi) e^{il\theta_x}.$$

-

$$\begin{aligned} b_l(\theta_\xi) &= \frac{1}{2\pi} \int_0^{2\pi} \int_{\partial D} e^{-ik_m|y|\cos(\theta_x - \theta_y)} \psi(y)\, d\sigma(y)\, e^{-il\theta_x}\, d\theta_x \\ &= \frac{1}{2\pi} \int_{\partial D} \int_0^{2\pi} e^{-ik_m|y|\cos(\theta_x - \theta_y)} e^{-il\theta_x}\, d\theta_x\, \psi(y)\, d\sigma(\theta_y)\,. \end{aligned}$$

- From

$$\frac{1}{2\pi} \int_0^{2\pi} e^{-ik_m|y|\cos(\theta_x - \theta_y)} e^{-il\theta_x}\, d\theta_x = J_l(k_m|y|) e^{-il(\theta_y + \frac{\pi}{2})},$$

- $\Rightarrow$

$$b_l(\theta_\xi) = \int_{\partial D} J_l(k_m|y|) e^{-il(\theta_y + \frac{\pi}{2})} \psi(y)\, d\sigma(\theta_y)\,.$$

Fundamental results in wave propagation

- Scattering cross-section: $\theta' \in [0, 2\pi]$,

$$Q^{\mathrm{s}}[\varepsilon,\mu,\omega](\theta') := -\frac{i}{2k_m}\int_{\partial B_R} [\overline{u}^s(x)\nabla u^s(x) - u^s(x)\nabla\overline{u}^s(x)]\,;$$

- Q^{s} satisfies

$$Q^{\mathrm{s}}[\varepsilon,\mu,\omega](\theta') = \int_0^{2\pi} \Big| A_\infty[\varepsilon,\mu,\omega](\theta,\theta') \Big|^2 \, d\theta\,.$$

- Absorption cross-section: $\theta' \in [0, 2\pi]$,

$$Q^{\mathrm{a}}[\varepsilon,\mu,\omega](\theta') := \frac{i}{2}\int_{\partial B_R} [\overline{u}(x)\nabla u(x) - u(x)\nabla\overline{u}(x)]\,;$$

- Extinction cross-section: $\theta' \in [0, 2\pi]$,

$$Q^{\mathrm{ext}}[\varepsilon,\mu,\omega](\theta') := Q^{\mathrm{a}}[\varepsilon,\mu,\omega](\theta') + Q^{\mathrm{s}}[\varepsilon,\mu,\omega](\theta').$$

- Extinction cross-section Q^{ext}: ratio of the sum of the mean powers absorbed and scattered by D to the mean intensity power flow in the incident field.

Fundamental results in wave propagation

- Optical theorem ($d = 2$): $\theta' \in [0, 2\pi]$,

$$\Im A_\infty[\varepsilon, \mu, \omega](\theta', \theta') = -\sqrt{\frac{k_m}{8\pi}} Q^{\mathrm{ext}}[\varepsilon, \mu, \omega](\theta') \,.$$

- $\omega \mapsto A_\infty[\varepsilon, \mu, \omega]$: analytic in $\mathbb{C}^+$, A_∞ vanishes sufficiently rapidly as $\omega \to +\infty$;
- $A_\infty[\varepsilon, \mu, -\omega] = \overline{A_\infty[\varepsilon, \mu, \omega]}$ for real values of ω;
- Real and imaginary parts of the scattering amplitude are connected by the Kramers-Kronig relations:

$$\Re A_\infty[\varepsilon, \mu, \omega](\xi, \xi) = c_d \, \mathrm{p.v.} \int_0^{+\infty} \frac{(\omega')^{(d+1)/2} Q^{\mathrm{ext}}[\varepsilon, \mu, \omega'](\xi)}{(\omega')^2 - \omega^2} \, d\omega' \,,$$

$$Q^{\mathrm{ext}}[\varepsilon, \mu, \omega](\xi) = -\frac{2}{\pi \sqrt{\varepsilon_m \mu_m}} \, \mathrm{p.v.} \int_0^{+\infty} \frac{\Re A_\infty[\varepsilon, \mu, \omega'](\xi, \xi)}{(\omega')^2 - \omega^2} \, d\omega' \,,$$

- $\xi \in \mathbb{R}^2, |\xi| = 1$; $c_2 = -\sqrt{\sqrt{\varepsilon_m \mu_m}/(2\pi^3)}$.

Fundamental results in wave propagation

- Limits as $\omega \to 0 \Rightarrow$ sum rules:

$$\Re A_\infty[\varepsilon, \mu, 0](\xi, \xi) = c_2 \, \mathrm{p.v.} \int_0^{+\infty} (\omega')^{-1/2} Q^{\mathrm{ext}}[\varepsilon, \mu, \omega'](\xi) \, d\omega' \,,$$

$$Q^{\mathrm{ext}}[\varepsilon, \mu, 0](\xi) = -\frac{2}{\pi\sqrt{\varepsilon_m \mu_m}} \, \mathrm{p.v.} \int_0^{+\infty} \frac{\Re A_\infty[\varepsilon, \mu, \omega'](\xi, \xi) - \Re A_\infty[\varepsilon, \mu, 0](\xi, \xi)}{(\omega')^2} \, d\omega' \,.$$

Fundamental results in wave propagation

- $Q^a = 0$ (non absorbing scatterers): $\theta' \in [0, 2\pi]$,

$$\Im \sum_{l,l' \in \mathbb{Z}} i^{l'-l} e^{i(l-l')\theta'} W_{ll'}[\varepsilon, \mu, \omega]$$

$$= -\sqrt{\frac{\pi k_m}{2}} \sum_{l' \in \mathbb{Z}} \left| \sum_{l \in \mathbb{Z}} i^{-l} W_{ll'}[\varepsilon, \mu, \omega] e^{il\theta'} \right|^2 .$$

Lecture 6: Scalar wave scattering by small particles

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Scalar wave scattering by small particles

- D: bounded smooth domain in $\mathbb{R}^d$.
- μ and ε: piecewise constant functions s.t. $\mu(x) = \mu_m$ and $\varepsilon(x) = \varepsilon_m$ for $x \in \mathbb{R}^d \setminus \overline{D}$ and $\mu(x) = \mu_c$ and $\varepsilon(x) = \varepsilon_c$ for $x \in D$.
- $\mu_m, \varepsilon_m, \mu_c,$ and ε_c: positive.
- $k_m = \omega\sqrt{\varepsilon_m \mu_m}$ and $k_c = \omega\sqrt{\varepsilon_c \mu_c}$.
- Transmission problem for the Helmholtz equation:

$$\begin{cases} \nabla \cdot \dfrac{1}{\mu}\nabla u + \omega^2 \varepsilon u = 0 \quad \text{in } \mathbb{R}^d, \\ u^s := u - u^{\mathrm{in}} \text{ satisfies the Sommerfeld radiation condition.} \end{cases}$$

- u^{in}: incident wave.
- Sommerfeld radiation condition:

$$\left| \frac{\partial u^s}{\partial r} - i k_m u^s \right| = O\left(r^{-(d+1)/2} \right) \quad \text{as } r = |x| \to +\infty \quad \text{uniformly in } \frac{x}{|x|}.$$

Scalar wave scattering by small particles

- Equivalent form:

$$\begin{cases} (\Delta + k_m^2)u = 0 \quad \text{in } \mathbb{R}^d \setminus \overline{D}, \\ (\Delta + k_c^2)u = 0 \quad \text{in } D, \\ u|_+ = u|_- \quad \text{on } \partial D, \\ \frac{1}{\mu_m}\frac{\partial u}{\partial \nu}|_+ = \frac{1}{\mu_c}\frac{\partial u}{\partial \nu}|_- \text{on } \partial D, \\ u^s := u - u^{\mathrm{in}} \text{ satisfies the Sommerfeld radiation condition.} \end{cases}$$

- Uniqueness result: $u^{\mathrm{in}} = 0 \Rightarrow u \equiv 0$ in $\mathbb{R}^d$.

Scalar wave scattering by small particles

- k_m^2: not a Dirichlet eigenvalue for $-\Delta$ on D.
- u can be represented using the single-layer potentials $\mathcal{S}_D^{k_m}$ and $\mathcal{S}_D^{k_c}$:

$$u(x) = \begin{cases} u^{\mathrm{in}}(x) + \mathcal{S}_D^{k_m}[\psi](x), & x \in \mathbb{R}^d \setminus \overline{D}, \\ \mathcal{S}_D^{k_c}[\varphi](x), & x \in D; \end{cases}$$

- $(\varphi, \psi) \in L^2(\partial D) \times L^2(\partial D)$: unique solution to

$$\begin{cases} \mathcal{S}_D^{k_c}[\varphi] - \mathcal{S}_D^{k_m}[\psi] = u^{\mathrm{in}} \\ \dfrac{1}{\mu_c} \dfrac{\partial (\mathcal{S}_D^{k_c}[\varphi])}{\partial \nu}\bigg|_- - \dfrac{1}{\mu_m} \dfrac{\partial (\mathcal{S}_D^{k_m}[\psi])}{\partial \nu}\bigg|_+ = \dfrac{1}{\mu_m} \dfrac{\partial u^{\mathrm{in}}}{\partial \nu} \end{cases} \quad \text{on } \partial D.$$

Scalar wave scattering by small particles

- $D = \delta B + z$; $\delta \to 0$.
- Asymptotic expansion of u as $\delta \to 0$.
- Consider $d = 3$.
- There exists $\delta_0 > 0$ s.t. for all $\delta \leq \delta_0$, there exists a constant C independent of δ s.t.

$$\|\varphi\|_{L^2(\partial D)} + \|\psi\|_{L^2(\partial D)} \leq C\left(\delta^{-1}\|u^{\mathrm{in}}\|_{L^2(\partial D)} + \|\nabla u^{\mathrm{in}}\|_{L^2(\partial D)}\right).$$

Scalar wave scattering by small particles

- Proof:
    - Scaling $x = z + \delta y \Rightarrow$

$$\begin{cases} \mathcal{S}_B^{k_c\delta}[\varphi_\delta] - \mathcal{S}_B^{k_m\delta}[\psi_\delta] = \dfrac{1}{\delta} u_\delta^{\mathrm{in}} \\ \dfrac{1}{\mu_c} \dfrac{\partial(\mathcal{S}_B^{k_c\delta}[\varphi_\delta])}{\partial \nu}\Big|_- - \dfrac{1}{\mu_m} \dfrac{\partial(\mathcal{S}_B^{k_m\delta}[\psi_\delta])}{\partial \nu}\Big|_+ = \dfrac{1}{\delta \mu_m} \dfrac{\partial u_\delta^{\mathrm{in}}}{\partial \nu} \end{cases} \quad \text{on } \partial B;$$

    - $\varphi_\delta(y) = \varphi(z + \delta y)$, $y \in \partial B$, *etc*;
    - $\mathcal{S}_B^{k_c\delta}$ and $\mathcal{S}_B^{k_m\delta}$: associated to the fundamental solutions $\Gamma_{k_c\delta}$ and $\Gamma_{k_m\delta}$, respectively.
    - For δ small enough:

$$\|\varphi_\delta\|_{L^2(\partial B)} + \|\psi_\delta\|_{L^2(\partial B)} \leq C\delta^{-1} \|u_\delta^{\mathrm{in}}\|_{H^1(\partial B)};$$

    - C independent of δ.

Scalar wave scattering by small particles

- Fix $n \in \mathbb{N}$.
- Define

$$u_n^{\mathrm{in}}(x) = \sum_{|l|=0}^{n} \frac{\partial^l u^{\mathrm{in}}(z)}{l!}(x-z)^l \, .$$

- (φ_n, ψ_n): unique solution of

$$\begin{cases} \mathcal{S}_D^{k_c}[\varphi_n] - \mathcal{S}_D^{k_m}[\psi_n] = u_{n+1}^{\mathrm{in}} \\ \frac{1}{\mu_c} \frac{\partial(\mathcal{S}_D^{k_c}[\varphi_n])}{\partial \nu}\Big|_- - \frac{1}{\mu_m} \frac{\partial(\mathcal{S}_D^{k_m}[\psi_n])}{\partial \nu}\Big|_+ = \frac{1}{\mu_m} \frac{\partial u_{n+1}^{\mathrm{in}}}{\partial \nu} \end{cases} \quad \text{on } \partial D.$$

- $(\varphi - \varphi_n, \psi - \psi_n)$: unique solution with the right-hand sides defined by $u^{\mathrm{in}} - u_{n+1}^{\mathrm{in}}$.

Scalar wave scattering by small particles

- $$\|\varphi - \varphi_n\|_{L^2(\partial D)} + \|\psi - \psi_n\|_{L^2(\partial D)} \leq C\left(\delta^{-1}\|u^{\rm in} - u^{\rm in}_{n+1}\|_{L^2(\partial D)} + \|\nabla(u^{\rm in} - u^{\rm in}_{n+1})\|_{L^2(\partial D)}\right).$$
- Definition of $u^{\rm in}_{n+1} \Rightarrow$
$$\|u^{\rm in} - u^{\rm in}_{n+1}\|_{L^2(\partial D)} \leq C|\partial D|^{1/2}\|u^{\rm in} - u^{\rm in}_{n+1}\|_{L^\infty(\partial D)} \leq C|\partial D|^{1/2}(\delta k_m)^{n+2},$$
and
$$\|\nabla(u^{\rm in} - u^{\rm in}_{n+1})\|_{L^2(\partial D)} \leq C|\partial D|^{1/2}(\delta k_m)^{n+1}.$$
- $\Rightarrow$
$$\|\varphi - \varphi_n\|_{L^2(\partial D)} + \|\psi - \psi_n\|_{L^2(\partial D)} \leq C(k_m)|\partial D|^{1/2}\delta^{n+1}.$$
- Representation formula $\Rightarrow$
$$u(x) = u^{\rm in}(x) + \mathcal{S}_D^{k_m}[\psi_n](x) + \mathcal{S}_D^{k_m}[\psi - \psi_n](x), \quad x \in K \Subset \mathbb{R}^d \setminus \overline{D}.$$

Scalar wave scattering by small particles

- $\text{dist}(D, K) \geq c_0 \Rightarrow$

$$\sup_{x \in K,\ y \in \partial D} \left| \Gamma_{k_m}(x - y) \right| \leq C$$

  for some constant C.

- For $x \in K$,

$$\left| \mathcal{S}_D^{k_m}[\psi - \psi_n](x) \right| \leq \left[\int_{\partial D} |\Gamma_{k_m}(x-y)|^2 \, d\sigma(y) \right]^{1/2} \|\psi - \psi_n\|_{L^2(\partial D)}$$

$$\leq C |\partial D|^{1/2} |\partial D|^{1/2} \delta^{n+1} \leq C' \delta^{n+d} \,;$$

- C and C': independent of $x \in K$ and δ.

-
$$u(x) = u^{\mathrm{in}}(x) + \mathcal{S}_D^{k_m}[\psi_n](x) + O(\delta^{n+d}) \,, \quad \text{uniformly in } x \in K \,.$$

Scalar wave scattering by small particles

- For l: multi-index, define (φ_l, ψ_l): unique solution to

$$\begin{cases} \mathcal{S}_B^{k_c\delta}[\varphi_l] - \mathcal{S}_B^{k_m\delta}[\psi_l] = x^l \\ \dfrac{1}{\mu_c}\dfrac{\partial(\mathcal{S}_B^{k_c\delta}[\varphi_l])}{\partial\nu}\Big|_- - \dfrac{1}{\mu_m}\dfrac{\partial(\mathcal{S}_B^{k_m\delta}[\psi_l])}{\partial\nu}\Big|_+ = \dfrac{1}{\mu_m}\dfrac{\partial x^l}{\partial\nu} \end{cases} \quad \text{on } \partial B\,.$$

- For $x \in \partial D$,

$$\mathcal{S}_D^{k_m}\left[\sum_{|l|=0}^{n+1}\delta^{|l|-1}\frac{\partial^l u^{\mathrm{in}}(z)}{l!}\varphi_l(\delta^{-1}(\cdot - z))\right](x)$$
$$= \sum_{|l|=0}^{n+1}\delta^{|l|}\frac{\partial^l u^{\mathrm{in}}(z)}{l!}(\mathcal{S}_B^{k_m\delta}[\varphi_l])(\delta^{-1}(x-z))\,;$$

- $\Rightarrow \varphi_n(x) = \sum_{|l|=0}^{n+1}\delta^{|l|-1}\frac{\partial^l u^{\mathrm{in}}(z)}{l!}\varphi_l(\delta^{-1}(x-z))$ and

$$\psi_n(x) = \sum_{|l|=0}^{n+1}\delta^{|l|-1}\frac{\partial^l u^{\mathrm{in}}(z)}{l!}\psi_l(\delta^{-1}(x-z))\,.$$

Scalar wave scattering by small particles

- $\Rightarrow$ uniformly in $x \in K$,

$$u(x) = u^{\mathrm{in}}(x) + \sum_{|l|=0}^{n+1} \delta^{|l|-1} \frac{\partial^l u^{\mathrm{in}}(z)}{l!} \mathcal{S}_D^{k_m}[\psi_l(\delta^{-1}(\cdot - z))](x) + O(\delta^{n+d}).$$

- $$\mathcal{S}_D^{k_m}[\psi_l(\delta^{-1}(\cdot - z))](x) = \int_{\partial D} \Gamma_{k_m}(x-y)\psi_l(\delta^{-1}(y-z))\, d\sigma(y) = \delta^{d-1} \int_{\partial B} \Gamma_{k_m}(x - (\delta w + z))\psi_l(w)\, d\sigma(w).$$

- For $x \in K$, $z \in D$, $w \in \partial B$, and sufficiently small δ:

$$\Gamma_{k_m}(x - (\delta w + z)) = \sum_{|l'|=0}^{\infty} \frac{\delta^{|l'|}}{l'!} \partial_z^{l'} \Gamma_{k_m}(x-z) w^{l'}.$$

- $\Rightarrow$

$$\mathcal{S}_D^{k_m}[\psi_l(\delta^{-1}(\cdot - z))](x) = \sum_{|l'|=0}^{\infty} \frac{\delta^{|l'|+d-1}}{l'!} \partial_z^{l'} \Gamma_{k_m}(x-z) \int_{\partial B} w^{l'} \psi_l(w)\, d\sigma(w).$$

Scalar wave scattering by small particles

- For multi-indices l and l' in $\mathbb{N}^d$, scattering tensors:

$$\widetilde{W}_{ll'} := \int_{\partial B} w^{l'} \psi_l(w)\, d\sigma(w)\,.$$

- Pointwise multipolar expansion in $K \Subset \mathbb{R}^d \setminus \overline{D}$:

$$u(x) = u^{\mathrm{in}}(x) + \delta^{d-2} \sum_{|l'|=0}^{n+1} \sum_{|l|=0}^{n-|l'|+1} \frac{\delta^{|l|+|l'|}}{l!l'!} \partial^l u^{\mathrm{in}}(z) \partial_z^{l'} \Gamma_{k_m}(x-z) \widetilde{W}_{ll'} + O(\delta^{n+d})\,;$$

- Remainder $O(\delta^{d+n})$: dominated by $C\delta^{d+n}$ for some C independent of $x \in K$.

Scalar wave scattering by small particles

- ψ_l and $\widetilde{W}_{ll'}$: depend on δ.
- Scattering tensors: basic building blocks for the full asymptotic expansion as $\delta \to 0$ of the scattering coefficients

$$W_{ll'} := \int_{\partial D} J_l(k_m|y|)e^{-il\theta_y}\psi_{l'}(y)d\sigma(y)\,.$$

- Scaling + Taylor expansions: For $p, q \in \mathbb{N}$,

$$W_{pq} = \frac{1}{k_m} \sum_{l,l' \in \mathbb{N}^3} \widetilde{W}_{ll'} \frac{(\delta k_m)^{|l|+|l'|+1}}{l!l'!} \partial^l \left[J_p(y)e^{ip\theta_y}\right]\Big|_{y=0} \partial^{l'} \left[J_q(y)e^{iq\theta_y}\right]\Big|_{y=0}.$$

Scalar wave scattering by small particles

- Expansion of $\widetilde{W}_{ll'}$ as $\delta \to 0$:
  - Introduce

$$T_\delta \begin{bmatrix} f \\ g \end{bmatrix} := \begin{bmatrix} \mathcal{S}_B^{k_c\delta}[f] - \mathcal{S}_B^{k_m\delta}[g] \\ \frac{1}{\mu_c}\frac{\partial(\mathcal{S}_B^{k_c\delta}[f])}{\partial\nu}\Big|_- - \frac{1}{\mu_m}\frac{\partial(\mathcal{S}_B^{k_m\delta}[g])}{\partial\nu}\Big|_+ \end{bmatrix} \text{ on } \partial B\,;$$

  - T_0 for $\delta = 0$.
  - (φ_l, ψ_l):

$$\begin{bmatrix} \varphi_l \\ \psi_l \end{bmatrix} = \Big[I + T_0^{-1}(T_\delta - T_0)\Big]^{-1} T_0^{-1} \begin{bmatrix} x^l \\ \frac{1}{\mu_m}\frac{\partial x^l}{\partial\nu} \end{bmatrix}.$$

Scalar wave scattering by small particles

- Expand $T_\delta - T_0$ in a power series of $\delta \Rightarrow (\widehat{\varphi}_l, \widehat{\psi}_l)$ leading-order term in the expansion of (φ_l, ψ_l):

$$\begin{cases} \mathcal{S}_B^0[\widehat{\varphi}_l] - \mathcal{S}_B^0[\widehat{\psi}_l] = x^l \\ \displaystyle \frac{1}{\mu_c} \frac{\partial(\mathcal{S}_B^0[\widehat{\varphi}_l])}{\partial \nu}\bigg|_- - \frac{1}{\mu_m} \frac{\partial(\mathcal{S}_B^0[\widehat{\psi}_l])}{\partial \nu}\bigg|_+ = \frac{1}{\mu_m} \frac{\partial x^l}{\partial \nu} \end{cases} \quad \text{on } \partial B\,.$$

- Take $n = 1$: find the leading-order term in the asymptotic expansion of $u - u^{\mathrm{in}}$ as $\delta \to 0$.
- Dependence of $\widetilde{W}_{ll'}$ on δ for $|l| \leq 1$ and $|l'| \leq 1$.

Scalar wave scattering by small particles

- $|l| \leq 1$:

$$\mathcal{S}_B^0[\widehat{\varphi}_l] - \mathcal{S}_B^0[\widehat{\psi}_l] = x^l \quad \text{in } B\,.$$

- $\Rightarrow$

$$\frac{\partial(\mathcal{S}_B^0[\widehat{\varphi}_l])}{\partial \nu}\bigg|_- - \frac{\partial(\mathcal{S}_B^0[\widehat{\psi}_l])}{\partial \nu}\bigg|_- = \frac{\partial x^l}{\partial \nu} \quad \text{on } \partial B\,.$$

- $\Rightarrow$

$$\frac{\mu_c}{\mu_m}\frac{\partial(\mathcal{S}_B^0[\widehat{\psi}_l])}{\partial \nu}\bigg|_+ - \frac{\partial(\mathcal{S}_B^0[\widehat{\psi}_l])}{\partial \nu}\bigg|_- = \left(1 - \frac{\mu_c}{\mu_m}\right)\frac{\partial x^l}{\partial \nu}\,.$$

- $(\mathcal{K}_B^0)^*$: Neumann–Poincaré operator,

$$\frac{\mu_c}{\mu_m}\left(\frac{1}{2}I + (\mathcal{K}_B^0)^*\right)[\widehat{\psi}_l] - \left(-\frac{1}{2}I + (\mathcal{K}_B^0)^*\right)[\widehat{\psi}_l] = \left(1 - \frac{\mu_c}{\mu_m}\right)\frac{\partial x^l}{\partial \nu}\,.$$

- $\Rightarrow$

$$\widehat{\psi}_l = (\lambda I - (\mathcal{K}_B^0)^*)^{-1}\left(\frac{\partial x^l}{\partial \nu}\bigg|_{\partial B}\right);$$

- Permeability contrast:

$$\lambda := \frac{\frac{\mu_m}{\mu_c} + 1}{2(\frac{\mu_m}{\mu_c} - 1)}\,.$$

Scalar wave scattering by small particles

- $|l| = 0$: $\widehat{\psi}_l = 0$ and $\mathcal{S}_B^0[\widehat{\varphi}_l] = 1$.
- $\Rightarrow \psi_l = O(\delta)$ and $\mathcal{S}_B^{k_c\delta}[\varphi_l] = 1 + O(\delta)$.
- $\mathcal{S}_B^{k_c\delta}[\varphi_l]$: depends on δ analytically $+$ $(\Delta + k_c^2\delta^2)\mathcal{S}_B^{k_c\delta}[\varphi_l] = 0$ in $B \Rightarrow$

$$\psi_l = O(\delta) \quad \text{and} \quad \mathcal{S}_B^{k_c\delta}[\varphi_l] = 1 + O(\delta^2)\,, \quad |l| = 0\,.$$

- $|l| = |l'| = 1$:

$$\widetilde{W}_{ll'} = \int_{\partial B} x^{l'} (\lambda I - (\mathcal{K}_B^0)^*)^{-1} \left(\frac{\partial y^l}{\partial \nu} \bigg|_{\partial B} \right)(x)\, d\sigma(x) + O(\delta)\,.$$

- Polarization tensor $M = (m_{pq})_{p,q=1}^3$:

$$m_{pq} := \int_{\partial B} y_q (\lambda I - (\mathcal{K}_B^0)^*)^{-1} [\nu_p](y)\, d\sigma(y);$$

- $\nu = (\nu_1, \ldots, \nu_3)$.

Scalar wave scattering by small particles

- $$\widetilde{W}_{ll'} = M + O(\delta)\,, \quad |l| = |l'| = 1\,.$$

- $l = 0$ or $l' = 0$:

$$\psi_l = \frac{\partial(\mathcal{S}_B^{k_m\delta}[\psi_l])}{\partial\nu}\Big|_+ - \frac{\partial(\mathcal{S}_B^{k_m\delta}[\psi_l])}{\partial\nu}\Big|_-$$
$$= \frac{\mu_m}{\mu_c}\frac{\partial(\mathcal{S}_B^{k_c\delta}[\varphi_l])}{\partial\nu}\Big|_- - \frac{\partial x^l}{\partial\nu} - \frac{\partial(\mathcal{S}_B^{k_m\delta}[\psi_l])}{\partial\nu}\Big|_-\,.$$

- Divergence theorem $\Rightarrow$

$$\int_{\partial B} x^{l'}\psi_l\,d\sigma = -k_c^2\delta^2\frac{\mu_m}{\mu_c}\int_B x^{l'}\mathcal{S}_B^{k_c\delta}[\varphi_l]\,dx + k_m^2\delta^2\int_B x^{l'}\mathcal{S}_B^{k_m\delta}[\psi_l]\,dx$$
$$+ \frac{\mu_m}{\mu_c}\int_{\partial B}\frac{\partial x^{l'}}{\partial\nu}\mathcal{S}_B^{k_c\delta}[\varphi_l]\,d\sigma - \int_{\partial B}\frac{\partial x^{l'}}{\partial\nu}\mathcal{S}_B^{k_m\delta}[\psi_l]\,d\sigma\,.$$

Scalar wave scattering by small particles

- $$\widetilde{W}_{ll'} = -k_c^2 \delta^2 \frac{\mu_m}{\mu_c} |B| + O(\delta^3) = -\delta^2 \omega^2 \varepsilon_c \mu_m |B| + O(\delta^3)\,, \quad |l| = |l'| = 0\,,$$
$$\widetilde{W}_{ll'} = O(\delta^2)\,, \quad |l| = 1\,,\ |l'| = 0\,,$$
$$\widetilde{W}_{ll'} = O(\delta^2)\,, \quad |l| = 0\,,\ |l'| = 1\,.$$

- $$\mathcal{S}_D^{k_m}[\psi](x) = O(\delta^d)\,, \quad \text{uniformly on } x \in K\,.$$

- $|l| = 2$ and $|l'| = 0$:
$$\int_{\partial B} \psi_l \, d\sigma = -\int_B \Delta x^l \, dx + O(\delta^2)\,.$$

- $|l'| = 0$:
$$\sum_{|l|=2} \frac{1}{l! l'!} \partial^l u^{\mathrm{in}}(z) \widetilde{W}_{ll'} = -\Delta u^{\mathrm{in}}(z)|B| + O(\delta^2) = k_m^2 u^{\mathrm{in}}(z)|B| + O(\delta^2)\,.$$

Scalar wave scattering by small particles

- Dipolar approximation: For any $x \in K$,

$$u(x) = u^{\mathrm{in}}(x)$$
$$+ \delta^d \left(\nabla u^{\mathrm{in}}(z) M \nabla_z \Gamma_{k_m}(x-z) + k_m^2 (\frac{\varepsilon_c}{\varepsilon_m} - 1)|B| u^{\mathrm{in}}(z) \Gamma_{k_m}(x-z) \right)$$
$$+ O(\delta^{d+1});$$

- M: polarization tensor.

Scalar wave scattering by small particles

- Several well-separated particles: $D := \cup_{s=1}^m (\delta B_s + z_s)$.
- There exists a positive constant C such that $|z_s - z_{s'}| \geq C$ for $s \neq s'$.
- Magnetic permeability and electric permittivity of the particle $\delta B_s + z_s$: $\mu_c^{(s)}$ and $\varepsilon_c^{(s)}$, $s = 1, \ldots, m$.
- Pointwise asymptotic expansion in K:

$$u(x) = u^{\mathrm{in}}(x)$$

$$+\delta^{d-2} \sum_{s=1}^{m} \sum_{|l'|=0}^{n+1} \sum_{|l|=0}^{n+1-|l'|} \frac{\delta^{|l|+|l'|}}{l!l'!} \partial^l u^{\mathrm{in}}(z_s) \partial_z^{l'} \Gamma_{k_m}(x - z_s) W_{ll'}^{(s)} + O(\delta^{n+d}) .$$

- $W_{ll'}^{(s)}$: scattering tensor.

Scalar wave scattering by small particles

- Closely spaced small particles:
  - $D := \cup_{s=1}^m (\delta B_s + z)$.
  - First-order dipolar expansion.
  - Overall polarization tensor of multiple particles $M = (m_{pq})_{p,q=1}^d$:

$$m_{pq} := \sum_{s=1}^m \int_{\partial B_s} x_p \phi_q^{(s)}(x)\, d\sigma(x).$$

Scalar wave scattering by small particles

- $\phi_q^{(s)}$: solution to the system of m equations

$$(\lambda_s I - (\mathcal{K}_{B_s}^0)^*)[\phi_q^{(s)}] - \sum_{s' \neq s} \frac{\partial \mathcal{S}_{B_{s'}}^0[\phi_q^{(s')}]}{\partial \nu^{(s)}} = \nu_q^{(s)} \quad \text{on } \partial B_s;$$

- λ_s: magnetic contrast associated to $\mu_c^{(s)}$.
- For any $x \in K$, as $\delta \to 0$,

$$u(x) = u^{\mathrm{in}}(x) + \delta^d \Big(\nabla u^{\mathrm{in}}(z) M \nabla_z \Gamma_{k_m}(x-z) + k_m^2 \big(\sum_{s=1}^{m} (\frac{\varepsilon_c^{(s)}}{\varepsilon_m} - 1)|B_s| \big) u^{\mathrm{in}}(z) \Gamma_{k_m}(x-z) \Big) + O(\delta^{d+1}).$$

Lecture 7: Imaging

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Imaging

- Direct Imaging of Small Particles:
  - Detect and localize small particles from multi-static measurements.
  - Multistatic imaging:
    - Record the waves generated by the particles on an array of receivers.
    - Process the recorded data in order to estimate some relevant features of the particles.
  - Small-volume asymptotic formulas.
  - Direct (non-iterative) reconstruction algorithms: MUltiple Signal Classification algorithm (MUSIC), reverse-time migration, and Kirchhoff migration.

Imaging

- Resolution and stability with respect to noise in the measurements:
  - Resolution analysis: estimate the size of the finest detail that can be reconstructed
  - Stability analysis is to quantify the localization error in the presence of noise.

Imaging

- Multistatic imaging:
  - $B_R := \{|x| < R\}$; D: small particle with location at $z \in B_R$ and material parameters ε_c and μ_c.
  - $x_i, i = 1, \ldots, N$: equi-distributed points along ∂B_R for $N \gg 1$.
  - Array of N elements $\{x_1, \ldots, x_N\}$: used to detect the particle.
  - $\{x_1, \ldots, x_N\}$: operating both in transmission and in reception.
  - u_j^s: scattered wave by D corresponding to the incident wave $\Gamma_{k_m}(x - x_j)$.
  - Small-volume expansion:

$$u_j^s(x) = \delta^d \Bigg(\nabla_z \Gamma_{k_m}(z - x_j) M \nabla_z \Gamma_{k_m}(x - z)$$

$$+ k_m^2 (\frac{\varepsilon_c}{\varepsilon_m} - 1) |B| \Gamma_{k_m}(z - x_j) \Gamma_{k_m}(x - z) \Bigg) + O(\delta^{d+1});$$

  - M: polarization tensor associated with the magnetic contrast μ_c / μ_m.

Imaging

- MUSIC-type Method:
  - Multistatic response matrix: $A^\omega := \left(u_j^s(x_i)\right)_{i,j=1}^N$.
  - D: disk.
  - N-dimensional vector fields $g^{(j)}(z^S)$, for $z^S \in B_R$ and $j = 1, \ldots, d$,

$$g^{(j)}(z^S) = \frac{1}{\sqrt{\sum_{i=1}^N |e_j \cdot \nabla_z \Gamma_{k_m}(z^S - x_i)|^2}} \times \left(e_j \cdot \nabla_z \Gamma_{k_m}(z^S - x_1), \ldots, e_j \cdot \nabla_z \Gamma_{k_m}(z - x_N) \right)^t,$$

$$g^{(d+1)}(z^S) = \frac{1}{\sqrt{\sum_{i=1}^N |\Gamma_{k_m}(z^S - x_i)|^2}} \times \left(\Gamma_{k_m}(z^S - x_1), \ldots, \Gamma_{k_m}(z^S - x_N) \right)^t.$$

  - t: transpose; $\{e_1, \ldots, e_d\}$: orthonormal basis of $\mathbb{R}^d$.

Imaging

- $g(z^S)$: $N \times d$ matrix whose columns are $g^{(1)}(z^S), \ldots, g^{(d)}(z^S)$.
- $$A^\omega \approx \tau_\mu g(z)\overline{g(z)}^t + \tau_\varepsilon g^{(d+1)}(z)\overline{g^{(d+1)}(z)}^t \, ;$$
- $$\tau_\mu := 2|D| \frac{\mu_m - \mu_c}{\mu_m + \mu_c} \Big(\sum_{i=1}^N |\nabla_z \Gamma_{k_m}(z - x_i)|^2 \Big) \, ,$$
  $$\tau_\varepsilon := |D| k_m^2 \big(\frac{\varepsilon_c}{\varepsilon_m} - 1 \big) \Big(\sum_{i=1}^N |\Gamma_{k_m}(z - x_i)|^2 \Big) \, .$$
- P: orthogonal projection onto the range of A^ω.
- MUSIC algorithm functional:
  $$\mathcal{I}_{\mathrm{MU}}(z^S, \omega) := \Big(\sum_{j=1}^{d+1} \|(I - P)[g^{(j)}](z^S)\|^2 \Big)^{-1/2} .$$
- $\mathcal{I}_{\mathrm{MU}}$: large peaks only at the locations of the particles.

Imaging

- Backpropagation-type imaging functional: For $z^S \in B_R$,

$$\mathcal{I}_{\rm BP}(z^S,\omega) := \sum_{j=1}^{d+1} u_j^s(x_j)\overline{g^{(j)}(z^S)} \cdot g^{(j)}(z^S)\,.$$

- For sufficiently large N,

$$\frac{1}{N}\sum_{j=1}^{N} \overline{\Gamma_{k_m}}(x_j - z^S)\Gamma_{k_m}(x_j - z^S) \sim \Im\Gamma_{k_m}(z - z^S),$$

$$\frac{1}{N}\sum_{j=1}^{N} \nabla_z\overline{\Gamma_{k_m}}(x_j - z^S)\cdot\nabla_z\Gamma_{k_m}(x_j - z^S)^t \sim \Im\Gamma_{k_m}(z - z^S)\,\frac{z - z^S}{|z - z^S|}\Big(\frac{z - z^S}{|z - z^S|}\Big)^t.$$

- $$\mathcal{I}_{\rm BP}(z^S,\omega) \sim \begin{cases} \mathrm{sinc}(k_m|z - z^S|) & \text{for } d = 3\,, \\ J_0(k_m|z - z^S|) & \text{for } d = 2. \end{cases}$$

- Resolution: of the order of half the wavelength $2\pi/k_m$.

Imaging

- $\mathcal{I}_{\mathrm{BP}}$: uses only the diagonal terms of the response matrix A^ω.
- Kirchhoff migration functional:

$$\mathcal{I}_{\mathrm{KM}}(z^S, \omega) = \sum_{j=1}^{d+1} \overline{g^{(j)}(z^S)} \cdot A^\omega g^{(j)}(z^S) \,.$$

Imaging

- Suppose that $\mu_c = \mu_m$:

$$A^\omega = \tau_\varepsilon g^{(d+1)}(z)\overline{g^{(d+1)}(z)}^t.$$

- $\mathcal{I}_{\mathrm{MU}}$: nonlinear function of $\mathcal{I}_{\mathrm{KM}}$;

$$\mathcal{I}_{\mathrm{KM}}(z^S,\omega) = \tau_\varepsilon \left(1 - \mathcal{I}_{\mathrm{MU}}^{-2}(z^S,\omega)\right).$$

- In the presence of measurement noise (additive measurement noise with variance $k_m^2\sigma_{\mathrm{noise}}^2$):

$$A^\omega = \tau_\varepsilon g^{(d+1)}(z)\overline{g^{(d+1)}(z)}^t + \sigma_{\mathrm{noise}} k_m W;$$

- W: complex symmetric Gaussian matrix with mean zero and variance 1.

Imaging

- $\mathbb{E}$ and Var: the mean and the variance.
- Signal-to-Noise Ratio (SNR) of $\mathcal{I}_{\mathrm{KM}}$:

$$\mathrm{SNR}(\mathcal{I}_{\mathrm{KM}}) = \frac{\mathbb{E}[\mathcal{I}_{\mathrm{KM}}(z,\omega)]}{\mathrm{Var}(\mathcal{I}_{\mathrm{KM}}(z,\omega))^{1/2}}\,.$$

- $$\mathrm{SNR}(\mathcal{I}_{\mathrm{KM}}) = \frac{\tau_\varepsilon}{k_m \sigma_{\mathrm{noise}}}\,.$$
- For the MUSIC algorithm, the peak of $\mathcal{I}_{\mathrm{MU}}$ is affected by measurement noise:

$$\mathcal{I}_{\mathrm{MU}}(z,\omega) = \begin{cases} \dfrac{|\tau_\varepsilon|}{\sigma_{\mathrm{noise}}} & \text{if } \tau_\varepsilon \gg \sigma_{\mathrm{noise}}, \\ 1 & \text{if } |\tau_\varepsilon| \ll k_m \sigma_{\mathrm{noise}}\,. \end{cases}$$

Imaging

- Joint sparse recovery.
- Lippmann-Schwinger representation of u_j^s:

$$u_j^s(x) = \int_D \left((\frac{1}{\mu_c} - \frac{1}{\mu_m}) \nabla_y \Gamma_{k_m}(x-y) \cdot \nabla_z u_j^s(y) + k_m^2 (\frac{\varepsilon_c}{\varepsilon_m} - 1) \Gamma_{k_m}(x-y) u_j^s(y) \right) dy,$$

- Approximate ∇u_j^s and u_j^s in the search domain Ω^S by either piecewise constant functions or splines:

$$\nabla u_j^s(y) = \begin{bmatrix} \sum_{l=1}^L \alpha_{l,j}^{(1)} \phi^{(1)}(y, y_l) \\ \vdots \\ \sum_{l=1}^L \alpha_{l,j}^{(d)} \phi^{(d)}(y, y_l) \end{bmatrix},$$

and

$$u_j^s(y) = \sum_{l=1}^L \alpha_{l,j}^{(d+1)} \phi^{(d+1)}(y, y_l).$$

- $\{y_l\}_{l=1}^L$, for some $L \in \mathbb{N}$, finite sampling points of Ω^S and $\phi^{(n)}(y, y_l)$: basis function of the nth coordinate with $n \in \{1, \ldots, d+1\}$.

Imaging

- Data matrix:

$$A^\omega = [S^{(1)}, \ldots, S^{(d+1)}] \begin{bmatrix} (\alpha_{l,j}^{(1)})_{l,j} \\ \vdots \\ (\alpha_{l,j}^{(d+1)})_{l,j} \end{bmatrix}.$$

- Sensing matrix $S = [S^{(1)}, \ldots, S^{(d+1)}]$:

$$(S^{(n)})_{i,l} = (\frac{1}{\mu_c} - \frac{1}{\mu_m}) \int_{\Omega^S} (\nabla_y \Gamma_{k_m}(x_i - y) \cdot e_n) \phi^{(n)}(y, y_l) dy$$

for $n = 1, \ldots, d$, and

$$(S^{(d+1)})_{i,l} = k_m^2 (\frac{\varepsilon_c}{\varepsilon_m} - 1) \int_{\Omega^S} \Gamma_{k_m}(x_i - y) \phi^{(d+1)}(y, y_l) dy.$$

Imaging

- $X = \begin{bmatrix} (\alpha_{l,j}^{(1)})_{l,j} \\ \vdots \\ (\alpha_{l,j}^{(d+1)})_{l,j} \end{bmatrix}$.
- Pairwise joint sparsity: $(\alpha_{l,j}^{(1)}), \ldots, (\alpha_{l,j}^{(d+1)})$ are nonzero at the rows corresponding to the particle's location.
- Joint sparse recovery problem:

$$\min_X \|X\|_0 \quad \text{subject to } \|A^\omega - SX\|_F^2 \leq \eta.$$

- $\|X\|_0$: number of rows that have nonzero elements in the matrix X; η: small regularization parameter; $\| \ \|_F$: Frobenius norm.

Imaging

- Super-resolution imaging
- Inverse source problems:

$$\begin{cases} \Delta u + k^2 n(x) u = f, \\ u \text{ satisfies the Sommerfeld radiation condition.} \end{cases}$$

- $n(x)$: refractive index; $n-1$: compactly supported in a bounded domain $D \Subset \mathbb{R}^d$ for $d = 2, 3$; assumed to be known.
- Image from the scattered field u in the far-field f in $L^2(D)$ or finite number of point sources supported in D.
- Outgoing fundamental solution $\Phi_k(x,y)$:

$$\begin{cases} \Delta_x \Phi_k(x,y) + k^2 n(x) \Phi_k(x,y) = \delta_y(x), \\ \Phi_k \text{ satisfies the Sommerfeld radiation condition.} \end{cases}$$

- Integral representation:

$$u(x) = K_D[f](x) := \int_D \Phi_k(x,y) f(y)\, dy.$$

Imaging

- Inverse source problem of reconstructing f from u at a fixed frequency: ill-posed for general sources.
- Methods of reconstructing f from u:
  - Time reversal based method;
  - Minimum L^2-norm solution;
  - Minimum L^1-norm solution.

Imaging

- Time reversal based method:

$$\mathcal{I}_{\rm TR}(x) := \int_{\partial B_R} \overline{\Phi_k(x,z)} u(z)\, ds(z) = K_D^* K_D[f](x),$$

- $K_D^* : L^2(\partial B_R) \mapsto L^2(D)$: adjoint of $K_D : L^2(D) \mapsto L^2(\partial B_R)$.
- K_D^*: time-reversing the observed field.
- Helmholtz-Kirchhoff identity $\Rightarrow$ resolution:

$$\mathcal{I}_{\rm TR}(x) \approx -\frac{1}{k} \int_D \Im \Phi_k(x,y) f(y)\, dy.$$

- f: point source $\Rightarrow$ resolution limited by $\Im \Phi_k(x,y)$.

Imaging

- Minimum L^2-norm solution:
- $f \in L^2(D)$,

$$\min \|g\|_{L^2(D)} \text{ subject to } \quad K_D[g] = u.$$

- Relaxation in the presence of noise:

$$\min \|g\|_{L^2(D)} \text{ subject to } \quad \|K_D[g] - u\|^2_{L^2(\Gamma)} < \delta;$$

- $\delta > 0$: given small regularization parameter.
- Singular value decomposition $K_D : L^2(D) \to L^2(\Gamma)$:

$$K_D = \sum_{l \geq 0} \sigma_l P_l;$$

- σ_l: lth singular value and P_l is the associated projection.
- Ill-posedness of the inverse source problem $\Leftarrow$ fast decay of the singular values to zero.

Imaging

- Minimum L^2-norm solution:

$$I(x) = \sum_{l \geq 0} \frac{P_l^* P_l}{\sigma_l^2} K_D^* K_D[f](x).$$

- Regularized solution:

$$I_\alpha(x) = \sum_{l \geq 0} \frac{P_l^* P_l}{\sigma_l^2 + \alpha} K_D^* K_D[f](x),$$

- α: function of δ; chosen by Morozov's discrepancy principle.

Imaging

- Minimum L^1-norm solution:
- f: superposition of separate point sources.
- Minimization problem:

$$\min \|g\|_{L^1(D)} \text{ subject to } K_D^* K_D[g] = K_D^*[u].$$

- Relaxed minimization problem:

$$\min \|g\|_{L^1(D)} \text{ subject to } \|K_D^* K_D[g] - K_D^*[u]\|_{L^2(\Gamma)}^2 < \delta.$$

Imaging

- Case of homogeneous medium
- $n \equiv 1$; $d = 3$:

$$\Phi_k(x,y) = \Gamma_k(x-y) = -\frac{e^{ik|x-y|}}{4\pi|x-y|}.$$

- Far-field: $k|y| = O(1)$ and $k|x| \gg 1 \Rightarrow |x-y| \approx |x| - \hat{x}\cdot y$, $\hat{x} = \frac{x}{|x|} \Rightarrow$

$$u(x) = -\int_D \frac{e^{ik|x-y|}}{4\pi|x-y|} f(y)\, dy \approx -\frac{e^{ik|x|}}{4\pi|x|}\hat{f}(k\hat{x});$$

- $\hat{f}$: Fourier transform of f.
- Measurements on ∂B_R:

$$u(x) = -\frac{e^{ikR}}{4\pi R}\hat{f}(k\hat{x}).$$

- Time-reversal method $\Rightarrow$

$$\mathcal{I}_{\mathrm{TR}}(z) \approx \frac{1}{16\pi^2 R^2}\int_{\partial B_R}\int_D e^{ik\hat{x}\cdot(y-z)} f(y)\, dy\, ds(x) = \frac{1}{4\pi}\int_D f(y)\frac{\sin k|z-y|}{k|z-y|}\, dy.$$

Imaging

- Green function in high-contrast media.
- $k = 1$; Helmholtz equation with a delta source term:

$$\Delta_x \Phi(x, x_0) + \Phi(x, x_0) + \tau n(x)\chi(D)(x)\Phi(x, x_0) = \delta(x - x_0) \quad \text{in } \mathbb{R}^d,$$

- $\chi(D)$: characteristic function of D; $n(x) \in \mathcal{C}^1(\overline{D})$: positive function of order one and $\tau \gg 1$: contrast.
- $\Phi_0(x, x_0)$: free-space Green's function $\Gamma_1(x - x_0)$.
- Write $\Phi = v + \Phi_0$,

$$\Delta v + v = -\tau n(x)\chi(D)(v + \Phi_0).$$

- $\Rightarrow$

$$v(x, x_0) = -\tau \int_D n(y)\Phi_0(x, y)\Big(v(y, x_0) + \Phi_0(y, x_0)\Big)\, dy.$$

Imaging

- Define

$$K_D[f](x) := -\int_D n(y)\Phi_0(x,y)f(y)\,dy.$$

- $v = v(x) = v(x, x_0)$ satisfies the integral equation:

$$(I - \tau K_D)[v] = \tau K_D[\Phi(\cdot, x_0)];$$

- $\Rightarrow$

$$v(x) = (\frac{1}{\tau} - K_D)^{-1} K_D[\Phi(\cdot, x_0)].$$

Imaging

- Properties of the integral operator K_D:
  - K_D: compact from $L^2(D)$ to $L^2(D)$ $\Leftarrow$ K_D: bounded from $L^2(D)$ to $H^2(D)$.
  - K_D: Hilbert-Schmidt operator.

Imaging

- Spectrum $\sigma(K_D)$ of K_D:
  - $\sigma(K_D) = \{0, \lambda_1, \lambda_2, \ldots, \lambda_n, \ldots\}$;
  - $|\lambda_1| \geq |\lambda_2| \geq |\lambda_3| \geq \ldots$ and $\lambda_n \to 0$;
  - $\{0\} = \sigma(K_D) \backslash \sigma_p(K_D)$; $\sigma_p(K_D)$: point spectrum of K_D.
- $\lambda \in \sigma(K_D)$ iff there is a non-trivial solution in $H^2_{\mathrm{loc}}(\mathbb{R}^d)$ to

$$\begin{cases} (\Delta + 1)u(x) = \frac{1}{\lambda} n(x)u(x) \quad \text{in } D, \\ (\Delta + 1)u = 0 \quad \text{in } \mathbb{R}^d \backslash D, \\ u \text{ satisfies the Sommerfeld radiation condition.} \end{cases}$$

- $\mathcal{H}_j$: generalized eigenspace of the operator K_D for the eigenvalue λ_j,

$$L^2(D) = \overline{\bigcup_{j=1}^{\infty} \mathcal{H}_j}.$$

- For $|\lambda| < 1$: resonant modes have sub-wavelength structures in D and can propagate into the far-field $\Rightarrow$ super-resolution.

Imaging

- Jordan theory applied to $K_D|_{\mathcal{H}_j} : \mathcal{H}_j \to \mathcal{H}_j$ on the finite dimensional space $\mathcal{H}_j \Rightarrow$
  - There exists a basis $\{u_{j,l,k}\}$, $1 \leq l \leq m_j, 1 \leq k \leq n_{j,l}$ for $\mathcal{H}_j$ s.t.

$$K_D(u_{j,1,1}, \ldots, u_{j,m_j,n_{j,m_j}}) = (u_{j,1,1}, \ldots, u_{j,m_j,n_{j,m_j}}) \begin{pmatrix} J_{j,1} & & \\ & \ddots & \\ & & J_{j,m_j} \end{pmatrix};$$

  - $J_{j,l}$: canonical Jordan matrix of size $n_{j,l}$

$$J_{j,l} = \begin{pmatrix} \lambda_j & 1 & & \\ & \ddots & \ddots & \\ & & \lambda_j & 1 \\ & & & \lambda_j \end{pmatrix}.$$

Imaging

- $\Gamma = \{(j,l,k) \in \mathbb{N} \times \mathbb{N} \times \mathbb{N}; 1 \leq l \leq m_j, 1 \leq k \leq n_{j,l}\}$: set of indices for the basis functions.
- Gram-Schmidt orthonormalization:
  - There exists an orthonormal basis $\{e_\gamma : \gamma \in \Gamma\}$ for $L^2(D)$ s.t.

$$e_\gamma = \sum_{\gamma' \preceq \gamma} a_{\gamma,\gamma'} u_{\gamma'};$$

  - $a_{\gamma,\gamma'}$: constants;
  - $a_{\gamma,\gamma} \neq 0$.

Imaging

- $A = \{a_{\gamma,\gamma'}\}_{\gamma,\gamma' \in \Gamma}$: viewed as a matrix.
- A: upper-triangular and has non-zero diagonal elements.
- $B = \{b_{\gamma,\gamma'}\}_{\gamma,\gamma' \in \Gamma}$ inverse of A: upper-triangular and has non-zero diagonal elements.
- $$u_\gamma = \sum_{\gamma' \preceq \gamma} b_{\gamma,\gamma'} e_{\gamma'}.$$
- $\{e_\gamma(x)\overline{e_{\gamma'}(y)}\}$ form a normal basis for the Hilbert space $L^2(D \times D)$.
- Completeness relation:

$$\delta_y(x) = \sum_\gamma e_\gamma(x)\overline{e_\gamma(y)}.$$

Imaging

- $\Phi(x, x_0) \in L^2(D \times D)$ for fixed $\tau \Rightarrow$
$$\Phi(x, x_0) = \sum_{\gamma,\gamma'} \alpha_{\gamma,\gamma'} e_\gamma(x)\overline{e_{\gamma'}}(x_0),$$
for some constants $\alpha_{\gamma,\gamma'}$:
$$\sum_{\gamma,\gamma'} |\alpha_{\gamma,\gamma'}|^2 = \|\Phi(x, x_0)\|^2_{L^2(D\times D)} < \infty.$$
- Analyze the Green function $\Phi \Leftarrow$ find the constants $\alpha_{\gamma,\gamma'}$.
- $$\Phi_0(x, x_0) = \frac{1}{n(x_0)} K_D[\delta(\cdot - x_0)].$$
- $$\begin{aligned}\Phi(x, x_0) &= \Phi_0(x, x_0) + (\frac{1}{\tau} - K_D)^{-1} K_D^2[\delta(\cdot - x_0)] \\ &= \Phi_0(x, x_0) + \frac{1}{n(x_0)} \sum_\gamma \overline{e_\gamma}(x_0)(\frac{1}{\tau} - K_D)^{-1} K_D^2[e_\gamma].\end{aligned}$$
- Compute $(\frac{1}{\tau} - K_D)^{-1} K_D^2[e_\gamma]$.

Imaging

- For $z \notin \sigma(K_D)$ ($z = 1/\mu$),

  $$(z - K_D)^{-1}[u_{j,l,k}] = \frac{1}{z - \lambda_j} u_{j,l,k} + \frac{1}{(z - \lambda_j)^2} u_{j,l,k-1} + \ldots + \frac{1}{(z - \lambda_j)^k} u_{j,l,1}.$$

- $$(z - K_D)^{-1} K_D^2 [u_{j,l,k}] = \sum_{\gamma'} d_{\gamma,\gamma'} u_{\gamma'}.$$

- Expansion of $\Phi(x, x_0)$ in the orthonormal basis $\{e_\gamma\}_{\gamma \in \Gamma}$:

  $$\Phi(x, x_0) = \Phi_0(x, x_0) + \sum_{\gamma \in \Gamma} \sum_{\gamma''' \in \Gamma} \alpha_{\gamma,\gamma'''} \overline{e_\gamma}(x_0) e_{\gamma'''}(x);$$

- $$\alpha_{\gamma,\gamma'''} = \frac{1}{n(x_0)} \sum_{\gamma' \preceq \gamma} \sum_{\gamma'' \preceq \gamma'} a_{\gamma,\gamma'} d_{\gamma',\gamma''} b_{\gamma'',\gamma'''}.$$

- For $\tau^{-1} \in I \Subset \mathbb{R} \setminus \big(\mathbb{R} \cap \sigma(K_D)\big)$, uniform bound:

  $$\sum_{\gamma,\gamma'} |\alpha_{\gamma,\gamma'}|^2 < \infty.$$

Imaging

- Expansion of $\Phi(x, x_0)$ in the basis of resonant modes $\{u_\gamma\}_{\gamma \in \Gamma}$:

$$\Phi(x, x_0) = \Phi_0(x, x_0) + \sum_{\gamma'' \in \Gamma} \sum_{\gamma''' \preceq \gamma''} \sum_{\gamma \preceq \gamma''} \beta_{\gamma'', \gamma, \gamma'''} u_\gamma(x) \overline{u_{\gamma'''}}(x_0);$$

- $$\beta_{\gamma'', \gamma, \gamma'''} = \frac{1}{n(x_0)} \sum_{\gamma' \preceq \gamma''} \bar{a}_{\gamma'', \gamma'''} a_{\gamma'', \gamma'} d_{\gamma', \gamma}.$$

- In $L^2(D \times D)$:

$$\lim_{\gamma_0 \to \infty} \sum_{\gamma'' \leq \gamma_0} \sum_{\gamma' \preceq \gamma''} \sum_{\gamma''' \preceq \gamma''} \beta_{\gamma'', \gamma, \gamma'''} u_\gamma(x) \overline{u_{\gamma'''}}(x_0) = \Phi(x, x_0) - \Phi_0(x, x_0).$$

Imaging

- Expansion of $\Phi_0(x, x_0)$ in the orthonormal basis $\{e_\gamma\}_{\gamma\in\Gamma}$:

$$\Phi_0(x, x_0) = \sum_{\gamma\in\Gamma} \sum_{\gamma'''\in\Gamma} \tilde{\alpha}_{\gamma,\gamma'''} \overline{e_\gamma}(x_0) e_{\gamma'''}(x),$$

- $$\tilde{\alpha}_{\gamma,\gamma'''} = \frac{1}{n(x_0)} \sum_{\gamma'\preceq\gamma} \sum_{\gamma''\preceq\gamma'} a_{\gamma,\gamma'} h_{\gamma',\gamma''} b_{\gamma'',\gamma'''}.$$

- Uniform bound:

$$\sum_{\gamma,\gamma'} |\tilde{\alpha}_{\gamma,\gamma'}|^2 < C < \infty.$$

- Expansions of $\Phi_0(x, x_0)$ in the basis of resonant modes $\{u_\gamma\}_{\gamma\in\Gamma}$:

$$\Phi_0(x, x_0) = \sum_{\gamma''\in\Gamma} \sum_{\gamma'''\preceq\gamma''} \sum_{\gamma\preceq\gamma''} \tilde{\beta}_{\gamma'',\gamma,\gamma'''} u_\gamma(x) \overline{u_{\gamma'''}}(x_0);$$

- $$\tilde{\beta}_{\gamma'',\gamma,\gamma'''} = \frac{1}{n(x_0)} \sum_{\gamma'\preceq\gamma''} \bar{a}_{\gamma'',\gamma'''} a_{\gamma'',\gamma'} h_{\gamma',\gamma}.$$

Imaging

- Resonance expansions of the Green functions in high-contrast media and in the free space $\Rightarrow$ explanation for the super-resolution phenomenon.
- Difference between the coefficients $\beta_{\gamma'',\gamma,\gamma'''}$ and $\tilde{\beta}_{\gamma'',\gamma,\gamma'''}$: quantities $d_{\gamma,\gamma'}$ and $h_{\gamma,\gamma'}$ ($a_{\gamma'',\gamma'}$ are constants).
- If $\mathcal{H}_j$ are of dimension one:

$$d_{\gamma,\gamma'} = \delta_{\gamma,\gamma'} \frac{\lambda_j^2}{z - \lambda_j}, \quad h_{\gamma,\gamma'} = \delta_{\gamma,\gamma'} \lambda_j,$$

- $\Rightarrow$

$$d_{\gamma,\gamma'} = \frac{1}{\frac{1}{\mu \lambda_j} - 1} h_{\gamma,\gamma'}.$$

- $\Rightarrow$ Contribution to the Green function Φ of the sub-wavelength resonant mode u_γ is amplified when $1/\tau$: close to λ_j.

Imaging

- Imaginary part of Φ: sharper peak than that of Φ_0 due to the excited sub-wavelength resonant modes.
- When the high contrast is properly chosen, one or several of these sub-wavelength resonance modes can be excited, and they dominate over the other ones in the expansion of the Green function Φ.
- It is those sub-wavelength modes that essentially determine the behavior of Φ and hence the associated resolution in the medium.
- Super-resolution occurs in this case.

Lecture 8: Maxwell's equations

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Maxwell's equations

- Layer potential formulation for electromagnetic scattering.
- Helmholtz-Kirchhoff theorem.
- Optical theorem.
- Scattering by small particles.

Maxwell's equations

- D: bounded, simply connected, and of class $\mathcal{C}^{1,\eta}$ for $\eta > 0$;
- Scattering problem of a time-harmonic electromagnetic wave incident on D.
- D: electric permittivity ε_c and magnetic permeability μ_c;
- Homogeneous medium: electric permittivity ε_m and magnetic permeability μ_m;
- $$k_m = \omega\sqrt{\varepsilon_m \mu_m}, \quad k_c = \omega\sqrt{\varepsilon_c \mu_c},$$
  and
  $$\varepsilon_D = \varepsilon_m \chi(\mathbb{R}^3 \setminus \overline{D}) + \varepsilon_c \chi(D), \quad \mu_D = \varepsilon_m \chi(\mathbb{R}^3 \setminus \overline{D}) + \varepsilon_c \chi(D).$$

Maxwell's equations

- Given incident plane wave $(E^{\text{in}}, H^{\text{in}})$, solution to the Maxwell equations in free space

$$\begin{cases} \nabla \times E^{\text{in}} &= i\omega\mu_m H^{\text{in}} \quad \text{in } \mathbb{R}^3, \\ \nabla \times H^{\text{in}} &= -i\omega\varepsilon_m E^{\text{in}} \quad \text{in } \mathbb{R}^3. \end{cases}$$

- Scattering problem:

$$\begin{cases} \nabla \times E &= i\omega\mu_D H \quad \text{in } \mathbb{R}^3 \setminus \partial D, \\ \nabla \times H &= -i\omega\varepsilon_D E \quad \text{in } \mathbb{R}^3 \setminus \partial D, \\ \nu \times E\big|_+ - \nu \times E\big|_- &= \nu \times H\big|_+ - \nu \times H\big|_- = 0 \quad \text{on } \partial D; \end{cases}$$

- Silver-Müller radiation condition:

$$\lim_{|x|\to\infty} |x| \left(\sqrt{\mu_m}(H - H^{\text{in}})(x) \times \frac{x}{|x|} - \sqrt{\varepsilon_m}(E - E^{\text{in}})(x) \right) = 0$$

uniformly in $x/|x|$.

Maxwell's equations

- Dyadic Green (matrix valued) function for the full Maxwell equations:

$$\mathbf{G}_{k_m}(x) = \varepsilon_m \left(\Gamma_{k_m}(x) I + \frac{1}{k_m^2} D_x^2 \Gamma_{k_m}(x) \right)$$

- $\mathbf{G}_{k_m}$ satisfies

$$\nabla \times \nabla \times \mathbf{G}_{k_m} - k_m^2 \mathbf{G}_{k_m} = \delta_0 I.$$

- $\mathbf{G}_{k_m}$ satisfies the Silver-Müller radiation condition.

Maxwell's equations

- Functional spaces: For $s = \pm 1/2$,

$$H^s_T(\partial D) = \left\{ \varphi \in \left(H^s(\partial D) \right)^3, \nu \cdot \varphi = 0 \right\}.$$

- Surface differential operators:
  - Surface gradient, surface divergence and Laplace-Beltrami operator: $\nabla_{\partial D}$, $\nabla_{\partial D} \cdot$ and $\Delta_{\partial D}$.
  - Vectorial surface curl: For $\varphi \in H^{\frac{1}{2}}(\partial D)$,

$$\vec{\mathrm{curl}}_{\partial D} \varphi = -\nu \times \nabla_{\partial D} \varphi.$$

  - Scalar surface curl: For $\varphi \in H_T^{\frac{1}{2}}(\partial D)$,

$$\mathrm{curl}_{\partial D} \varphi = -\nabla_{\partial D} \cdot (\nu \times \varphi).$$

Maxwell's equations

- $\Delta_{\partial D} : H_0^{\frac{3}{2}}(\partial D) \to H_0^{-\frac{1}{2}}(\partial D)$: invertible.
- $H_0^{\frac{3}{2}}(\partial D)$ and $H_0^{-\frac{1}{2}}(\partial D)$: zero mean subspaces of $H^{\frac{3}{2}}(\partial D)$ and $H^{-\frac{1}{2}}(\partial D)$.
- Vector identities:

$$\begin{aligned}
\nabla_{\partial D} \cdot \nabla_{\partial D} &= \Delta_{\partial D}, \\
\mathrm{curl}_{\partial D} \vec{\mathrm{curl}}_{\partial D} &= -\Delta_{\partial D}, \\
\vec{\mathrm{curl}}_{\partial D} \mathrm{curl}_{\partial D} &= -\Delta_{\partial D} + \nabla_{\partial D} \nabla_{\partial D} \cdot, \\
\nabla_{\partial D} \cdot \vec{\mathrm{curl}}_{\partial D} &= 0, \\
\mathrm{curl}_{\partial D} \nabla_{\partial D} &= 0.
\end{aligned}$$

- Functional space:

$$H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D) = \left\{ \varphi \in H_T^{-\frac{1}{2}}(\partial D), \nabla_{\partial D} \cdot \varphi \in H^{-\frac{1}{2}}(\partial D) \right\}.$$

Maxwell's equations

- Trace theorems:
  - $u \in H(\text{div}, D) := \{u \in L^2(D) : \nabla \cdot u \in L^2(D)\}$

    $$u \cdot \nu \in H^{-\frac{1}{2}}(\partial D).$$

  - $u \in H(\text{curl}, D) := \{u \in L^2(D) : \nabla \times u \in L^2(D)\}$

    $$u \times \nu \in H_T^{-\frac{1}{2}}(\partial D).$$

  - ν: outward normal to ∂D.

Maxwell's equations

- $H_0(\mathrm{div}, D) := \{u \in H(\mathrm{div}, D) : u \cdot \nu = 0 \text{ on } \partial D\}$.
- $H_0(\mathrm{curl}, D) := \{u \in H(\mathrm{curl}, D) : u \times \nu = 0 \text{ on } \partial D\}$.
- $H_0^1(D) := \{u \in H^1(D) : u = 0 \text{ on } \partial D\}$.
- Characterization of $H_0^1(D)$:

$$H_0^1(D) = H_0(\mathrm{div}, D) \cap H_0(\mathrm{curl}, D).$$

- Characterization of $H^1(D)$:

$$H^1(D) = H(\mathrm{div}, D) \cap H(\mathrm{curl}, D) \cap \{u \cdot \nu \in H^{\frac{1}{2}}(\partial D) \text{ or } u \times \nu \in H_T^{\frac{1}{2}}(\partial D)\}.$$

Maxwell's equations

- Helmholtz decomposition:

$$H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D) = \nabla_{\partial D} H_0^{\frac{3}{2}}(\partial D) \oplus \vec{\mathrm{curl}}_{\partial D} H^{\frac{1}{2}}(\partial D).$$

  - For $u \in H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)$: $u^{(1)}$ and $u^{(2)}$ two functions in $H_0^{\frac{3}{2}}(\partial D)$ and $H^{\frac{1}{2}}(\partial D)$ s.t.

$$u = \nabla_{\partial D} u^{(1)} + \vec{\mathrm{curl}}_{\partial D} u^{(2)}.$$

  - $u^{(1)}$: uniquely defined and $u^{(2)}$: defined up to a constant function.

Maxwell's equations

- Boundary integral operators:
  -
    $$\begin{aligned}\vec{\mathcal{S}}_D^k[\varphi] : H_T^{-\frac{1}{2}}(\partial D) &\longrightarrow H_T^{\frac{1}{2}}(\partial D) \text{ or } H^1_{\mathrm{loc}}(\mathbb{R}^3)^3 \\ \varphi &\longmapsto \vec{\mathcal{S}}_D^k[\varphi](x) = \int_{\partial D} \Gamma_k(x-y)\varphi(y)d\sigma(y);\end{aligned}$$
  -
    $$\mathcal{M}_D^k[\varphi] : H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D) \longrightarrow H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)$$
    $$\varphi \longmapsto \mathcal{M}_D^k[\varphi](x) = \int_{\partial D} \nu(x) \times \nabla_x \times \big(\Gamma_k(x-y)\varphi(y)\big)\, d\sigma(y);$$
  -
    $$\mathcal{L}_D^k[\varphi] : H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D) \longrightarrow H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)$$
    $$\varphi \longmapsto \mathcal{L}_D^k[\varphi](x) = \nu(x) \times \left(k^2 \vec{\mathcal{S}}_D^k[\varphi](x) + \nabla \mathcal{S}_D^k[\nabla_{\partial D} \cdot \varphi](x)\right).$$

Maxwell's equations

- Jump relations for $\vec{\mathcal{S}}_D^k$: For $\varphi \in H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)$,
  - $$\left(\nu \times \nabla \times \vec{\mathcal{S}}_D^k[\varphi]\right)\Big|_{\pm} = (\mp \frac{1}{2} I + \mathcal{M}_D^k)[\varphi];$$
  - $$\left(\nu \times \nabla \times \nabla \times \vec{\mathcal{S}}_D^k[\varphi]\right)\Big|_{\partial D} = \mathcal{L}_D^k[\varphi].$$

Maxwell's equations

- Relation to the Neumann-Poincaré operator:
  - $k = 0$;
  - $\mathcal{M}_D^0 : H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D) \longrightarrow H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)$: compact;
  - For $\varphi \in H^{\frac{1}{2}}(\partial D)$,

$$\mathcal{M}_D^0[\vec{\mathrm{curl}}_{\partial D}\varphi] = \vec{\mathrm{curl}}_{\partial D}\mathcal{K}_D^0[\varphi];$$

  - For $\varphi \in H^{\frac{3}{2}}(\partial D)$,

$$\mathcal{M}_D^0[\nabla_{\partial D}\varphi] = -\nabla_{\partial D}\Delta_{\partial D}^{-1}(\mathcal{K}_D^0)^*[\Delta_{\partial D}\varphi] + \vec{\mathrm{curl}}_{\partial D}\mathcal{R}_D[\varphi];$$

  - $$\mathcal{R}_D = -\Delta_{\partial D}^{-1}\mathrm{curl}_{\partial D}\mathcal{M}_D^0\nabla_{\partial D}.$$

Maxwell's equations

- $\sigma(\mathcal{M}_D^0)$: spectrum of $\mathcal{M}_D^0$.
- For $(\psi, \varphi) \in \left(H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)\right)^2$ and $\lambda \notin \sigma(\mathcal{M}_D^0)$,

$$\left(\lambda I - \mathcal{M}_D^0\right)[\psi] = \varphi.$$

- Helmholtz decompositions of $\psi, \varphi \in H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)$:
  - $\psi^{(1)}$ and $\psi^{(2)}$ in $H_0^{\frac{3}{2}}(\partial D)$ and $H^{\frac{1}{2}}(\partial D)$ s.t.

$$\psi = \nabla_{\partial D}\psi^{(1)} + \vec{\mathrm{curl}}_{\partial D}\psi^{(2)}.$$

  - $\varphi^{(1)}$ and $\varphi^{(2)}$ in $H_0^{\frac{3}{2}}(\partial D)$ and $H^{\frac{1}{2}}(\partial D)$ s.t.

$$\varphi = \nabla_{\partial D}\varphi^{(1)} + \vec{\mathrm{curl}}_{\partial D}\varphi^{(2)}.$$

Maxwell's equations

- Assume $\lambda \neq \frac{1}{2}$,

$$\left(\lambda I - \mathcal{M}_D^0\right)[\psi] = \varphi.$$

$\Leftrightarrow$ $(\psi^{(1)}, \psi^{(2)}) \in H_0^{\frac{3}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)$:

$$\underbrace{\begin{pmatrix} \lambda I + \Delta_{\partial D}^{-1}(\mathcal{K}_D^0)^* \Delta_{\partial D} & 0 \\ \mathcal{R}_D & \lambda I - \mathcal{K}_D^0 \end{pmatrix}}_{:=\widetilde{\mathcal{M}}_D} \begin{pmatrix} \psi^{(1)} \\ \psi^{(2)} \end{pmatrix} = \begin{pmatrix} \varphi^{(1)} \\ \varphi^{(2)} \end{pmatrix}.$$

- $H(\partial D) := H_0^{\frac{3}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)$, equipped with the inner product

$$\langle u, v \rangle_{H(\partial D)} = \langle \Delta_{\partial D} u^{(1)}, \Delta_{\partial D} v^{(1)} \rangle_{\mathcal{H}^*} + \langle u^{(2)}, v^{(2)} \rangle_{\mathcal{H}}.$$

- Equivalent to the $H_0^{\frac{3}{2}}(\partial D) \times H^{\frac{1}{2}}(\partial D)$-norm.
- Spectrum $\sigma(\widetilde{\mathcal{M}}_D) = \sigma(-(\mathcal{K}_D^0)^*) \cup \sigma((\mathcal{K}_D^0)^*) \backslash \{-\frac{1}{2}\}$ in $H(\partial D)$.

Maxwell's equations

- Integral representations:

$$E(x) = \begin{cases} E^{\text{in}}(x) + \mu_m \nabla \times \vec{\mathcal{S}}_D^{k_m}[\psi](x) + \nabla \times \nabla \times \vec{\mathcal{S}}_D^{k_m}[\phi](x), & x \in \mathbb{R}^3 \setminus \overline{D}, \\ \mu_c \nabla \times \vec{\mathcal{S}}_D^{k_c}[\psi](x) + \nabla \times \nabla \times \vec{\mathcal{S}}_D^{k_c}[\phi](x), & x \in D, \end{cases}$$

$$H(x) = -\frac{i}{\omega \mu_D}(\nabla \times E)(x), \quad x \in \mathbb{R}^3 \setminus \partial D;$$

- $(\phi, \psi) \in \left(H_T^{-\frac{1}{2}}(\text{div}, \partial D)\right)^2$ satisfies

$$\begin{pmatrix} \frac{\mu_c + \mu_m}{2} I + \mu_c \mathcal{M}_D^{k_c} - \mu_m \mathcal{M}_D^{k_m} & \mathcal{L}_D^{k_c} - \mathcal{L}_D^{k_m} \\ \mathcal{L}_D^{k_c} - \mathcal{L}_D^{k_m} & \left(\frac{k_c^2}{2\mu_c} + \frac{k_m^2}{2\mu_m}\right) I + \frac{k_c^2}{\mu_c} \mathcal{M}_D^{k_c} - \frac{k_m^2}{\mu_m} \mathcal{M}_D^{k_m} \end{pmatrix}$$

$$= \left[\begin{array}{c} \nu \times E^{\text{in}} \\ i\omega \nu \times H^{\text{in}} \end{array} \right] \Bigg|_{\partial D}.$$

Maxwell's equations

- Unique solution on $H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D) \times H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)$;
- There exists there a positive constant $C = C(\varepsilon_c, \mu_c, \omega)$ s.t.

$$\|\psi\|_{H_T^{-\frac{1}{2}}(\mathrm{div},\partial D)} + \|\phi\|_{H_T^{-\frac{1}{2}}(\mathrm{div},\partial D)} \leq C\Big(\|E^{\mathrm{in}} \times \nu\|_{H_T^{-\frac{1}{2}}(\mathrm{div},\partial D)} + \|H^{\mathrm{in}} \times \nu\|_{H_T^{-\frac{1}{2}}(\mathrm{div},\partial D)}\Big).$$

Maxwell's equations

- Low-frequency asymptotic expansions of layer potentials: $\mathcal{M}_D^k$ and $\mathcal{L}_D^k$ as $k \to 0$.
  - For $\varphi \in H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)$,

$$\mathcal{M}_D^k[\varphi](x) = \mathcal{M}_D^0[\varphi](x) - \sum_{j=2}^{\infty} (ik)^j \mathcal{M}_D^j[\varphi](x);$$

  -

$$\mathcal{M}_D^j[\varphi](x) = \int_{\partial D} \frac{1}{4\pi j!} \nu(x) \times \nabla_x \times |x-y|^{j-1} \varphi(y) d\sigma(y).$$

  - $\|\mathcal{M}_D^j\|_{\mathcal{L}\left(H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)\right)}$: uniformly bounded with respect to j.
  - Convergence in $\mathcal{L}\left(H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)\right)$ and $\mathcal{M}_D^k$: analytic in k.

Maxwell's equations

- For $\varphi \in H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)$,

$$(\mathcal{L}_D^{k_c} - \mathcal{L}_D^{k_m})[\varphi](x) = \sum_{j=1}^{\infty} \omega^{j+1} \mathcal{L}_D^j[\varphi](x);$$

- $$\mathcal{L}_D^j[\varphi](x) = C_j \nu(x) \times \Big(\int_{\partial D} |x-y|^{j-2} \varphi(y) d\sigma(y) - \int_{\partial D} \frac{|x-y|^{j-2}(x-y)}{j+1} \nabla_{\partial D} \cdot \varphi(y) d\sigma(y) \Big),$$

- $$C_j = \frac{(i)^j ((\sqrt{\varepsilon_c \mu_c})^{j+1} - (\sqrt{\varepsilon_m \mu_m})^{j+1})}{4\pi (j-1)!}.$$

- $\|\mathcal{L}_D^j\|_{\mathcal{L}\left(H_T^{-\frac{1}{2}}(\mathrm{div},\partial D)\right)}$: uniformly bounded with respect to j.
- Convergence in $\mathcal{L}\left(H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D)\right)$ and $\mathcal{L}_D^k$: analytic in k.

Maxwell's equations

- Helmholtz-Kirchhoff theorem:
  - Dyadic outgoing Green function:

$$\mathbf{G}_{k_m}(x) = \varepsilon_m \left(\Gamma_{k_m}(x) I + \frac{1}{k_m^2} D_x^2 \Gamma_{k_m}(x) \right)$$

  - ∂B_R: sphere of radius R and center 0.
  - Integration by parts $\Rightarrow$

$$\int_{\partial B_R} \left(\frac{\partial \overline{\mathbf{G}_{k_m}}}{\partial \nu}(x-y) \mathbf{G}_{k_m}(z-y) - \overline{\mathbf{G}_{k_m}}(x-y) \frac{\partial \mathbf{G}_{k_m}}{\partial \nu}(z-y) \right) d\sigma(y)$$
$$= 2i \Im \mathbf{G}_{k_m}(x-z)\,;$$

  - Silver-Müller radiation condition $\Rightarrow$

$$\lim_{R \to +\infty} \int_{\partial B_R} \overline{\mathbf{G}_{k_m}}(x-y) \mathbf{G}_{k_m}(z-y)\, d\sigma(y) = -\frac{1}{k_m} \Im \mathbf{G}_{k_m}(x-z)\,.$$

Maxwell's equations

- Optical cross-section theorem:
  - Incident plane waves: $c \in \mathbb{R}^3$ and $d \in S$ s.t. $c \cdot d = 0$,

$$E^{\rm in}(x) = c e^{ik_m d\cdot x}, \quad H^{\rm in}(x) = \sqrt{\frac{\varepsilon_m}{\mu_m}} d \times c e^{ik_m d \cdot x}.$$

  - Extinction cross-section Q^{ext}:

$$Q^{ext} := -\frac{1}{|c|^2}\sqrt{\frac{\mu_m}{\varepsilon_m}} \Re\Big[\int_{\partial D} (\overline{E^i} \times (H - H^i) + (E - E^i) \times \overline{H^i}) \cdot \nu \, d\sigma \Big].$$

  - Scattering amplitude $A_\infty(c, d; \hat{x})$: $(\hat{x} = x/|x|)$

$$E(x) - E^{\rm in}(x) = \frac{e^{ik_m|x|}}{k_m|x|} A_\infty(c, d; \hat{x}) + o(\frac{1}{|x|}), \quad |x| \to +\infty.$$

  - Optical theorem:

$$Q^{ext} = \frac{4\pi}{k_m} \Im\left[\frac{c \cdot A_\infty(c, d; d)}{|c|^2}\right].$$

Maxwell's equations

- Electromagnetic scattering by small particles:
- $D = z + \delta B$ where B contains the origin and $|B| = O(1)$.
- Leading-order term in the asymptotic expansion of the scattered electric field $E^s := E - E^{\mathrm{in}}$ far-away from the particle:

$$\begin{aligned} E^s(x) \quad = \quad & -\frac{i\omega\mu_m}{\varepsilon_m} \nabla \times \mathbf{G}_{k_m}(x-z) M(\lambda_\mu, D) H^i(z) \\ & -\omega^2 \mu_m \mathbf{G}_{k_m}(x-z) M(\lambda_\varepsilon, D) E^i(z) + O(\delta^4). \end{aligned}$$

- $\mathbf{G}_{k_m}(x-z)$: Dyadic Green (matrix valued) function for the full Maxwell equations;
- $M(\lambda_\mu, D)$ and $M(\lambda_\varepsilon, D)$: polarization tensors associated with D and the contrasts λ_μ and λ_ε.
-

$$\lambda_\mu := \frac{\frac{\mu_m}{\mu_c} + 1}{2(\frac{\mu_m}{\mu_c} - 1)}, \quad \lambda_\varepsilon := \frac{\frac{\varepsilon_c}{\varepsilon_m} + 1}{2(\frac{\varepsilon_c}{\varepsilon_m} - 1)}.$$

Maxwell's equations

- Spherical particle:

$$M(\lambda_\mu, D) = 3\frac{\frac{\mu_m}{\mu_c} - 1}{2 + \frac{\mu_m}{\mu_c}} I, \quad M(\lambda_\varepsilon, D) = 3\frac{\frac{\varepsilon_c}{\varepsilon_m} - 1}{2 + \frac{\varepsilon_c}{\varepsilon_m}} I.$$

- $\mu_m = \mu_c$, $E^{\mathrm{in}}(x) = \mathbf{G}_{k_m}(x - x_j)\theta_j$:

$$E^s(x) = 3k_m^2 \frac{\varepsilon_m - \varepsilon_c}{2\varepsilon_m + \varepsilon_c} \mathbf{G}_{k_m}(x - x_j)\mathbf{G}_{k_m}(z - x_j)\theta_j + O(\delta^4).$$

Maxwell's equations

- Direct electromagnetic imaging:
  - $x_i, i = 1, \ldots, N$: equi-distributed points on $\partial B_R := \{|x| = R\}$ for $N \gg 1$.
  - Array of N elements $\{x_1, \ldots, x_N\}$: used to detect the spherical particle D.
  - $\theta_1, \ldots, \theta_N$: corresponding unit directions of the incident fields/observation directions.
  - $$E^{\mathrm{in}}(x) = \mathbf{G}_{k_m}(x - x_j)\theta_j, \quad x \in \mathbb{R}^3.$$
  - Asymptotic expansion:
  $$\begin{aligned} E_j^s(x) \quad = \quad & 3k_m^2 \frac{\varepsilon_m - \varepsilon_c}{2\varepsilon_m + \varepsilon_c} |D| \mathbf{G}_{k_m}(x - z) \mathbf{G}_{k_m}(z - x_j)\theta_j \\ & + O(\delta^4). \end{aligned}$$
  - Measured data: $N \times N$ matrix
  $$\mathbf{A}^\omega := \Big(E_j^s(x_i) \cdot \theta_i \Big)_{i,j}.$$

Maxwell's equations

- N-dimensional vector fields $g^{(j)}(z^S)$, for $z^S \in B_R$ and $j = 1, 2, 3$,

$$g^{(j)}(z^S) = \frac{1}{\sqrt{\sum_{i=1}^{N} |e_j \cdot \mathbf{G}_{k_m}(z^S - x_i)\theta_i|^2}}$$
$$\times \Big(e_j \cdot \mathbf{G}_{k_m}(z^S - x_1)\theta_1, \ldots, e_j \cdot \mathbf{G}_{k_m}(z^S - x_N)\theta_N \Big)^t .$$

- MUSIC, reverse-time migration, Kirchhoff, and joint sparse recovery algorithms: extended to the electromagnetic case.

Lecture 9: Diffraction gratings

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Diffraction gratings

- Periodic structures with tiny features used as optical devices:
  - antireflective interfaces;
  - beam splitters;
  - sensors
- Small features: Light propagation governed by diffraction.
- Time-harmonic Maxwell's equations: reduced to two scalar Helmholtz equations (transverse electric and transverse magnetic modes).
- Two classes of grating structures:
  - Linear grating (one-dimensional gratings),
  - Crossed gratings (biperiodic or two-dimensional gratings).

Diffraction gratings

- Time-harmonic electromagnetic fields:

$$\begin{aligned} E(x,t) &= \Re E(x) e^{-i\omega t}, \\ H(x,t) &= \Re H(x) e^{-i\omega t} \end{aligned}$$

- Operating frequency $\omega > 0$; E and H: electric and magnetic fields.
- Time-harmonic Maxwell equations:

$$\begin{aligned} \nabla \times E &= i\omega\mu H, \\ \nabla \times H &= -i\omega\varepsilon E. \end{aligned}$$

- μ: magnetic permeability and ε: electric permittivity.

Diffraction gratings

- $$\begin{aligned} \nabla \cdot (\varepsilon E) &= 0, \\ \nabla \cdot (\mu H) &= 0. \end{aligned}$$
- Jump conditions ($\mu = \mu_0$):
  - Tangential components of E and H: continuous crossing an interface;
  - Normal components of εE and H: continuous crossing an interface.
- Homogeneous, nonmagnetic, and isotropic medium:

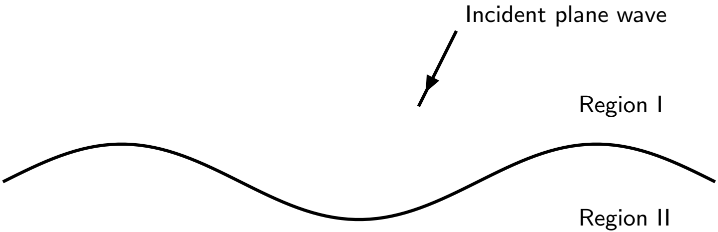
$$-\Delta E + \nabla(\nabla \cdot E) = i\omega\mu_0 \nabla \times H.$$

- $\Rightarrow$

$$-\Delta E + \nabla(\nabla \cdot E) = \omega^2 \varepsilon \mu_0 E$$

Diffraction gratings

- Grating geometry and fundamental polarizations



Grating geometry.

- Λ, h, and θ: period, height, and incident angle.
- (e_1, e_2, e_3): orthonormal basis of $\mathbb{R}^3$.

Diffraction gratings

- One-dimensional grating:

$$\varepsilon(x_1 + n\Lambda, x_2) = \varepsilon(x_1, x_2), \quad n \in \mathbb{Z}.$$

- Two-dimensional grating with period $\Lambda = (\Lambda_1, \Lambda_2)$:

$$\varepsilon(x_1 + n_1\Lambda_1,\ x_2 + n_2\Lambda_2,\ x_3) = \varepsilon(x_1, x_2, x_3),\ \forall\ n_1, n_2 \in \mathbb{Z}.$$

- Incident vector: $k_1(\sin\theta, -\cos\theta, 0)$.
- Fundamental cases of polarization: *TE* (transverse electric) and *TM* (transverse magnetic):
    - TE polarization:

$$E = u(x_1, x_2)e_3.$$

    - u: scalar function.
    - TM polarization:

$$H = u(x_1, x_2)e_3.$$

Diffraction gratings

- Perfectly conducting gratings
- $u = E_3(x_1, x_2)$ in TE polarization; $= H_3(x_1, x_2)$ in TM polarization.
- Grating: $x_2 = f(x_1) \Rightarrow u = 0$ in Region II ($x_2 < f(x_1)$).
- In Region I, u:

$$\Delta u + k^2 u = 0 \text{ if } x_2 > f(x_1).$$

- Boundary condition of u on $x_2 = f(x_1)$:
  - ν: outward normal to Region II,

$$\nu \times E = 0 \quad \text{on } x_2 = f(x_1).$$

  - In TE polarization: homogeneous Dirichlet boundary condition,

$$u(x_1, f(x_1)) = 0.$$

  - In TM polarization: homogeneous Neumann boundary condition,

$$\frac{\partial u}{\partial \nu}\bigg|_{x_2 = f(x_1)} = 0.$$

Diffraction gratings

- Incident field: $u^{\mathrm{in}} = e^{i(\alpha x_1 - \beta x_2)}$; scattered field: $u^s = u - u^{\mathrm{in}}$.
- $$\begin{cases} \alpha = k_1 \sin\theta, \\ \beta = k_1 \cos\theta. \end{cases}$$
- $$\Delta u^s + k_1^2 u^s = 0 \text{ for } x_2 > f(x_1).$$
- Boundary conditions:
  - TE polarization: $u^s = -u^{\mathrm{in}}$ on $x_2 = f(x_1)$.
  - TM polarization: $\dfrac{\partial u^s}{\partial \nu} = -\dfrac{\partial u^{\mathrm{in}}}{\partial \nu}$ on $x_2 = f(x_1)$.

Diffraction gratings

- Radiation condition:
  - Assume u^s: bounded when $x_2 \to +\infty$ and consisted of outgoing plane waves.
- Quasi–periodic solutions.
- $u^s(x_1, x_2)e^{-i\alpha x_1}$: periodic function of period Λ with respect to x_1 for every x_2:

$$u^s(x_1 + \Lambda, x_2)e^{-i\alpha\Lambda} = u^s(x_1, x_2).$$

Diffraction gratings

- Grating formula.
- Define
$$\alpha_n = \alpha + \frac{2\pi n}{\Lambda} = k_1 \sin\theta + n\frac{2\pi}{\Lambda}.$$
- Fourier series expansion:
$$\begin{aligned} u^s(x_1, x_2) &= e^{i\alpha x_1} \sum_{n\in\mathbb{Z}} V_n(x_2) e^{in\frac{2\pi}{\Lambda}x_1} \\ &= \sum_{n\in\mathbb{Z}} V_n(x_2) e^{i\alpha_n x_1}. \end{aligned}$$
- Determine $V_n(x_2)$.
- $u^s(x_1, x_2)$ satisfies the Helmholtz equation in $\{x_2 > \max\{f(x_1)\}\} \Rightarrow$
$$\sum_{n\in\mathbb{Z}} \left[\frac{d^2 V_n(x_2)}{dx_2^2} + (k_1^2 - \alpha_n^2) V_n(x_2) \right] e^{in\frac{2\pi}{\Lambda}x_1} = 0.$$
- $\Rightarrow$
$$\frac{d^2 V_n(x_2)}{dx_2^2} + (k_1^2 - \alpha_n^2) V_n(x_2) = 0.$$

Diffraction gratings

- Define

$$\beta_n = \begin{cases} \sqrt{k_1^2 - \alpha_n^2} & k_1^2 > \alpha_n^2, \\ i\sqrt{\alpha_n^2 - k_1^2} & k_1^2 \leq \alpha_n^2. \end{cases}$$

- $$V_n(x_2) = A_n e^{-i\beta_n x_2} + B_n e^{i\beta_n x_2}.$$

- Radiation condition $\Rightarrow A_n = 0$.
- Rayleigh expansion:

$$\begin{aligned} u^s(x_1, x_2) &= \sum_{|\alpha_n| < k_1} B_n e^{i\alpha_n x_1 + i\beta_n x_2} \quad \text{outgoing waves} \\ &+ \sum_{|\alpha_n| \geq k_1} B_n e^{i\alpha_n x_1 + i\beta_n x_2} \quad \text{evanescent waves}. \end{aligned}$$

Diffraction gratings

- $U = \{n, |\alpha_n| < k_1\}$: propagating plane wave (or scattered wave in the nth order).
- If $|n|$: large ($n \notin U$), $B_n e^{-|\beta_n| x_2} e^{i\alpha_n x_1}$: evanescent wave.
- Scattered wave in the nth order:

$$\psi_n(x_1, x_2) = B_n e^{i\alpha_n x_1 + i\sqrt{k_1^2 - \alpha_n^2}\; x_2} \quad \text{for } n \in U.$$

- Since $|\alpha_n / k_1| < 1$, angle of diffraction θ_n:

$$\frac{\alpha_n}{k_1} = \sin\theta_n = \sin\theta + \frac{2\pi n}{k_1 \Lambda}, \quad -\frac{\pi}{2} < \theta_n < \frac{\pi}{2}.$$

- Scattered wave in the nth order:

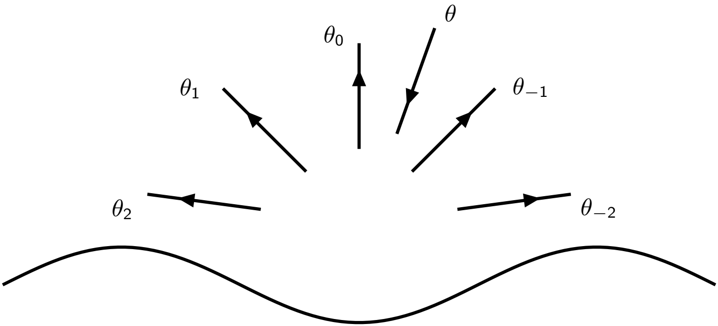
$$\psi_n(x_1, x_2) = B_n e^{ik_1(x_1 \sin\theta_n + x_2 \cos\theta_n)}.$$

Diffraction gratings

- Grating formula:

$$\sin\theta_n = \sin\theta + n\frac{\lambda_1}{\Lambda} \text{ or } k_1\sin\theta_n = k_1\sin\theta + \frac{n2\pi}{\Lambda}.$$

- λ_1: wavelength in Region I and $k_1 = \frac{2\pi}{\lambda_1}$.



Geometric interpretation of the grating formula.

Diffraction gratings

- Reciprocity property:
  - θ and θ_n: angle of incidence and the angle of diffraction of the nth order.
  - Angle of incidence: $\theta' = -\theta_n \Rightarrow n$th scattered order propagates in the direction: $\theta'_n = -\theta$.

Reciprocity theorem.

Diffraction gratings

- Grating efficiency:
  - ϕ^{in} and ϕ_n^s: fluxes of the Poynting vectors associated with the incident wave and the nth scattered wave, respectively.
  - Measurement of energy in the nth propagating order:

$$E_n = \frac{\phi_n^s}{\phi^{\text{in}}}.$$

-

$$E_n = |B_n|^2 \frac{\cos\theta_n}{\cos\theta}.$$

- The conservation of energy:

$$\sum_{n \in U} E_n = 1.$$

- Incident energy = the scattered energy.

Diffraction gratings

- Assume that u_1 and u_2:
$$\Delta u + k^2 u = 0$$
and either a homogeneous Dirichlet or a Neumann boundary condition.
- For any $x_2 > \max f(x_1)$,
$$\int_0^\Lambda (u_1 \frac{\partial u_2}{\partial x_2} - u_2 \frac{\partial u_1}{\partial x_2}) dx_1 = 0.$$
- Apply to u and $\overline{u}$:
$$\frac{1}{\Lambda} \int_0^\Lambda \left(\frac{\partial \overline{u}}{\partial x_2} - \overline{u} \frac{\partial u}{\partial x_2} \right) dx_1 = 0 \text{ for } x_2 > \max f(x_1)$$
- $\Rightarrow$
$$\frac{1}{\Lambda} \Im \left\{ \int_0^\Lambda u \frac{\partial \overline{u}}{\partial x_2} \right\} = 0 \text{ for } x_2 > \max f(x_1).$$

Diffraction gratings

- $$u = e^{i\alpha x_1 - i\beta x_2} + \sum_{n\in U} B_n e^{i\alpha_n x_1 + i\beta_n x_2} + \sum_{n\notin U} B_n e^{i\alpha_n x_1 + i\beta_n x_2}$$

- $$\overline{u} = e^{-i\alpha x_1 + i\beta x_2} + \sum_{n\in U} \overline{B}_n e^{-i\alpha_n x_1 - i\beta_n x_2} + \sum_{n\notin U} \overline{B}_n e^{-i\alpha_n x_1 - i\beta_n x_2}.$$

- $\Rightarrow$
$$\beta = \sum_{n\in U} \beta_n |B_n|^2,$$
or equivalently $\sum_{n\in U} E_n = 1$.

Diffraction gratings

- Dielectric gratings
- Region I: filled with a material of real permittivity ε_1;
- Region II: filled with a material of real permittivity ε_2.
- In Region I,
$$\Delta u + k_1^2 u = 0 \qquad \text{if } x_2 > f(x_1).$$
- In Region II,
$$\Delta u + k_2^2 u = 0 \qquad \text{if } x_2 < f(x_1).$$
- Outgoing wave conditions satisfied by $u^s = u - u^{\text{in}}$ (for $x_2 \to +\infty$) and by u (for $x_2 \to -\infty$).
- Jump conditions $\Rightarrow$ u: continuous, $\partial u/\partial \nu$: continuous in TE polarization, and $(1/\varepsilon)\partial u/\partial \nu$: continuous in TM polarization.

Diffraction gratings

- Quasi-periodicity of the field.
- For $x_2 > \max f(x_1)$,

$$u(x_1, x_2) = e^{i\alpha x_1} \sum_{n \in \mathbb{Z}} V_n(x_2) e^{in\frac{2\pi}{\Lambda} x_1}.$$

- Rayleigh expansion:

$$u(x_1, x_2) = e^{(i\alpha x_1 - i\beta x_2)} + \sum R_n e^{i\alpha_n x_1 + i\beta_{n1} x_2}.$$

- $\alpha_n = k_1 \sin\theta + n\frac{2\pi}{\Lambda}$ and $\beta_{n1}^2 = k_1^2 - \alpha_n^2$.
- If $x_2 < \min f(x_1)$,

$$u(x_1, x_2) = \sum_{n \in \mathbb{Z}} T_n \ e^{i\alpha_n x_1 - i\beta_{n2} x_2}$$

- $$\beta_{n2}^2 = k_2^2 - \alpha_n^2.$$

- Expansions contain propagating and evanescent waves depending on n.

Diffraction gratings

- For $j = 1, 2,\ U_j = \{n, \beta_{nj}^2 > 0\}$.
- If $n \in U_1,\ \alpha_n^2 < k_1^2$,

$$\alpha_n = k_1 \sin\theta + n\frac{2\pi}{\Lambda} = k_1 \sin\theta_{n1}, \qquad -\frac{\pi}{2} < \theta_{n1} < \frac{\pi}{2},$$

- $$\beta_{n1} = k_1 \cos\theta_{n1};$$
- $R_n e^{i\alpha_n x_1 + i\beta_{n1} x_2}$: plane wave propagating in the θ_{n1} direction.
- If $n \in U_2$,

$$\alpha_n = k_2 \sin\theta + n\frac{2\pi}{\Lambda} = k_2 \sin\theta_{n2}, \quad -\frac{\pi}{2} < \theta_{n2} < \frac{\pi}{2};$$

- $$\beta_{n2} = k_2 \cos\theta_{n2};$$
- $T_n e^{i\alpha_n x_1 - i\beta_{n2} x_2}$: transmitted plane wave propagating in the θ_{n2} direction.

Diffraction gratings

- Variational formulations.
- Model problem:
  - $\Omega_1 = \{x = (x_1, x_2) \in \mathbb{R}^2 : x_2 > b\}$;
    $\Omega_2 = \{x = (x_1, x_2) \in \mathbb{R}^2 : x_2 < -b\}$;
    $\Omega = \{(x_1, x_2) \in \mathbb{R}^2 : -b < x_2 < b\}$.
  - Periodic slab: $q_0(x_1 + \Lambda, x_2) = q_0(x_1, x_2)$ $(q = \sqrt{\varepsilon \mu_0})$

$$q(x) = \begin{cases} q_1 & \text{in } \Omega_1 \cup \overline{\Omega}_1, \\ q_0(x) & \text{in } \Omega, \\ q_2 & \text{in } \Omega_2 \cup \overline{\Omega}_2. \end{cases}$$

Diffraction gratings

- Incoming plane wave
$$u^{\mathrm{in}}(x_1, x_2) = e^{i\alpha x_1 - i\beta x_2}.$$
-
$$\nabla \cdot (\frac{1}{q^2} \nabla u) + \omega^2 u = 0 \quad \text{in } \mathbb{R}^2.$$
- $u_\alpha(x_1, x_2) = u(x_1, x_2) e^{-i\alpha x_1}$.
- u_α:
$$\nabla_\alpha \cdot (\frac{1}{q^2} \nabla_\alpha u_\alpha) + \omega^2 u_\alpha = 0 \qquad \text{in } \mathbb{R}^2.$$
- $\nabla_\alpha = \nabla + i(\alpha, 0)$.

Diffraction gratings

- Expand u_α in a Fourier series:

$$u_\alpha(x_1,x_2)=\sum_{n\in\mathbb{Z}} u_\alpha^{(n)}(x_2)e^{i\frac{2\pi n}{\Lambda}x_1}.$$

- $$u_\alpha^{(n)}(x_2)=\frac{1}{\Lambda}\int_0^\Lambda u_\alpha(x_1,x_2)e^{-i\frac{2\pi n}{\Lambda}x_1}dx_1.$$

- Sets

$$\Gamma_1'=\{x\in\mathbb{R}^2 : x_2=b_1\},\ \ \Gamma_2'=\{x_2=-b_1\},$$

with $0<b_1<b$ s.t. $\Omega_0\subseteq\{-b_1<x_2<b_1\}$.

- $$D_1=\{x\in\mathbb{R}^2 : x_2>b_1\}\quad\text{and}\quad D_2=\{x\in\mathbb{R}^2 : x_2<-b_1\}.$$

- For $j=1,2$,

$$\beta_j^n(\alpha)=e^{i\gamma_j^n/2}|k_j^2-\alpha_n^2|^{1/2}=e^{i\gamma_j^n/2}|\omega^2 q_j^2-\alpha_n^2|^{1/2},\quad n\in\mathbb{Z}.$$

- $$\gamma_j^n=\arg(k_j^2-\alpha_n^2),\ \ 0\le\gamma_j^n<2\pi.$$

Diffraction gratings

- Exclude Wood's anomalies:

$$k_j^2 \neq \alpha_n^2 \quad \text{for all } n \in \mathbb{Z}, j = 1, 2.$$

- $$\beta_j^n(\alpha) = \begin{cases} \sqrt{k_j^2 - \alpha_n^2}, & k_j^2 > \alpha_n^2, \\ i\sqrt{\alpha_n^2 - k_j^2}, & k_j^2 < \alpha_n^2. \end{cases}$$

- Inside D_1 and D_2: u_α can be expressed as a sum of plane waves:

$$u_\alpha|_{D_j} = \sum_{n \in \mathbb{Z}} a_j^n e^{\pm i \beta_j^n(\alpha) x_2 + i \frac{2\pi n}{\Lambda} x_1}, \quad j = 1, 2.$$

- a_j^n: complex scalars.

Diffraction gratings

- Radiation condition.
- β_j^n: real for at most finitely many $n \Rightarrow$ there are only a finite number of propagating plane waves as $|x_2| \to \infty$.
- $u_\alpha^{(n)}(x_2)$

$$
= \begin{cases} u_\alpha^{(n)}(b)e^{i\beta_1^n(\alpha)(x_2-b)} & \text{in } D_1 \quad \text{for } n \neq 0, \\ u_\alpha^{(0)}(b)e^{i\beta(x_2-b)} + e^{-i\beta x_2} - e^{i\beta(x_2-2b)} & \text{in } D_1 \quad \text{for } n = 0, \\ u_\alpha^{(n)}(-b)e^{-i\beta_2^n(\alpha)(x_2+b)} & \text{in } D_2. \end{cases}
$$

Diffraction gratings

- Compute the normal derivative of $u_\alpha^n(x_2)$ on $\Gamma_j, j = 1, 2$:

$$\left.\frac{\partial u_\alpha^{(n)}}{\partial \nu}\right|_{\Gamma_j} = \begin{cases} i\beta_1^n(\alpha) u_\alpha^{(n)}(b) & \text{on } \Gamma_1 \quad \text{for } n \neq 0, \\ i\beta u_\alpha^{(0)}(b) - 2i\beta e^{-i\beta b} & \text{on } \Gamma_1 \quad \text{for } n = 0, \\ i\beta_2^n(\alpha) u_\alpha^{(n)}(-b) & \text{on } \Gamma_2. \end{cases}$$

- $\Rightarrow$

$$\left.\frac{\partial u_\alpha}{\partial \nu}\right|_{\Gamma_1} = \sum_{n\in\mathbb{Z}} i\beta_1^n(\alpha) u_\alpha^{(n)}(b) e^{i\frac{2\pi n}{\Lambda}x_1} - 2i\beta e^{-i\beta b};$$

$$\left.\frac{\partial u_\alpha}{\partial \nu}\right|_{\Gamma_2} = \sum_{n\in\mathbb{Z}} i\beta_2^n(\alpha) u_\alpha^{(n)}(-b) e^{i\frac{2\pi n}{\Lambda}x_1}.$$

- Outward normal vector $\nu = (0, 1)$ on Γ_1 and $= (0, -1)$ on Γ_2.

Diffraction gratings

- Suppose that $\alpha_n^2 > k_1^2$. Then

$$u_\alpha^{(n)}(b) = u_\alpha^{(n)}(b_1) e^{-(b-b_1)\sqrt{\alpha_n^2 - k_1^2}}.$$

- If $\alpha_n^2 > |k_2|^2$, then

$$|u_\alpha^{(n)}(-b)| = |u_\alpha^{(n)}(-b_1)| e^{-(b-b_1)\sin(\gamma_2^n/2)\sqrt[4]{(\alpha_n^2 - \Re(k_2^2))^2 + (\Im(k_2^2))^2}}.$$

- For functions $f \in H^{\frac{1}{2}}(\Gamma_j)$ (Sobolev space of Λ-periodic complex valued functions),

$$T_j^\alpha[f](x_1) = \sum_{n\in\mathbb{Z}} i\beta_j^n(\alpha) f^{(n)} e^{i\frac{2\pi n}{\Lambda}x_1};$$

-

$$f^{(n)} = \frac{1}{\Lambda}\int_0^\Lambda f(x_1) e^{-i\frac{2\pi n}{\Lambda}x_1}\, dx_1.$$

- For $j = 1, 2$, $T_j^\alpha : H^{\frac{1}{2}}(\Gamma_j) \to H^{-\frac{1}{2}}(\Gamma_j)$: continuous.

Diffraction gratings

- Find $u_\alpha \in H^1(\Omega)$:

$$\begin{cases} \nabla_\alpha \cdot (\frac{1}{q^2} \nabla_\alpha u_\alpha) + \omega^2 u_\alpha & = & 0 \text{ in } \Omega, \\ T_1^\alpha[u_\alpha] - \frac{\partial u_\alpha}{\partial \nu} & = & 2i\beta e^{-i\beta b} \text{ on } \Gamma_1, \\ T_2^\alpha[u_\alpha] - \frac{\partial u_\alpha}{\partial \nu} & = & 0 \text{ on } \Gamma_2. \end{cases}$$

- Equivalent form:

$$\begin{aligned} \nabla_\alpha \cdot (\frac{1}{q^2} \nabla_\alpha \widetilde{u}_\alpha) + \omega^2 \widetilde{u}_\alpha &= -f \text{ in } \Omega, \\ T_1^\alpha[\widetilde{u}_\alpha] - \frac{\partial \widetilde{u}_\alpha}{\partial \nu} &= 0 \text{ on } \Gamma_1, \\ T_2^\alpha[\widetilde{u}_\alpha] - \frac{\partial \widetilde{u}_\alpha}{\partial \nu} &= 0 \text{ on } \Gamma_2. \end{aligned}$$

- $f \in (H^1(\Omega))'$ and $\widetilde{u}_\alpha = u_\alpha - u_0$ with u_0 a fixed smooth function.

Diffraction gratings

- Denote $\widetilde{u}_\alpha$ by u_α.
- Variational form: Given $f \in (H^1(\Omega))'$, find $u_\alpha \in H^1(\Omega)$ s.t.

$$a(u_\alpha, \phi) = \langle f, \phi \rangle, \quad \forall \phi \in H^1(\Omega).$$

- Sesquilinear form:

$$\begin{aligned} a(w_1, w_2) \quad = \quad & \int_\Omega \frac{1}{q^2} \nabla w_1 \cdot \nabla \overline{w_2} - \int_\Omega (\omega^2 - \frac{\alpha^2}{q^2}) w_1 \overline{w_2} \\ & -i\alpha \int_\Omega \frac{1}{q^2} (\partial_{x_1} w_1) \overline{w_2} + i\alpha \int_\Omega \frac{1}{q^2} w_1 \overline{\partial_{x_1} w_2} \\ & - \int_{\Gamma_1} \frac{1}{q_1^2} T_1^\alpha [w_1] \overline{w_2} - \int_{\Gamma_2} \frac{1}{q_2^2} T_2^\alpha [w_1] \overline{w_2}. \end{aligned}$$

- $\int_{\Gamma_j}$: dual pairing of $H^{-\frac{1}{2}}(\Gamma_j)$ with $H^{\frac{1}{2}}(\Gamma_j)$.

Diffraction gratings

- For all but a countable set of frequencies ω_j, $|\omega_j| \to +\infty$, the diffraction problem has a unique solution $u_\alpha \in H^1(\Omega)$.
- Write $a(w_1, w_2) = B_1(w_1, w_2) + \omega^2 B_2(w_1, w_2)$.
-

$$\begin{aligned} B_1(w_1, w_2) &= \int_\Omega \frac{1}{q^2} \nabla w_1 \cdot \nabla \overline{w_2} + 2 \int_\Omega \frac{\alpha^2}{q^2} w_1 \overline{w_2} - i\alpha \int_\Omega \frac{1}{q^2} (\partial_{x_1} w_1) \overline{w_2} \\ &\quad + i\alpha \int_\Omega \frac{1}{q^2} w_1 \overline{\partial_{x_1} w_2} - \int_{\Gamma_1} \frac{1}{q_1^2} T_1[w_1] \overline{w_2} - \int_{\Gamma_2} \frac{1}{q_2^2} T_2[w_1] \overline{w_2}, \\ B_2(w_1, w_2) &= - \int_\Omega (1 + \frac{\alpha^2}{k^2}) w_1 \overline{w_2} \, . \end{aligned}$$

- $\Rightarrow$

$$B_1(u, u) = \int_\Omega \frac{1}{q^2} |\nabla u|^2 + 2 \int_\Omega \frac{\alpha^2}{q^2} |u|^2 - 2\alpha \int_\Omega \frac{1}{q^2} \Im(u \, \overline{\partial_{x_1} u})$$
$$- \int_{\Gamma_1} \frac{1}{q_1^2} T_1[u] \overline{u} - \int_{\Gamma_2} \frac{1}{q_2^2} T_2[u] \overline{u}.$$

Diffraction gratings

- Denote $\frac{1}{q^2} = \frac{1}{\varepsilon \mu_0}$ by $\sigma' - i\sigma''$.
- Denote $\frac{1}{q_2^2}$ by $\sigma_2' - i\sigma_2''$, where $\sigma_2' > 0$ and $\sigma_2'' \geq 0$.
- $\Rightarrow$

$$\begin{aligned} \Re\{B_1(u,u)\} &= \int_\Omega \sigma' |\nabla u|^2 + 2\int_\Omega \alpha^2 \sigma' |u|^2 - 2\alpha \int_\Omega \sigma' \Im(u\, \overline{\partial_{x_1} u}) \\ &\quad -\Re\{\int_{\Gamma_1} \frac{1}{q_1^2} T_1[u]\overline{u} + \int_{\Gamma_2} \frac{1}{q_2^2} T_2[u]\overline{u}\} \\ &\geq \int_\Omega \frac{\sigma'}{2} |\nabla u|^2 - \Re\{\int_{\Gamma_1} \frac{1}{q_1^2} T_1[u]\overline{u} + \int_{\Gamma_2} \frac{1}{q_2^2} T_2[u]\overline{u}\}. \end{aligned}$$

-

$$\begin{aligned} -\Im\{B_1(u,u)\} &= \int_\Omega \sigma'' |\nabla u|^2 + 2\int_\Omega \alpha^2 \sigma'' |u|^2 - 2\alpha \int_\Omega \sigma'' \Im(u\, \overline{\partial_{x_1} u}) \\ &\quad +\Im\{\int_{\Gamma_1} \frac{1}{q_1^2} T_1[u]\overline{u} + \int_{\Gamma_2} \frac{1}{q_2^2} T_2[u]\overline{u}\} \\ &\geq \int_\Omega \frac{\sigma''}{2} |\nabla u|^2 + \Im\{\int_{\Gamma_1} \frac{1}{q_1^2} T_1[u]\overline{u} + \int_{\Gamma_2} \frac{1}{q_2^2} T_2[u]\overline{u}\}. \end{aligned}$$

Diffraction gratings

- $$
\begin{aligned}
-\int_{\Gamma_1} \frac{1}{q_1^2} T_1[u]\overline{u} &= -\sum \frac{1}{q_1^2} \Lambda i \beta_1^n |u^{(n)}|^2 \\
&= \sum \frac{1}{q_1^2} \Lambda (\Im \beta_1^n) \, |u^{(n)}|^2 - i \sum \frac{1}{n_1^2} \Lambda \Re \beta_1^n |u^{(n)}|^2 .
\end{aligned}
$$

- $$
\begin{aligned}
-\int_{\Gamma_2} \frac{1}{q_2^2} T_2[u]\overline{u} &= -\sum \frac{1}{q_2^2} i \Lambda \beta_2^n |u^{(n)}(-b)|^2 \\
&= \sum_n \Lambda |\beta_2^n| |u^{(n)}(-b)|^2 p_n \, .
\end{aligned}
$$

- $p_n = p_n' - i p_n''$ with

$$
p_n' = -\sigma_2'' \cos(\gamma_2^n/2) + \sigma_2' \sin(\gamma_2^n/2)
$$

and

$$
p_n'' = \sigma_2' \cos(\gamma_2^n/2) + \sigma_2'' \sin(\gamma_2^n/2).
$$

Diffraction gratings

- $$\gamma_2^n = \arg(\Re(k_2^2) - \alpha_n^2 + i\Im(k_2^2))$$

  and $0 \leq \gamma_2^n < 2\pi$.
- $\Rightarrow p_n'' > 0$ for all n and $\{n : p_n' < 0\}$: finite.
- $|p_n''| > |p_n'|$ for $n \in \{n : p_n' < 0\}$.

Diffraction gratings

- Fix $\omega \notin \mathcal{B}$:
$$\mathcal{B} := \{\omega : \beta_j^n(\omega) = 0, \quad j = 1, 2\}.$$
-
$$|\beta_j^n| \geq C(1 + |n|^2)^{1/2}, \; j = 1, 2.$$
-
$$\begin{aligned} |B_1(u,u)| &\geq C\Big[\int_\Omega |\nabla u|^2 + ||u||^2_{H^{1/2}(\Gamma_1)} + \sum_{n\in\Lambda}(|p_n''| - |p_n'|)|u^{(n)}(-b)|^2 \\ &\quad + \sum_{n\notin\Lambda}|p_n''||u^{(n)}(-b)|^2\Big] \\ &\geq C[\int_\Omega |\nabla u|^2 + ||u||^2_{H^{1/2}(\Gamma_1)} + ||u||^2_{H^{1/2}(\Gamma_2)}] \\ &\geq C||u||^2_{H^1(\Omega)}. \end{aligned}$$

Diffraction gratings

- B_1: bounded coercive sesquilinear form over $H^1(\Omega)$:

$$|B_1(u,u)| \geq C\|u\|^2_{H^1(\Omega)}.$$

- Lax-Milgram lemma $\Rightarrow$ existence of a bounded invertible map $A_1 = A_1(\omega) : H^1(\Omega) \to (H^1(\Omega))'$ s.t. $\langle A_1 u, v\rangle = B_1(u,v)$;
- $'$: dual space.
- A_1^{-1}: bounded.
- $A_2 : H^1(\Omega) \to (H^1(\Omega))'$ $\langle A_2 u, v\rangle = B_2(u,v)$: compact and independent of ω.
- Fix $\omega_0 \notin \mathcal{B}$;
- Consider $A(\omega_0,\omega) = A_1(\omega_0) + \omega^2 A_2$.
- A_1: bounded invertible and A_2: compact $\Rightarrow$ $A(\omega_0,\omega)^{-1}$ exists by Fredholm theory for all $\omega \notin$ some discrete set $\mathcal{E}(\omega_0)$.
-

$$\|A_1(\omega) - A_1(\omega_0)\| \to 0, \quad \text{as } \omega \to \omega_0.$$

Diffraction gratings

- $\|A(\omega,\omega) - A(\omega_0,\omega)\| = \|A_1(\omega) - A_1(\omega_0)\|$: small for $|\omega - \omega_0|$ sufficiently small.
- Stability of bounded invertibility $\Rightarrow A(\omega,\omega)^{-1}$: exists and bounded for $|\omega - \omega_0|$ sufficiently small, $\omega \notin \mathcal{E}(\omega_0)$.
- $\omega_0 > 0$: arbitrary real number $\Rightarrow A(\omega,\omega)^{-1}$ exists for all but a discrete set of points.

Diffraction gratings

- Boundary integral formulations.
- Period Λ; $\Gamma = \{x_2 = f(x_1)\}/(\Lambda\mathbb{Z} \setminus \{0\})$.
- Quasi-periodic Green's function for the grating:

$$(\Delta + k^2)G^{\alpha,k}(x,y) = \sum_{n\in\mathbb{Z}} \delta_0(x - y - (n\Lambda, 0))e^{in\alpha\Lambda}.$$

- $$G^{\alpha,k}(x,y) = -\frac{i}{4}\sum_{n\in\mathbb{Z}} H_0^{(1)}(k|x - (n\Lambda,0) - y|)e^{in\alpha\Lambda}.$$

Diffraction gratings

- If $k \neq |\alpha_n|, \forall\, n \in \mathbb{Z}$ Poisson's summation formula

$$\sum_{n\in\mathbb{Z}} e^{i(\frac{2\pi n}{\Lambda}+\alpha)x_1} = \sum_{n\in\mathbb{Z}} \delta_0(x_1 - n\Lambda)e^{in\alpha\Lambda},$$

- Equivalent representation of $G^{\alpha,k}$:

$$G^{\alpha,k}(x,y) = \sum_{n\in\mathbb{Z}} \frac{e^{i\alpha_n(x_1-y_1)+i\beta_n(x_2-y_2)}}{k^2-\alpha_n^2}.$$

- β_n:

$$\beta_n = \begin{cases} \sqrt{k^2-\alpha_n^2} & k^2 > \alpha_n^2, \\ i\sqrt{\alpha_n^2-k^2} & k^2 < \alpha_n^2. \end{cases}$$

Diffraction gratings

- $\mathcal{S}_\Gamma^{\alpha,k}$: quasi-periodic single-layer potential associated with $G^{\alpha,k}$ on Γ.
- Integral representation of u:

$$u(x) = \begin{cases} u^i(x) + \mathcal{S}_\Gamma^{\alpha,k_1}[\psi](x), & x \in \{x = (x_1, x_2) : x_2 > f(x_1)\}, \\ \mathcal{S}_\Gamma^{\alpha,k_2}[\varphi](x), & x \in \{x = (x_1, x_2) : x_2 < f(x_1)\}, \end{cases}$$

- $(\varphi, \psi) \in L^2(\Gamma) \times L^2(\Gamma)$:

$$\begin{cases} \mathcal{S}_\Gamma^{\alpha,k_2}[\varphi] - \mathcal{S}_\Gamma^{\alpha,k_1}[\psi] = u^i \\ \dfrac{\partial(\mathcal{S}_\Gamma^{\alpha,k_2}[\varphi])}{\partial\nu}\Big|_- - \dfrac{\partial(\mathcal{S}_\Gamma^{\alpha,k_1}[\psi])}{\partial\nu}\Big|_+ = \dfrac{\partial u^i}{\partial\nu} \end{cases} \quad \text{on } \Gamma.$$

- For all but possibly a countable set of frequencies ω_j, $\omega_j \to +\infty$, the system of integral equations has a unique solution $(\varphi, \psi) \in H^{-1/2}(\Gamma) \times H^{-1/2}(\Gamma)$.

Lecture 10: Photonic crystals

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Photonic crystals

- Photonic crystals (also known as photonic band-gap materials):
  - Periodic dielectric structures that have a band gap that forbids propagation of a certain frequency range of light.
  - Band gap calculations: high-contrast materials, periodicity of the same order as the wavelength; efficient numerical schemes.
  - Control light and produce effects that are impossible with conventional optics.
  - Resonant cavities: making point defects in a photonic crystal $\rightarrow$ light can be localized, trapped in the defect. The frequency, symmetry, and other properties of the defect mode can be easily tuned to anything desired.

Photonic crystals

- Mathematically speaking:
  - Appearance of bandgaps in the spectrum of the associated operator.
  - Spectral techniques to analyze bandgaps:
    - High-contrast models.
    - Characterization of the bandgap (Floquet theory).
    - Sensitivity analysis of the bandgap with respect to material and geometry of the structure (based on generalized argument principle).
- Bandgap calculations: involve a family of eigenvalue problems (as the quasi-periodicity is varying).
- Muller's method.

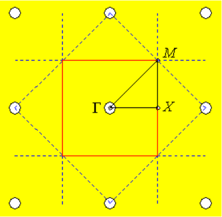
Photonic crystals

- Floquet transform: $f(x)$: function decaying sufficiently fast,

$$\mathcal{U}[f](x,\alpha) = \sum_{n\in\mathbb{Z}^d} f(x-n)e^{i\alpha\cdot n}.$$

- $\mathcal{U}$: analogue of the Fourier transform for the periodic case.
- $\alpha \in$ Brillouin zone $\mathbb{R}^d/(2\pi\mathbb{Z}^d)$: quasi-momentum.
- Expansion into a direct integral of operators:

$$L = \int_{\mathbb{R}^d/(2\pi\mathbb{Z}^d)}^{\oplus} L(\alpha)\, d\alpha, \quad L(\alpha)[f] = \mathcal{U}[L[f]].$$



Photonic crystals

- Spectral theorem for a self-adjoint operator:

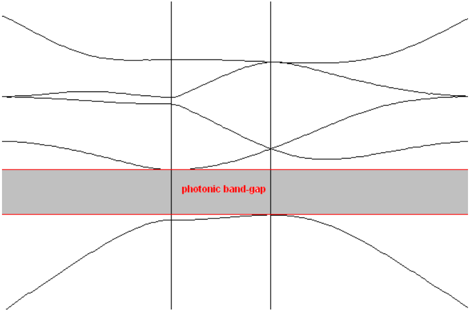
$$\sigma(L) = \bigcup_{\alpha \in \mathbb{R}^d/(2\pi\mathbb{Z}^d)} \sigma(L(\alpha)),$$

- $\sigma(L)$: spectrum of L.
- L: elliptic $\to$ $L(\alpha)$: compact resolvents $\to$ discrete spectra $(\mu_l(\alpha))_l$,

$$\sigma(L) = \left[\min_\alpha \mu_l(\alpha), \max_\alpha \mu_l(\alpha) \right].$$

Photonic crystals

- Gohberg-Sigal theory:
  - Sensitivity analysis of band gaps with respect to changes of the coefficients of L.
  - Analysis of photonic crystal cavities: defect mode inside the band gap.



Photonic crystals

- Floquet transform:
  - Plays in the periodic case the role of the Fourier transform.
  - Structure of spectra of periodic elliptic operators.
- $f(x)$: function decaying sufficiently fast.
- Floquet transform of f:

$$\mathcal{U}[f](x,\alpha) = \sum_{n\in\mathbb{Z}^d} f(x-n)e^{i\alpha\cdot n}.$$

- α: quasi-momentum; analogue of the dual variable in the Fourier transform.
- x shifted by a period $m \in \mathbb{Z}^d \Rightarrow$ Floquet condition:

$$\mathcal{U}[f](x+m,\alpha) = e^{i\alpha\cdot m}\mathcal{U}[f](x,\alpha).$$

Photonic crystals

- It suffices to know $\mathcal{U}[f](x,\alpha)$ on the unit cell $Y :=]0,1[^d$ in order to recover it completely as a function of the x-variable.
- $\mathcal{U}[f](x,\alpha)$: periodic with respect to the quasi-momentum α:

$$\mathcal{U}[f](x,\alpha+2\pi m) = \mathcal{U}[f](x,\alpha), \quad m \in \mathbb{Z}^d.$$

- α can be considered as an element of the torus $\mathbb{R}^d/(2\pi\mathbb{Z}^d)$.
- All information about $\mathcal{U}[f](x,\alpha)$: contained in its values for α in the Brillouin zone B of the dual lattice $2\pi\mathbb{Z}^d$.

Photonic crystals

- Analogue of the Plancherel theorem:
  - Suppose that the measures $d\alpha$ and the dual torus $\mathbb{R}^d/(2\pi\mathbb{Z}^d)$ are normalized;
  - $$\mathcal{U} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d/(2\pi\mathbb{Z}^d), L^2(Y)) : \textit{isometric}.$$
  - Its inverse:
  $$\mathcal{U}^{-1}[g](x) = \int_{\mathbb{R}^d/(2\pi\mathbb{Z}^d)} g(x,\alpha)\, d\alpha;$$
  - $g(x,\alpha) \in L^2(\mathbb{R}^d/(2\pi\mathbb{Z}^d), L^2(Y))$: extended from Y to all $x \in \mathbb{R}^d$ according to the Floquet condition.

Photonic crystals

- Spectrum of self-adjoint operators.
- L: linear self-adjoint operator in the Hilbert space H with domain $D(L), \overline{D(L)} = H$.
- Resolvent:

$$\rho(L) := \left\{ z \in \mathbb{C} : (zI - L)^{-1} \text{exists as a bounded operator } : H \to D(L) \right\}.$$

- Spectrum of L: complement of the resolvent,

$$\sigma(L) = \mathbb{C} \setminus \rho(L).$$

- L: self-adjoint $\Rightarrow z \in \rho(L)$ iff there exists a constant $C(z)$ s.t. for all $u \in D(L)$,

$$\|(zI - L)u\|_H \geq C(z)\|u\|_H.$$

- $\sigma(L) \neq \emptyset$ and $\sigma(L) \subset \mathbb{R}$.
- Weyl's criteron for characterizing $\sigma(l)$: $z \in \sigma(L)$ iff there exists $u_n \in D(L)$ s.t.

$$\lim_{n \to +\infty} \|(zI - L)u_n\|_H = 0.$$

Photonic crystals

- Point spectrum $\sigma_p(L)$ of L:

  $$\sigma_p(L) := \{z \in \sigma(L) : (zI - L)^{-1} \text{does not exist or equivalently } \ker(zI - L) \neq \emptyset\}.$$

- Continuous spectrum $\sigma_c(L) := \sigma(L) \setminus \sigma_p(L)$.
  If $z \in \sigma_c(L)$, then $(zI - L)^{-1}$ does exist but is not bounded.
- Discrete spectrum spectrum $\sigma_d(L)$:

  $$\sigma_d(L) := \{z \in \sigma_p(L) : \dim \ker(zI - L) < \infty \text{ and } z \text{ is isolated in } \sigma(L)\}.$$

- Essential spectrum: $\sigma_{ess}(L) := \sigma(L) \setminus \sigma_d(L)$.
- L: self-adjoint $\Rightarrow$

  $$\begin{aligned} \sigma_{ess}(L) = & \overline{\sigma_c(L)} \\ & \cup \{ \text{ eigenvalues of infinite multiplicity and their accumulation points } \} \\ & \cup \{ \text{ accumulation points of } \sigma_d(L) \}. \end{aligned}$$

Photonic crystals

- A family of operators $\{\mathcal{E}(t)\}_{t=-\infty}^{+\infty}$: spectral family (also called resolution of identity) if the following conditions are satisfied:
  - $\mathcal{E}(t)$: projector for all $t \in \mathbb{R}$;
  - $\mathcal{E}(t) \leq \mathcal{E}(s)$ for all $t < s$;
  - $\{\mathcal{E}(t)\}$: right continuous with respect to the strong topology,

$$\lim_{s \to t+0} \|\mathcal{E}(s)u - \mathcal{E}(t)u\|_H = 0 \quad \text{for all } u \in H;$$

  - Normalization of $\{\mathcal{E}(t)\}$:

$$\lim_{t \to +\infty} \|\mathcal{E}(t)u - u\|_H = 0 \quad \text{for all } u \in H.$$

Photonic crystals

- $u, v \in H$, $\langle \mathcal{E}(t)u, v\rangle_H$: function of bounded variation with respect to t.
- L: self-adjoint operator $\Rightarrow$ unique spectral representation.
- There is a unique spectral family $\mathcal{E}(t)$ s.t.

$$Lu = \int_{-\infty}^{+\infty} t \, d\mathcal{E}(t)u \quad \text{for all } u \in D(L).$$

- Spectral theorem $\Rightarrow$
  - $$(zI - L)^{-1} = \int_{-\infty}^{+\infty} \frac{1}{z-t} \, d\mathcal{E}(t) \quad \text{for all } z \in \rho(L);$$
  - $z \in \sigma_p(L)$ iff $\mathcal{E}(z) - \mathcal{E}(z-0) \neq 0$;
  - $z \in \sigma_c(L)$ iff $\mathcal{E}(z) - \mathcal{E}(z-0) = 0$;
  - $\mathcal{E}(z-0) := \lim_{\epsilon \to 0+} \mathcal{E}(z-\epsilon)$ in the sense of strong operator topology.

Photonic crystals

- $\mathcal{C}(\sigma(L))$: set of continuous functions on $\sigma(L)$.
- $$f(L) := \lim_{n \to +\infty} P_n(L)$$
  with $\{P_n\}$ being a sequence of polynomials converging uniformly to f as $n \to +\infty$.
- For any $u \in H$, $f \mapsto \langle u, f(L)u \rangle_H$: positive linear function on $\mathcal{C}(\sigma(L))$.
- $\Rightarrow$ There exists a unique Radon measure $\mu(u)$ on $\sigma(L)$ (called the spectral measure associated to u and L) s.t.
  $$\int_{\sigma(L)} f \, d\mu(u) = \langle u, f(L)u \rangle_H \quad \text{for all } f \in \mathcal{C}(\sigma(L)).$$
- $\Rightarrow \mu(u)(\sigma(L)) = \|u\|_H^2 \Rightarrow \mu(u)$: finite measure.

Photonic crystals

- $\mu(u)$: invariant under linear transformations and can be decomposed into three parts:

$$\mu(u) = \mu_{ac} + \mu_{sc} + \mu_{pp}.$$

  - μ_{pp}: pure point measure;
  - μ_{ac}: absolutely continuous;
  - μ_{sc}: singular with respect to the Lebesgue measure.

Photonic crystals

- $$H_{pp} := \{u \in H : \mu(u) \text{ is pure point }\},$$
  $$H_{ac} := \{u \in H : \mu(u) \text{ is absolutely continuous }\},$$
  $$H_{sc} := \{u \in H : \mu(u) \text{ is singulary continuous }\}.$$
- $H = H_{pp} \oplus H_{ac} \oplus H_{sc}$.
- Each subspace is invariant under L.
- $$\sigma(L) = \overline{\sigma_{pp}}(L) \cup \sigma_{ac}(L) \cup \sigma_{sc}(L);$$
- $$\overline{\sigma_{pp}}(L) = \sigma(L|_{H_{pp}}), \sigma_{ac}(L) = \sigma(L|_{H_{ac}}), \quad \text{and } \sigma_{sc}(L) = \sigma(L|_{H_{sc}}),$$
- Union may not be disjoint.
- $$\langle u, (z-L)^{-1} u \rangle_H = \int_{\mathbb{R}} \frac{d\mu(u)(t)}{z-t}.$$
- $\Rightarrow d\mu(u)(t) = \langle d\mathcal{E}(t) u, u \rangle_H$ for all $t \in \mathbb{R}$.

Photonic crystals

- L: self-adjoint and compact.
  - Sequence of eigenvalues $\lambda_j \neq 0, j \in \mathbb{N}$:

$$|\lambda_0| \geq |\lambda_1| \geq \ldots \geq |\lambda_j| \geq \ldots;$$

  - If there are infinitely many eigenvalues then $\lim_{j\to+\infty} \lambda_j = 0$ and 0 is the only accumulation point of $\{\lambda_j\}_{j\in\mathbb{N}}$;
  - Multiplicity of λ_j: finite;
  - φ_j: normalized eigenvector for $\lambda_j \Rightarrow \{\varphi_j\}_{j=0}^{+\infty}$: orthonormal basis on $R(L)$ and the spectral theorem $\Rightarrow$

$$Lu = \sum_{j=0}^{+\infty} \lambda_j \langle u, \varphi_j \rangle_H \varphi_j, \quad u \in H.$$

  - $\sigma(L) = \{0, \lambda_0, \lambda_1, \ldots, \lambda_j, \ldots\}$ while 0: not necessarily an eigenvalue of L.

Photonic crystals

- Structure of spectra of periodic elliptic operators.
- $L(x, \partial_x)$: linear partial differential operator whose coefficients are periodic with respect to $\mathbb{Z}^d, d = 2, 3$.
- Periodicity $\Rightarrow L(x, \partial_x)$ commutes with the Floquet transform:

$$\mathcal{U}[Lf](x, \alpha) = L(x, \partial_x)\mathcal{U}[f](x, \alpha).$$

- $\forall \alpha$, $L(x, \partial_x)$ now acts on functions satisfying the Floquet condition.
- $L(\alpha)$ (its domain changes with α);
- $L : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$: expanded into the direct integral of operators:

$$L = \int_{\mathbb{R}^d/(2\pi\mathbb{Z}^d)}^{\oplus} L(\alpha)\, d\alpha.$$

Photonic crystals

- L: self-adjoint $\Rightarrow$

$$\sigma(L) = \bigcup_{\alpha \in B} \sigma(L(\alpha)).$$

- L: self-adjoint + elliptic $\Rightarrow$ $L(\alpha)$: compact resolvent $\Rightarrow$ discrete spectra.
- L: bounded from below $\Rightarrow$ $\sigma(L(\alpha))$ accumulates only at $+\infty$.
- $\mu_n(\alpha)$: nth eigenvalue of $L(\alpha)$ (counted in increasing order with their multiplicity).
- Band function function $\alpha \mapsto \mu_n(\alpha)$: continuous in B.
- One branch of the dispersion relations.
- $\sigma(L)$ consists of the closed intervals (called the spectral bands)

$$\sigma(L) = \bigcup_n \left[\min_\alpha \mu_n(\alpha), \max_\alpha \mu_n(\alpha) \right];$$

- $\min_\alpha \mu_n(\alpha) \to +\infty$ when $n \to +\infty$.
- $d \geq 2$: spectral bands do overlap in general.
- Opening gaps in the spectrum of L: high contrast materials.

Photonic crystals

- Boundary integral formulation:
- $d = 2$; $Y :=]0,1[^2$: unit cell; $\chi(Y \setminus \overline{D})$: indicator function of $Y \setminus \overline{D}$.
- Seek eigenfunctions u of

$$\begin{cases} \nabla \cdot (1 + (k-1)\chi(Y \setminus \overline{D}))\nabla u + \omega^2 u = 0 \quad \text{in } Y, \\ e^{-i\alpha \cdot x} u : \text{ periodic in the whole space.} \end{cases}$$

- Equivalently,

$$\begin{cases} k\Delta u + \omega^2 u = 0 & \text{in } Y \setminus \overline{D}, \\ \Delta u + \omega^2 u = 0 & \text{in } D, \\ u|_+ = u|_- & \text{on } \partial D, \\ k \dfrac{\partial u}{\partial \nu}\Big|_+ = \dfrac{\partial u}{\partial \nu}\Big|_- & \text{on } \partial D, \\ e^{-i\alpha \cdot x} u : \text{ periodic in the whole space.} \end{cases}$$

Photonic crystals

- $\forall \alpha$, $\sigma_\alpha(D,k)$: (discrete) spectrum.
- Spectral band of the photonic crystal:

$$\bigcup_{\alpha \in [0,2\pi]^2} \sigma_\alpha(D,k).$$

- Investigate behavior of $\sigma_\alpha(D,k)$ when $k \to +\infty$.
- D: invariant under the transformations

$$(x_1,x_2) \mapsto (-x_1,-x_2), \qquad (x_1,x_2) \mapsto (-x_1,x_2), \qquad (x_1,x_2) \mapsto (x_2,x_1).$$

- α restricted to the reduced Brillouin zone

$$T := \Big\{ \alpha = (\alpha_1,\alpha_2) : 0 \le \alpha_1 \le \pi, 0 \le \alpha_2 \le \alpha_1 \Big\}.$$

- Take $\alpha \in T$ rather than $\alpha \in [0,2\pi]^2$.

Photonic crystals

- Assumptions:
  - ω^2: not an eigenvalue of $-\Delta$ in $Y \setminus \overline{D}$ with the Dirichlet boundary condition on ∂D and the quasi-periodic condition on ∂Y;
  - ω^2/k: not an eigenvalue of $-\Delta$ in D with the Dirichlet boundary condition.
- Representation formula: $\phi, \psi \in L^2(\partial D)$,

$$u(x) = \begin{cases} \mathcal{S}^{\alpha,\omega}[\phi](x), & x \in D, \\ H(x) + \mathcal{S}^{\alpha,\frac{\omega}{\sqrt{k}}}[\psi](x). & x \in Y \setminus \overline{D}, \end{cases}$$

- H:

$$H(x) = -\mathcal{S}_Y^{\alpha,\frac{\omega}{\sqrt{k}}}[\frac{\partial u}{\partial \nu}|_{\partial Y}] + \mathcal{D}_Y^{\alpha,\frac{\omega}{\sqrt{k}}}[u|_{\partial Y}], \quad x \in Y.$$

Photonic crystals

- u, v: quasi-periodic in $Y \Rightarrow \int_{\partial Y} \frac{\partial u}{\partial \nu} \overline{v} = 0$.
- $\Rightarrow H \equiv 0 \Rightarrow$ representation formula:

$$u = \begin{cases} \mathcal{S}^{\alpha,\omega}[\phi], & \text{in } D, \\ \mathcal{S}^{\alpha,\frac{\omega}{\sqrt{k}}}[\psi], & \text{in } Y \setminus \overline{D}. \end{cases}$$

- Transmission conditions $\Rightarrow (\phi, \psi) \in L^2(\partial D) \times L^2(\partial D)$ solution to the system of integral equations:

$$\begin{cases} \mathcal{S}^{\alpha,\omega}[\phi] - \mathcal{S}^{\alpha,\frac{\omega}{\sqrt{k}}}[\psi] = 0 & \text{on } \partial D, \\ \Big(-\frac{1}{2} I + (\mathcal{K}^{-\alpha,\omega})^* \Big)[\phi] - k\Big(\frac{1}{2} I + (\mathcal{K}^{-\alpha,\frac{\omega}{\sqrt{k}}})^* \Big)[\psi] = 0 & \text{on } \partial D. \end{cases}$$

- Converse true: $(\phi, \psi) \in L^2(\partial D) \times L^2(\partial D)$: nonzero solution $\Rightarrow \omega$: eigenvalue.

Photonic crystals

- Proof of the Representation Formula:
  - u: eigenfunction $\Rightarrow \exists ! \; (\phi, \psi) \in L^2(\partial D) \times L^2(\partial D)$ s.t. u has the representation formula.
  - (ϕ, ψ): solution to the system of integral equations.
  - $u \longmapsto (\phi, \psi)$: one-to-one.

Photonic crystals

- $\mathcal{S}^{-\alpha,\omega} : L^2(\partial D) \to H^1(\partial D)$.
- u: eigenfunction $\Rightarrow$

$$u|_{\partial D} \perp \ker(\mathcal{S}^{-\alpha,\omega}).$$

- Proof:
    - $(\Delta + \omega^2)u = 0$ in $D \Rightarrow$

$$u(x) = \mathcal{D}^{\alpha,\omega}\left[u|_{\partial D}\right](x) - \mathcal{S}^{\alpha,\omega}\left[\frac{\partial u}{\partial \nu}\Big|_-\right](x), \quad x \in D.$$

    - $\Rightarrow$

$$\frac{1}{2}u|_{\partial D} = \mathcal{K}^{\alpha,\omega}\left[u|_{\partial D}\right] - \mathcal{S}^{\alpha,\omega}\left[\frac{\partial u}{\partial \nu}\Big|_-\right].$$

    - $\phi \in \ker(\mathcal{S}^{-\alpha,\omega})$.
    - Assumption on $\omega^2 \Rightarrow \mathcal{S}^{-\alpha,\omega}[\phi] = 0$ in $Y \setminus \overline{D}$.

Photonic crystals

- $\Rightarrow$

$$\begin{cases} \mathcal{S}^{-\alpha,\omega}[\phi] = 0, \\ \frac{1}{2}\phi + (\mathcal{K}^{\alpha,\omega})^*[\phi] = 0 \end{cases} \quad \text{on } \partial D.$$

- $\Rightarrow$

$$\begin{aligned} \frac{1}{2}\langle u|_{\partial D}, \phi\rangle &= \langle \mathcal{K}^{\alpha,\omega}[u|_{\partial D}], \phi\rangle - \left\langle \mathcal{S}^{\alpha,\omega}\left[\frac{\partial u}{\partial \nu}\Big|_-\right], \phi\right\rangle \\ &= \langle u|_{\partial D}, (\mathcal{K}^{\alpha,\omega})^*[\phi]\rangle - \left\langle \frac{\partial u}{\partial \nu}\Big|_-, \mathcal{S}^{-\alpha,\omega}[\phi]\right\rangle \\ &= -\frac{1}{2}\langle u|_{\partial D}, \phi\rangle - 0. \end{aligned}$$

Photonic crystals

- Finding $(\phi, \psi) \Leftrightarrow$

$$(*) \begin{cases} \mathcal{S}^{\alpha,\omega}[\phi] = u|_{\partial D} & \text{on } \partial D, \\ \Big(-\dfrac{1}{2}I + (\mathcal{K}^{-\alpha,\omega})^*\Big)[\phi] = \dfrac{\partial u}{\partial \nu}\Big|_{-} & \text{on } \partial D, \end{cases}$$

$$\begin{cases} \mathcal{S}^{\alpha,\frac{\omega}{\sqrt{k}}}[\psi] = u|_{\partial D} & \text{on } \partial D, \\ \Big(\dfrac{1}{2}I + (\mathcal{K}^{-\alpha,\frac{\omega}{\sqrt{k}}})^*\Big)[\psi] = \dfrac{\partial u}{\partial \nu}\Big|_{+} & \text{on } \partial D. \end{cases}$$

Photonic crystals

- $u|_{\partial D} \perp \ker(\mathcal{S}^{-\alpha,\omega}) \Rightarrow \exists \phi_0 \in L^2(\partial D)$ s.t.

$$\mathcal{S}^{\alpha,\omega}[\phi_0 + \phi] = u|_{\partial D} \quad \text{on } \partial D, \quad \forall \phi \in \ker(\mathcal{S}^{\alpha,\omega}).$$

- To show existence of a solution to $(*)$, it suffices to prove that $\exists \phi \in \ker(\mathcal{S}^{\alpha,\omega})$ s.t.

$$\big(-\frac{1}{2}I + (\mathcal{K}^{-\alpha,\omega})^*\big)[\phi + \phi_0] = \frac{\partial u}{\partial \nu}\Big|_- \text{ on } \partial D.$$

- $\Rightarrow$

$$\phi = \frac{\partial\left(\mathcal{S}^{\alpha,\omega}[\phi_0] - u\right)}{\partial \nu}\Big|_- .$$

- $\mathcal{S}^{\alpha,\omega}[\phi_0] - u$: solution to $\Delta + \omega^2$ in D with the Dirichlet boundary condition $\Rightarrow$

$$\frac{\partial\left(\mathcal{S}^{\alpha,\omega}[\phi_0] - u\right)}{\partial \nu}\Big|_- \in \ker(\mathcal{S}^{\alpha,\omega}).$$

Photonic crystals

- ϕ_1 and ϕ_2: two solutions.
- Assumption on $\omega^2 \Rightarrow \mathcal{S}^{\alpha,\omega}[\phi_1 - \phi_2] = 0$ in $Y \setminus \overline{D} \Rightarrow$

$$\Big(\frac{1}{2} I + (\mathcal{K}^{-\alpha,\omega})^*\Big)[\phi_1 - \phi_2] = 0 \quad \text{on } \partial D.$$

- $\Big(-\frac{1}{2} I + (\mathcal{K}^{-\alpha,\omega})^*\Big)[\phi_1 - \phi_2] = 0$ on $\partial D \Rightarrow \phi_1 = \phi_2$.

Photonic crystals

- Converse: (ϕ, ψ): (nontrivial) solution to the system of integral equations. One only needs to prove: u given by the representation formula is not trivial.
- Suppose $u = 0$ in $Y \Rightarrow \mathcal{S}^{\alpha,\omega}[\phi] = 0$ in D.
- Assumption on $\omega^2 \Rightarrow \mathcal{S}^{\alpha,\omega}[\phi] = 0$ in $Y \setminus \overline{D} \Rightarrow \phi = 0$ on ∂D. Assumption on $\omega^2/k \Rightarrow \psi = 0$ on ∂D.

Photonic crystals

- Suppose $\alpha \neq 0$.

$$\mathcal{A}^{\alpha,k}(\omega) := \begin{pmatrix} \mathcal{S}^{\alpha,\omega} & -\mathcal{S}^{\alpha,\frac{\omega}{\sqrt{k}}} \\ \frac{1}{k}\left(\frac{1}{2}I - (\mathcal{K}^{-\alpha,\omega})^*\right) & \frac{1}{2}I + (\mathcal{K}^{-\alpha,\frac{\omega}{\sqrt{k}}})^* \end{pmatrix}.$$

- ω^2: eigenvalue corresponding to u with a given quasi-momentum α iff ω: characteristic value of $\mathcal{A}^{\alpha,k}$.
- For $\alpha = 0$,

$$\widetilde{\mathcal{A}}^{0,k}(\omega) := \begin{pmatrix} \mathcal{S}^{0,\omega} & -\frac{1}{k}\mathcal{S}^{0,\frac{\omega}{\sqrt{k}}} \\ \frac{1}{2}I - (\mathcal{K}^{0,\omega})^* & \frac{1}{2}I + (\mathcal{K}^{0,\frac{\omega}{\sqrt{k}}})^* \end{pmatrix}.$$

- By a change of functions, ω: eigenvalue corresponding to u for $\alpha = 0$ iff ω^2: characteristic value of $\widetilde{\mathcal{A}}^{0,k}$.

Photonic crystals

- Characteristic values of $\mathcal{A}^{\alpha,k}$ and $\widetilde{\mathcal{A}}^{0,k}$.
- $\mathcal{A}^{\alpha,k}$: Fredholm analytic with index 0 in $\mathbb{C} \setminus i\mathbb{R}^-$.
- $\omega \mapsto (\mathcal{A}^{\alpha,k})^{-1}(\omega)$: meromorphic function and its poles are on the real axis.
- Proof: logarithmic behavior of quasi-periodic Green's functions $\Rightarrow$ define $\mathcal{A}^{\alpha,k}$ on $\mathbb{C} \setminus i\mathbb{R}^-$.

Photonic crystals

- $\mathcal{A}^{\alpha,k}$: Fredholm analytic with index 0 in $\mathbb{C} \setminus i\mathbb{R}^- \Leftarrow$

$$\mathcal{A}^{\alpha,k}(\omega) = \begin{pmatrix} \mathcal{S}^{\alpha,0} & -\mathcal{S}^{\alpha,0} \\ \frac{1}{2k} I & \frac{1}{2} I \end{pmatrix} + \begin{pmatrix} \mathcal{S}^{\alpha,\omega} - \mathcal{S}^{\alpha,0} & -\mathcal{S}^{\alpha,\frac{\omega}{\sqrt{k}}} + \mathcal{S}^{\alpha,0} \\ \frac{1}{k}(\mathcal{K}^{-\alpha,\omega})^* & (\mathcal{K}^{-\alpha,\omega})^* \end{pmatrix}$$
$$:= \mathcal{A}^{\alpha} + \mathcal{B}^{\alpha}(\omega).$$

- $\mathcal{A}^{\alpha}$: invertible and $\mathcal{B}^{\alpha}$: compact and analytic in $\omega \Rightarrow \mathcal{A}^{\alpha,k}$: Fredholm analytic with index 0.
- Steinberg's theorem $\Rightarrow$ invertibility of $\mathcal{A}^{\alpha,k}(\omega)$ at $\omega = 0$ shows that $\omega \mapsto (\mathcal{A}^{\alpha,k})^{-1}(\omega)$: meromorphic function.

Photonic crystals

- ω_0: pole of $(\mathcal{A}^{\alpha,k})^{-1}(\omega)$. Then ω_0: characteristic value of $\mathcal{A}^{\alpha,k}$.
- (ϕ,ψ): root function associated with ω_0. Define

$$u(x) = \begin{cases} \mathcal{S}^{\alpha,\omega_0}[\phi](x), & x \in D, \\ \mathcal{S}^{\alpha,\frac{\omega_0}{\sqrt{k}}}[\psi](x), & x \in Y \setminus \overline{D}. \end{cases}$$

- Integrating by parts $\Rightarrow$

$$\int_Y (1+(k-1)\chi(Y\setminus\overline{D}))|\nabla u|^2 - \omega_0^2 \int_Y |u|^2 = 0.$$

- $\Rightarrow$ ω_0: real.
- Same result holds for $\widetilde{\mathcal{A}}^{0,k}$.

Photonic crystals

- Numerical approach for band structure calculations:
  - Discretization $\Rightarrow$ linear system in the form $\mathcal{A}^{\alpha,k}(\omega)[x] = 0$.
  - Unknown vector x: represents point values of the densities ϕ and ψ on ∂D.
  - Muller's method for

$$f(\omega) := \frac{1}{x \cdot \mathcal{A}^{\alpha,k}(\omega)^{-1}[y]};$$

  - x and y: two fixed random vectors.

Photonic crystals

- Sensitivity analysis with respect to the contrast and/or the shape of the inclusion: use of the generalized Rouché's theorem.
- Asymptotic expansion asymptotic expansion of $\mathcal{A}^{\alpha,k}$ for $\alpha \neq 0$ as $k \to +\infty$:

$$\mathcal{A}^{\alpha,k}(\omega) = \mathcal{A}_0^{\alpha}(\omega) + \sum_{l=1}^{+\infty} \frac{1}{k^l} \mathcal{A}_l^{\alpha}(\omega).$$

- $$\mathcal{A}_0^{\alpha}(\omega) = \begin{pmatrix} \mathcal{S}^{\alpha,\omega} & -\mathcal{S}^{\alpha,0} \\ 0 & \frac{1}{2}I + (\mathcal{K}^{-\alpha,0})^* \end{pmatrix};$$

$$\mathcal{A}_1^{\alpha}(\omega) = \begin{pmatrix} 0 & -\mathcal{S}_1^{\alpha,\omega} \\ \left(\frac{1}{2}I - (\mathcal{K}^{-\alpha,\omega})^*\right) & (\mathcal{K}_1^{-\alpha,\omega})^* \end{pmatrix};$$

- For $l \geq 2$,

$$\mathcal{A}_l^{\alpha}(\omega) = \begin{pmatrix} 0 & -\mathcal{S}_l^{\alpha,\omega} \\ 0 & (\mathcal{K}_l^{-\alpha,\omega})^* \end{pmatrix}.$$

Photonic crystals

- $\alpha \neq 0$. $\omega_0^\alpha \in \mathbb{R}$: characteristic value of $\mathcal{A}_0^\alpha$ iff $(\omega_0^\alpha)^2$: either an eigenvalue of $-\Delta$ in D with the Dirichlet boundary condition or an eigenvalue of $-\Delta$ in $Y \setminus \overline{D}$ with the Dirichlet boundary condition on ∂D and the quasi-periodic condition on ∂Y.
- Proof:
  - $\omega = \omega_0^\alpha \in \mathbb{R}$: characteristic value of $\mathcal{A}_0^\alpha \Rightarrow \exists (\phi, \psi) \neq 0$ s.t.

$$(**) \left\{ \begin{array}{l} \mathcal{S}^{\alpha,\omega}[\phi] - \mathcal{S}^{\alpha,0}[\psi] = 0, \\ \left(\frac{1}{2} I + (\mathcal{K}^{-\alpha,0})^*\right)[\psi] = 0 \end{array} \right. \quad \text{on } \partial D.$$

  - $\Rightarrow \psi = 0 \Rightarrow \mathcal{S}^{\alpha,\omega}[\phi] = 0$ on ∂D.
  - $\phi \neq 0$, $\mathcal{S}^{\alpha,\omega}[\phi] \neq 0$ either in D or in $Y \setminus \overline{D} \Rightarrow (\omega_0^\alpha)^2$: either an eigenvalue of $-\Delta$ in D with the Dirichlet boundary condition or an eigenvalue of $-\Delta$ in $Y \setminus \overline{D}$ with the Dirichlet boundary condition on ∂D and the quasi-periodic condition on ∂Y, and $\mathcal{S}^{\alpha,\omega}[\phi]$: associated eigenfunction.

Photonic crystals

- Converse:
  - $(\omega_0^\alpha)^2$: eigenvalue of $-\Delta$ in D with the Dirichlet boundary condition $\Rightarrow$ by Green's representation formula,

$$u(x) = -\mathcal{S}^{\alpha,\omega}\left[\frac{\partial u}{\partial \nu}\Big|_{\partial D}\right], \quad x \in D.$$

  - $\Rightarrow$ $(**)$ holds with $(\phi, \psi) = (\partial u/\partial \nu|_{\partial D}, 0)$.
  - Other case: treated similarly.

Photonic crystals

- Generalized Rouché's theorem:

$$\omega^{\alpha,k} - \omega^0 = \frac{1}{2i\pi} \operatorname{tr} \int_{\partial V} (\omega - \omega^0)(\mathcal{A}_k^\alpha)^{-1}(\omega) \frac{d}{d\omega} \mathcal{A}^{\alpha,k}(\omega) d\omega.$$

- Asymptotic expansion for the eigenvalue perturbations $\omega^{\alpha,k} - \omega^0$. Suppose $\alpha \neq 0$:

$$\omega^{\alpha,k} - \omega^0 = \frac{1}{2i\pi k} \operatorname{tr} \int_{\partial V} (\mathcal{A}_0^\alpha)^{-1}(\omega) \mathcal{A}_1^\alpha(\omega) d\omega;$$

$$(\mathcal{A}_0^\alpha)^{-1}(\omega) = \begin{pmatrix} (\mathcal{S}^{\alpha,\omega})^{-1} & (\mathcal{S}^{\alpha,\omega})^{-1} \mathcal{S}^{\alpha,0} (\frac{1}{2} I + (\mathcal{K}^{-\alpha,0})^*)^{-1} \\ 0 & (\frac{1}{2} I + (\mathcal{K}^{-\alpha,0})^*)^{-1} \end{pmatrix}.$$

Photonic crystals

- Explicit calculations of the leading-order term.
- u^0: (normalized) eigenvector associated to the simple eigenvalue $(\omega^0)^2$; $\varphi := \partial u^0/\partial\nu|_- \Rightarrow u^0(x) = -\mathcal{S}^{\alpha,\omega^0}[\varphi](x)$ for $x \in D$.
- $\Rightarrow$

$$\langle \varphi, \frac{d}{d\omega}\mathcal{S}^{\alpha,\omega}[\varphi]|_{\omega=\omega^0}\rangle = -2\omega^0 \int_D |u^0|^2.$$

- Proof:
  - $$\Delta \frac{d}{d\omega} G^{\alpha,\omega}(x,y) + \omega^2 \frac{d}{d\omega} G^{\alpha,\omega}(x,y) = -2\omega G^{\alpha,\omega}(x,y).$$
  - $$\frac{d}{d\omega} G^{\alpha,\omega}(x,y) = -2\omega \int_Y G^{\alpha,\omega}(x,z) G^{\alpha,\omega}(z,y) dz.$$

Photonic crystals

- $\forall \psi \in L^2(\partial D)$,

$$
\begin{aligned}
\frac{d\mathcal{S}^{\alpha,\omega}[\psi](x)}{d\omega} =& \frac{d}{d\omega}\int_{\partial D} G^{\alpha,\omega}(x,y)\psi(y)\, d\sigma(y) \\
=& \int_{\partial D} \frac{d}{d\omega} G^{\alpha,\omega}(x,y)\psi(y)\, d\sigma(y) \\
=& -2\omega \int_Y G^{\alpha,\omega}(x,z) \int_{\partial D} G^{\alpha,\omega}(z,y)\psi(y)\, d\sigma(y) dz \\
=& -2\omega \int_Y G^{\alpha,\omega}(x,z)\mathcal{S}^{\alpha,\omega}[\psi](z) dz.
\end{aligned}
$$

Photonic crystals

- From
$$\mathcal{S}^{\alpha,\omega^0}[\varphi] = \begin{cases} -u^0 & \text{in } D, \\ 0 & \text{in } Y \setminus \overline{D}, \end{cases}$$
- $\Rightarrow$
$$\left\langle \varphi, \frac{d\mathcal{S}^{\alpha,\omega}[\varphi]}{d\omega}\Big|_{\omega=\omega^0} \right\rangle = \int_{\partial D} \varphi(x) \frac{d\mathcal{S}^{-\alpha,\omega}}{d\omega}[\overline{\varphi}](x)\Big|_{\omega=\omega^0} d\sigma(x)$$
$$= -2\omega^0 \int_{\partial D} \varphi(x) \int_Y G^{\alpha,\omega^0}(x,z) \mathcal{S}^{-\alpha,\omega^0}[\overline{\varphi}](z) dz \, d\sigma(x)$$
$$= -2\omega^0 \int_{\partial D} \int_{\partial D} \int_Y G^{\alpha,\omega^0}(x,z) G^{-\alpha,\omega^0}(y,z) \varphi(x) \overline{\varphi}(y) dz d\sigma(x) \, d\sigma(y)$$
$$= -2\omega^0 \int_Y \left| \int_{\partial D} G^{\alpha,\omega^0}(x,z) \varphi(x) d\sigma(x) \right|^2 dz$$
$$= -2\omega^0 \int_Y \left| \mathcal{S}^{\alpha,\omega^0}[\varphi](z) \right|^2 dz$$
$$= -2\omega^0 \int_D |u^0(z)|^2 \, dz.$$

Photonic crystals

- v^α: unique α-quasi-periodic solution to

$$(***) \begin{cases} \Delta v^\alpha = 0 & \text{in } Y \setminus \overline{D}, \\ \dfrac{\partial v^\alpha}{\partial \nu}\Big|_+ = \dfrac{\partial u^0}{\partial \nu}\Big|_- & \text{on } \partial D. \end{cases}$$

- Leading-order term:

$$\omega^{\alpha,k} - \omega^0 = -\frac{1}{k} \frac{\displaystyle\int_{Y\setminus\overline{D}} |\nabla v^\alpha|^2}{\displaystyle 2\omega^0 \int_D |u^0|^2} + O(\frac{1}{k^2}) \quad \text{as } k \to +\infty.$$

Photonic crystals

- $u^0(x) = -\mathcal{S}^{\alpha,\omega^0}[\varphi](x) \quad \text{for } x \in D \Rightarrow (\frac{1}{2}I - (\mathcal{K}^{-\alpha,\omega^0})^*)[\varphi] = \varphi.$
- ω^0: only simple pole in V of $\omega \mapsto (\mathcal{S}^{\alpha,\omega})^{-1} \Rightarrow$

$$(\mathcal{S}^{\alpha,\omega})^{-1} = \frac{1}{\omega - \omega^0} T + \mathcal{Q}^{\alpha;\omega}.$$

- $\mathcal{Q}^{\alpha,\omega}$: holomorphic in ω in V;
- $T : L^2(\partial D) \to \text{ span}\{\varphi\}$ s.t. $T\mathcal{S}^{\alpha,\omega^0} = \mathcal{S}^{\alpha,\omega^0} T = 0$;

$$T \frac{d}{d\omega} \mathcal{S}^{\alpha,\omega}\Big|_{\omega=\omega^0} = \frac{1}{||\varphi||^2_{L^2}} \langle \varphi, \cdot \rangle \varphi \quad (\text{orthogonal projection}).$$

-

$$T = \frac{1}{\left\langle \varphi, \frac{d}{d\omega} \mathcal{S}^{\alpha,\omega}[\varphi]\big|_{\omega=\omega^0} \right\rangle} \langle \varphi, \cdot \rangle \, \varphi.$$

- Residue theorem $\Rightarrow$

$$\frac{1}{2i\pi} \text{ tr} \int_{\partial V} (\mathcal{A}_0^\alpha)^{-1}(\omega) \mathcal{A}_1^\alpha(\omega) d\omega = \text{tr} \left[T\mathcal{S}^{\alpha,0} \big(\frac{1}{2}I + (\mathcal{K}^{-\alpha,0})^*\big)^{-1} \big(\frac{1}{2}I - (\mathcal{K}^{-\alpha,\omega^0})^*\big) \right].$$

Photonic crystals

- $$v^\alpha(x) := \mathcal{S}^{\alpha,0}\Big(\frac{1}{2}I + (\mathcal{K}^{-\alpha,0})^*\Big)^{-1}[\varphi](x), \quad x \in Y \setminus \overline{D}.$$
- v^α: unique α-quasi-periodic solution to $(***)$ and
$$\frac{1}{2i\pi} \text{ tr } \int_{\partial V} (\mathcal{A}_0^\alpha)^{-1}(\omega)\mathcal{A}_1^\alpha(\omega) d\omega = \frac{1}{||\varphi||^2_{L^2}} \langle \varphi, Tv^\alpha \rangle.$$
- $\Rightarrow$
$$\omega^{\alpha,k} - \omega^0 = -\frac{1}{k||\varphi||^2_{L^2}} \langle \varphi, Tv^\alpha \rangle + O(\frac{1}{k^2}) \quad \text{as } k \to +\infty.$$
- $$\frac{1}{||\varphi||^2_{L^2}} \langle \varphi, Tv^\alpha \rangle = \frac{1}{\Big\langle \varphi, \frac{d}{d\omega} \mathcal{S}^{\alpha,\omega}[\varphi]\Big|_{\omega=\omega^0} \Big\rangle} \Big\langle \varphi, v^\alpha \Big\rangle.$$
- Integration by parts $\Rightarrow$
$$\langle \varphi, v^\alpha \rangle = -\int_{Y \setminus \overline{D}} |\nabla v^\alpha|^2.$$

Photonic crystals

- Periodic case ($\alpha = 0$):
  - $\widetilde{\Delta}$: acting on span$\{\chi(Y), H_0^1(D)\}$,

$$\widetilde{\Delta} u := \begin{cases} -\Delta(u|_D) & \text{in } D, \\ \dfrac{1}{|Y \setminus \overline{D}|} \displaystyle\int_{\partial D} \frac{\partial}{\partial \nu}(u|_D) & \text{in } Y \setminus \overline{D}. \end{cases}$$

  - Eigenvalue problem for $\widetilde{\Delta}$:

$$\begin{cases} \Delta u + \omega^2 u = 0 & \text{in } D, \\ u + \dfrac{1}{|Y \setminus \overline{D}|} \displaystyle\int_D u = 0 & \text{on } \partial D. \end{cases}$$

  - $$\widetilde{\mathcal{A}}_0^0(\omega) = \begin{pmatrix} \mathcal{S}^{0,\omega} & -\dfrac{1}{\omega^2} \displaystyle\int_{\partial D} \cdot \\ \dfrac{1}{2} I - (\mathcal{K}^{0,\omega})^* & \dfrac{1}{2} I + (\mathcal{K}^{0,0})^* \end{pmatrix}.$$

Photonic crystals

- $$\widetilde{\mathcal{A}}_1^0(\omega) = \begin{pmatrix} 0 & -\mathcal{S}^{0,0} \\ 0 & (\mathcal{K}_1^{0,\omega})^* \end{pmatrix}.$$

- Asymptotic expansion of $\widetilde{\mathcal{A}}^{0,k}$ as $k \to +\infty$:

$$\widetilde{\mathcal{A}}^{0,k}(\omega) = \widetilde{\mathcal{A}}_0^0(\omega) + \frac{1}{k}\widetilde{\mathcal{A}}_1^0(\omega) + O(\frac{1}{k^2}).$$

- $(\widetilde{\omega}^0)^2$ (with $\widetilde{\omega}^0 > 0$): not an eigenvalue of $-\Delta$ in $Y \setminus \overline{D}$ with Dirichlet boundary condition on ∂D and the periodic condition on ∂Y. Then $(\widetilde{\omega}^0)^2$: eigenvalue of $\widetilde{\Delta}$ iff $\widetilde{\omega}^0$: characteristic value of $\widetilde{\mathcal{A}}_0^0$.

- Suppose $\alpha = 0$; $(\widetilde{\omega}^0)^2$ (with $\widetilde{\omega}^0 > 0$): simple eigenvalue of $\widetilde{\Delta}$. There exists a unique eigenvalue $(\omega^{0,k})^2$ lying in a small complex neighborhood of $(\widetilde{\omega}^0)^2$.

- V: small complex neighborhood of $\widetilde{\omega}^0$; Asymptotic expansion:

$$\omega^{0,k} - \widetilde{\omega}^0 = \frac{1}{2i\pi k}\ \mathrm{tr} \int_{\partial V} \widetilde{\mathcal{A}}_0^0(\omega)^{-1}\widetilde{\mathcal{A}}_1^0(\omega) d\omega + O(\frac{1}{k^2}).$$

Photonic crystals

- Characterization of the eigenvalues of $\widetilde{\Delta}$.
- $\widetilde{\omega}_0$: characteristic value characteristic value of $\widetilde{\mathcal{A}}_0^0$.
- (ϕ, ψ): root function associated with $\widetilde{\omega}_0$.
- Set
$$u = \mathcal{S}^{0,\omega}[\phi] - \frac{1}{\widetilde{\omega}_0^2} \int_{\partial D} \psi;$$
- $$c = \frac{1}{\widetilde{\omega}_0^2 |Y \setminus \overline{D}|} \int_{\partial D} (-\frac{1}{2} I + (\mathcal{K}^{0,\omega})^*)[\phi].$$
- $(\frac{1}{2} I + \mathcal{K}^{0,0})[1] = |Y \setminus \overline{D}| \Rightarrow$
$$c = \frac{1}{\widetilde{\omega}_0^2} \int_{\partial D} \psi;$$
- $\Rightarrow -\Delta(u + c) = \widetilde{\omega}_0^2 (u + c)$ in D and $u = 0$ on ∂D.
- $\Rightarrow \widetilde{\omega}_0^2$: eigenvalue of $\widetilde{\Delta}$.

Photonic crystals

- Converse:
  Assume $\widetilde{\omega}_0^2$ (with $\widetilde{\omega}_0 > 0$): an eigenvalue of $\widetilde{\Delta}$ associated with $u + c$, where $u \in H_0^1(D)$, and
  $$c = \frac{1}{|Y \setminus \overline{D}|\widetilde{\omega}_0^2} \int_{\partial D} \frac{\partial u}{\partial \nu}.$$
- ϕ: solution to
  $$(\frac{1}{2} I - (\mathcal{K}^{0,\widetilde{\omega}_0})^*)[\phi] = \frac{\partial u}{\partial \nu} \quad \text{on } \partial D.$$
  ($\exists$ because $\partial u/\partial \nu$: orthogonal in L^2 to the associated Neumann eigenvector).

Photonic crystals

- Set
$$\psi = -(\frac{1}{2}I + (\mathcal{K}^{0,0})^*)^{-1}\left[\frac{\partial u}{\partial \nu}\right].$$
- Then, (ϕ, ψ) satisfies
$$\begin{pmatrix} \mathcal{S}^{0,\widetilde{\omega}_0} & -\frac{1}{\widetilde{\omega}_0^2}\int_{\partial D}\cdot \\ \frac{1}{2}I - (\mathcal{K}^{0,\widetilde{\omega}_0})^* & \frac{1}{2}I + (\mathcal{K}^{0,0})^* \end{pmatrix}\begin{pmatrix} \phi \\ \psi \end{pmatrix} = 0.$$
- $\Rightarrow \widetilde{\omega}_0$: characteristic value of $\widetilde{\mathcal{A}}_0^0$.

Photonic crystals

- Photonic band gap opening.
- ω_j: eigenvalues of $-\Delta$ in D with Dirichlet conditions;
- $\widetilde{\omega}_j$: eigenvalues of $\widetilde{\Delta}$.
- $E(u, v) := \int_D \nabla u \cdot \nabla \overline{v}$; Min-max characterizations:
  - $$\omega_j^2 = \min_{N_j} \max_{u \in N_j, \|u\|_{L^2(D)}=1} E(u, u),$$
    $$\widetilde{\omega}_j^2 = \min_{N_j} \max_{u \in N_j, \|\mathbf{u}\|_{L^2(D)}=1} \frac{E(u, u)}{1 - \left| \int_D u \right|^2}.$$
  - N_j: j -dimensional subspaces of $H_0^1(D)$.
  - Interlacing relation:
    $$\omega_j \leq \widetilde{\omega}_j \leq \omega_{j+1}, \quad j = 1, 2, \ldots .$$
  - For any $\varepsilon > 0$ and j, there exist c_1 and c_2 sufficiently small s.t. $\widetilde{\omega}_j - \epsilon \leq \omega_{j+1}^{\alpha,k} \leq \omega_{j+1}$ for $|\alpha| \leq c_1$ and $k > 1/c_2$.

Photonic crystals

- 0: eigenvalue of the periodic problem with multiplicity 1 $\Rightarrow$ the spectral bands converge, as $k \to +\infty$, to

$$[0, \omega_1] \cup [\widetilde{\omega}_1, \omega_2] \cup [\widetilde{\omega}_2, \omega_3] \cup \ldots ,$$

- Band gap iff

$$\omega_j < \widetilde{\omega}_j \quad \text{for some } j.$$

- Identity holds provided that $\int_D u_j \neq 0$ where u_j: eigenfunction corresponding to ω_j^2.

Photonic crystals

- Small perturbations in the geometry of the holes.
- D: $\mathcal{C}^2$.
- D_ε ϵ-perturbation of D:

$$\partial D_\varepsilon = \left\{ \widetilde{x} : \widetilde{x} = x + \varepsilon h(x)\nu(x),\ x \in \partial D \right\}, \quad h \in \mathcal{C}^1(\partial D).$$

-
$$\mathcal{A}_\varepsilon^\alpha : \omega \mapsto \begin{pmatrix} \mathcal{S}_{D_\varepsilon}^{\alpha,\omega} & -\mathcal{S}_{D_\varepsilon}^{\alpha,\frac{\omega}{\sqrt{k}}} \\ \frac{1}{k}\left(\frac{1}{2}I - (\mathcal{K}_{D_\varepsilon}^{-\alpha,\omega})^*\right) & \frac{1}{2}I + (\mathcal{K}_{D_\varepsilon}^{-\alpha,\frac{\omega}{\sqrt{k}}})^* \end{pmatrix}.$$

- $\exists\ R^{\alpha,\omega}(x,y)$ smooth for all x and y s.t.

$$\frac{\partial G^{\alpha,\omega}}{\partial \nu(x)}(x,y) = \frac{1}{2\pi}\frac{\langle x-y, \nu(x)\rangle}{|x-y|^2} + R^{\alpha,\omega}(x,y).$$

Photonic crystals

- Photonic cavities:

$$k(x) = \begin{cases} k & \text{in } Y \setminus \overline{D}, \quad 0 < k \neq 1 < +\infty, \\ 1 & \text{in } D. \end{cases}$$

- u: solution to

$$\nabla \cdot k(x) \nabla u + \omega^2 n(x) u = 0.$$

- $n(x) - 1$: compactly supported in a bounded domain $\Omega \subset \mathbb{R}^2$.
- Ω: localized defect inserted into the photonic crystal.
- Introduction of a localized defect does not change the essential spectrum of the operator.
- Assume that the operator $\nabla \cdot k(x) \nabla$ has a gap in the spectrum and seek for ω inside the bandgap s.t. u: nontrivial solution.
-

$$u(x) + \omega^2 \int_\Omega (n(y) - 1) G_\omega(x, y) u(y) dy = 0, \quad x \in \mathbb{R}^2.$$

- G_ω: Green's function of $\nabla \cdot k(x) \nabla + \omega^2$ in $\mathbb{R}^2$.

Photonic crystals

- For frequencies in the band gap, G_ω is exponentially decaying:

$$|G_\omega(x,y)| = O\left(e^{-C\mathrm{dist}(\omega^2, \sigma(-\nabla\cdot k(x)\nabla))}\right) \quad \text{as } |x-y| \to \infty.$$

- C: positive constant and $\sigma(-\nabla \cdot k(x)\nabla)$: spectrum of $-\nabla \cdot k(x)\nabla$.
- Exponentially localized defect mode.

Lecture 11: Plasmonic nanoparticles

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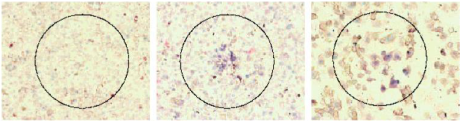
Plasmonic nanoparticles

- Gold nano-particles: accumulate selectively in tumor cells; bio-compatible; reduced toxicity.
- Detection: localized enhancement in radiation dose (strong scattering).
- Ablation: localized damage (strong absorption).
- Functionalization: targeted drugs.



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Plasmonic nanoparticles

- Particles with unsual scattering and absorption properties at certain frequencies (called resonant frequencies).
- Applications: biomedical imaging (nanodetection), nanothermotheraphy, photonic devices, . . .
- Math. modeling: quantify the scattering and absorption enhancement.

Plasmonic nanoparticles

- D: nanoparticle in $\mathbb{R}^d, d = 2, 3$; $\mathcal{C}^{1,\alpha}$ boundary ∂D, $\alpha > 0$.
- $\varepsilon_c(\omega)$: complex electric permittivity of D; $\varepsilon_m > 0$: electric permittivity of the background medium;
- μ_m: magnetic permeability of the background medium and of D;
- Quasi-static resonance: $\omega \to 0$
  - $\nabla \times E = i\omega\mu H \Rightarrow \nabla \times E = 0$;
  - $\nabla \times H = -i\omega\varepsilon E \Rightarrow \nabla \cdot \varepsilon E = 0$;
  - $E = \nabla u$, $u^{\rm in}$: harmonic,

$$\begin{cases} \nabla \cdot \varepsilon \nabla u = 0 \quad \text{in } \mathbb{R}^3, \\ (u - u^{\rm in})(x) \to 0 \quad |x| \to +\infty. \end{cases}$$

Plasmonic nanoparticles

- Permittivity contrast: $\lambda(\omega) = (\varepsilon_c(\omega) + \varepsilon_m)/(2(\varepsilon_c(\omega) - \varepsilon_m))$;
- Integral representation of u:

$$u = \mathcal{S}_D(\lambda I - \mathcal{K}_D^*)^{-1}[\frac{\partial u^{\mathrm{in}}}{\partial \nu}];$$

- $\varepsilon_c > 0 \Rightarrow |\lambda| > \frac{1}{2} \Rightarrow \lambda I - \mathcal{K}_D^*$: invertible.
- $\Re\varepsilon_c < 0$, $\Re\lambda \sim \sigma(\mathcal{K}_D^*) \Rightarrow (\lambda I - \mathcal{K}_D^*)^{-1}$: large.
- Quasi-static plasmonic resonance: $\mathrm{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))$ minimal ($\Re\,\varepsilon_c(\omega) < 0$).

Plasmonic nanoparticles

- Causality $\Rightarrow$ Kramer-Krönig relations (Hilbert transform), $\varepsilon_c(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)$:

$$\varepsilon'(\omega) - \varepsilon_\infty = -\frac{2}{\pi}\text{p.v.} \int_0^{+\infty} \frac{s\varepsilon''(s)}{s^2 - \omega^2} ds,$$

$$\varepsilon''(\omega) = \frac{2\omega}{\pi}\text{p.v.} \int_0^{+\infty} \frac{\varepsilon'(s) - \varepsilon_\infty}{s^2 - \omega^2} ds.$$

- Drude model for the dielectric permittivity $\varepsilon_c(\omega)$:

$$\varepsilon_c(\omega) = \varepsilon_\infty(1 - \frac{\omega_p^2}{\omega^2 + i\tau\omega}), \qquad \varepsilon'(\omega) \leq 0 \quad \text{for} \quad \omega \leq \omega_p.$$

ω_p, τ: positive constants.

Plasmonic nanoparticles

- Scalar model for wave propagation.
- u^{in}: incident plane wave; Helmholtz equation:

$$\begin{cases} \nabla\cdot\Big(\varepsilon_m\chi(\mathbb{R}^d\setminus\bar{D})+\varepsilon_c(\omega)\chi(\overline{D})\Big)\nabla u+\omega^2 u=0, \\ u^s:=u-u^{\text{in}} \text{ satisfies the outgoing radiation condition.}\end{cases}$$

- Uniform small volume expansion with respect to the contrast: $D=z+\delta B$, $\delta\to 0$, $|x-z|\gg 2\pi/k_m$,

$$u^s=-M(\lambda(\omega),D)\nabla_z\Gamma_{k_m}(x-z)\cdot\nabla u^{\text{in}}(z)+O\Big(\frac{\delta^{d+1}}{\mathrm{dist}(\lambda(\omega),\sigma(\mathcal{K}_D^*))}\Big).$$

- Γ_{k_m}: outgoing fundamental solution to $\Delta+k_m^2$; $k_m:=\omega/\sqrt{\varepsilon_m}$;
- Polarization tensor:

$$M(\lambda(\omega),D):=\int_{\partial D}x(\lambda(\omega)I-\mathcal{K}_D^*)^{-1}[\nu](x)\,ds(x).$$

- Scaling and translation properties: $M(\lambda(\omega),z+\delta B)=\delta^d M(\lambda(\omega),B)$.

Plasmonic nanoparticles

Representation by equivalent ellipses and ellipsoids:

- Nanoparticle's permittivity: $\varepsilon_c(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)$.
- $\varepsilon'(\omega) > 0$ and $\varepsilon''(\omega) = 0$: canonical representation; equivalent ellipse or ellipsoid with the same polarization tensor.
- Plasmonic nanoparticles: non Hermitian case.
- $\Im M(\lambda(\omega), D)$: equivalent frequency depending ellipse or ellipsoid with the same imaginary part of the polarization tensor.

Plasmonic nanoparticles

- Spectral decomposition: (l, m)-entry

$$M_{l,m}(\lambda(\omega), D) = \sum_{j=1}^{\infty} \frac{(\nu_m, \varphi_j)_{\mathcal{H}^*} (\nu_l, \varphi_j)_{\mathcal{H}^*}}{(1/2 - \lambda_j)(\lambda(\omega) - \lambda_j)}.$$

- $(\nu_m, \varphi_0)_{\mathcal{H}^*} = 0$; φ_0: eigenfunction of $\mathcal{K}_D^*$ associated to $1/2$.
- Quasi-static far-field approximation: $\delta \to 0$,

$$u^s = -\delta^d M(\lambda(\omega), B) \nabla_z \Gamma_{k_m}(x - z) \cdot \nabla u^{\text{in}}(z) + O\Big(\frac{\delta^{d+1}}{\text{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))}\Big).$$

- Quasi-static plasmonic resonance: $\text{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))$ minimal ($\Re \varepsilon_c(\omega) < 0$).

Plasmonic nanoparticles

- $M(\lambda(\omega), B) = (\frac{\varepsilon_c(\omega)}{\varepsilon_m} - 1) \int_B \nabla v(y) dy$:

$$\begin{cases} \nabla \cdot \Big(\varepsilon_m \chi(\mathbb{R}^d \setminus \bar{B}) + \varepsilon_c(\omega) \chi(\overline{B}) \Big) \nabla v = 0, \\ v(y) - y \to 0, \qquad |y| \to +\infty. \end{cases}$$

- Corrector v:

$$v(y) = y + \mathcal{S}_B (\lambda(\omega) I - \mathcal{K}_B^*)^{-1} [\nu](y), \quad y \in \mathbb{R}^d.$$

- Inner expansion: $\delta \to 0$, $|x - z| = O(\delta)$,

$$u(x) = u^{\text{in}}(z) + \delta v(\frac{x-z}{\delta}) \cdot \nabla u^{\text{in}}(z) + O(\frac{\delta^2}{\text{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))}).$$

- Monitoring of temperature elevation due to nanoparticle heating:

$$\begin{cases} \rho C \frac{\partial T}{\partial t} - \nabla \cdot \tau \nabla T = \frac{\omega}{2\pi} \Im(\varepsilon_c(\omega)) \, |u|^2 \chi(D), \\ T\big|_{t=0} = 0. \end{cases}$$

ρ: mass density; C: thermal capacity; τ: thermal conductivity.

Plasmonic nanoparticles

- Scattering amplitude:

$$u^s(x) = -ie^{-\frac{\pi i}{4}} \frac{e^{ik_m|x|}}{\sqrt{8\pi k_m |x|}} A_\infty[D, \varepsilon_c, \varepsilon_m, \omega](\theta, \theta') + o(|x|^{-\frac{1}{2}}),$$

$|x| \to \infty$; θ, θ': incident and scattered directions.

- Scattering cross-section:

$$Q^s[D, \varepsilon_c, \varepsilon_m, \omega](\theta') := \int_0^{2\pi} \left| A_\infty[D, \varepsilon_c, \varepsilon_m, \omega](\theta, \theta') \right|^2 d\theta.$$

- Enhancement of the absorption and scattering cross-sections Q^a and Q^s at plasmonic resonances:

$$Q^a + Q^s (= \text{extinction cross-section } Q^e) \propto \Im\, \mathrm{tr}(M(\lambda(\omega), D));$$

$$Q^s \propto \left| \mathrm{tr}(M(\lambda(\omega), D)) \right|^2.$$

Plasmonic nanoparticles

- Quasi-plasmonic resonances for multiple particles: D_1 and D_2: $\mathcal{C}^{1,\alpha}$-bounded domains; $\mathrm{dist}(D_1, D_2) > 0$; $\nu^{(1)}$ and $\nu^{(2)}$: outward normal vectors at ∂D_1 and ∂D_2.
- Neumann-Poincaré operator $\mathbb{K}^*_{D_1 \cup D_2}$ associated with $D_1 \cup D_2$:

$$\mathbb{K}^*_{D_1 \cup D_2} := \begin{pmatrix} \mathcal{K}^*_{D_1} & \frac{\partial}{\partial \nu^{(1)}} \mathcal{S}_{D_2} \\ \frac{\partial}{\partial \nu^{(2)}} \mathcal{S}_{D_1} & \mathcal{K}^*_{D_2} \end{pmatrix}.$$

- Symmetrization of $\mathbb{K}^*_{D_1 \cup D_2}$.
- Behavior of the eigenvalues of $\mathbb{K}^*_{D_1 \cup D_2}$ as $\mathrm{dist}(D_1, D_2) \to 0$.
- Blow-up of ∇u between the disks at plasmonic resonances.

Plasmonic nanoparticles

- (m, l)-entry of the polarization tensor M:

$$M_{l,m}(\lambda(\omega), D) = \sum_{j=1}^{\infty} \frac{\alpha_{l,m}^{(j)}}{\lambda(\omega) - \lambda_j},$$

$$\alpha_{l,m}^{(j)} := \frac{(\nu_m, \varphi_j)_{\mathcal{H}^*}(\nu_l, \varphi_j)_{\mathcal{H}^*}}{(1/2 - \lambda_j)}, \quad \alpha_{l,l}^{(j)} \geq 0, \quad j \geq 1.$$

- Sum rules for the polarization tensor:

$$\sum_{j=1}^{\infty} \alpha_{l,m}^{(j)} = \delta_{l,m}|D|; \qquad \sum_{j=1}^{\infty} \lambda_i \sum_{l=1}^{d} \alpha_{l,l}^{(j)} = \frac{(d-2)}{2}|D|.$$

$$\sum_{j=1}^{\infty} \lambda_j^2 \sum_{l=1}^{d} \alpha_{l,l}^{(j)} = \frac{(d-4)}{4}|D| + \sum_{l=1}^{d} \int_D |\nabla \mathcal{S}_D[\nu_l]|^2 dx.$$

- f holomorphic function in an open set $U \subset \mathbb{C}$ containing $\sigma(\mathcal{K}_D^*)$:

$$f(\mathcal{K}_D^*) = \sum_{j=1}^{\infty} f(\lambda_j)(\cdot, \varphi_j)_{\mathcal{H}^*} \varphi_j.$$

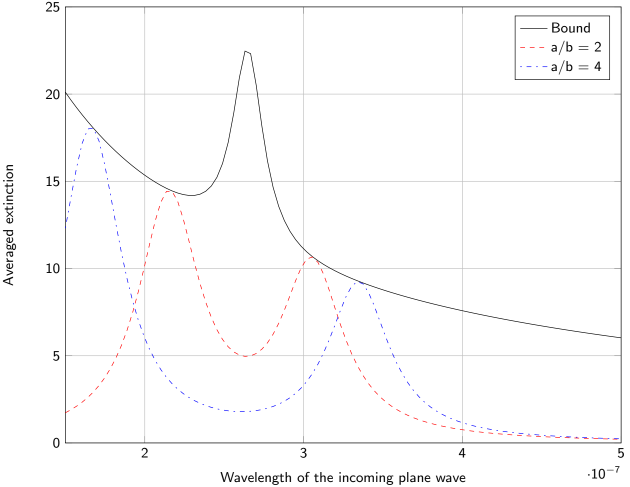
Plasmonic nanoparticles

- Upper bound for the averaged extinction cross-section Q_m^e of a randomly oriented nanoparticle:

$$
\begin{aligned}
&\left|\Im(\mathrm{tr}(M(\lambda, D)))\right| \leq \frac{d|\lambda''||D|}{\lambda''^2 + 4\lambda'^2} \\
&+ \frac{1}{|\lambda''|(\lambda''^2 + 4\lambda'^2)}\Big(d\lambda'^2|D| + \frac{(d-4)}{4}|D| \\
&+ \sum_{l=1}^{d} \int_D |\nabla \mathcal{S}_D[\nu_l]|^2 dx + 2\lambda' \frac{(d-2)}{2}|D|\Big) + O\Big(\frac{\lambda''^2}{4\lambda'^2 + \lambda''^2}\Big).
\end{aligned}
$$

$\lambda' = \Re\lambda, \lambda'' = \Im\lambda.$

Plasmonic nanoparticles



Plasmonic nanoparticles

Hadamard's formula for $\mathcal{K}_D^*$:

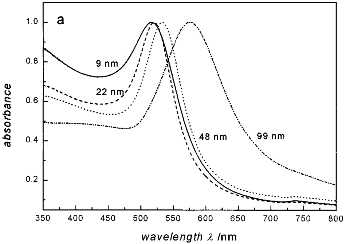
- ∂D: class $\mathcal{C}^2$; $\partial D := \{x = X(t), t \in [a, b]\}$.
- $\Psi_\eta : \partial D \mapsto \partial D_\eta := \{x + \eta h(t)\nu(x)\}$; Ψ_η: diffeomorphism.
- Hadamard's formula for $\mathcal{K}_D^*$:

$$||\mathcal{K}_{D_\eta}^*[\tilde{\phi}] \circ \Psi_\eta - \mathcal{K}_D^*[\phi] - \eta \mathcal{K}_D^{(1)}[\phi]||_{L^2(\partial D)} \leq C\eta^2 ||\phi||_{L^2(\partial D)},$$

  C: depends only on $||X||_{\mathcal{C}^2}$ and $||h||_{\mathcal{C}^1}$; $\phi := \tilde{\phi} \circ \Psi_\eta$.
- $\mathcal{K}_D^{(1)}$: explicit kernel.
- Hadamard's formula for the eigenvalues of $\mathcal{K}_D^*$.
- Shape derivative of plasmonic resonances for nanoparticles.

Plasmonic nanoparticles

- $\mathcal{K}_D^*$: scale invariant $\Rightarrow$ Quasi-static plasmonic resonances: size independent.
- Analytic formula for the first-order correction to quasi-static plasmonic resonances in terms of the particle's characteristic size δ:



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Plasmonic nanoparticles

- Helmholtz equation:

$$\begin{cases} \nabla\cdot\Big(\varepsilon_m\chi(\mathbb{R}^d\setminus\bar{D})+\varepsilon_c(\omega)\chi(\overline{D})\Big)\nabla u+\omega^2 u=0, \\ u^s:=u-u^{\mathrm{in}} \text{ satisfies the outgoing radiation condition.} \end{cases}$$

  u^{in}: incident plane wave; $k_m := \omega\sqrt{\varepsilon_m}$, $k_c := \omega\sqrt{\varepsilon_c(\omega)}$.

- Integral formulation on ∂D:

$$\begin{cases} \mathcal{S}_D^{k_c}[\phi]-\mathcal{S}_D^{k_m}[\psi]=u^{\mathrm{in}}, \\ \varepsilon_c\big(\frac{I}{2}-(\mathcal{K}_D^{k_c})^*\big)[\phi]-\varepsilon_m\big(\frac{I}{2}+(\mathcal{K}_D^{k_m})^*\big)[\psi]=\varepsilon_m\partial u^i/\partial\nu. \end{cases}$$

- Operator-Valued function $\delta\mapsto\mathcal{A}_\delta(\omega)\in\mathcal{L}(\mathcal{H}^*(\partial B),\mathcal{H}^*(\partial B))$:

$$\mathcal{A}_\delta(\omega)=\overbrace{(\lambda(\omega)I-\mathcal{K}_B^*)}^{\mathcal{A}_0(\omega)}+(\omega\delta)^2\mathcal{A}_1(\omega)+O((\omega\delta)^3).$$

- Quasi-static limit:

$$\mathcal{A}_0(\omega)[\psi]=\sum_{j=0}^{\infty}\tau_j(\omega)(\psi,\varphi_j)_{\mathcal{H}^*}\varphi_j,\quad \tau_j(\omega):=\frac{1}{2}(\varepsilon_m+\varepsilon_c(\omega))-(\varepsilon_c(\omega)-\varepsilon_m)\lambda_j.$$

Plasmonic nanoparticles

- Shift in the plasmonic resonance:

$$\arg\min_{\omega} \left| \frac{1}{2}\big(\varepsilon_m + \varepsilon_c(\omega)\big) - \big(\varepsilon_c(\omega) - \varepsilon_m\big)\lambda_j + (\omega\delta)^2 \tau_{j,1} \right|;$$

- $\tau_{j,1} := (\mathcal{A}_1(\omega)[\varphi_j], \varphi_j)_{\mathcal{H}^*}$.
- Gohberg-Sigal theory.

Plasmonic nanoparticles

- Full Maxwell's equations:

$$\begin{cases} \nabla \times \nabla \times E - \omega^2 \Big(\varepsilon_m \chi(\mathbb{R}^d \setminus \bar{D}) + \varepsilon_c(\omega)\chi(\overline{D}) \Big) E = 0, \\ E^s := E - E^{\mathrm{in}} \text{ satisfies the outgoing radiation condition.} \end{cases}$$

- Small-volume expansion:

$$E^s(x) = -\delta^3 \omega^2 \mathbf{G}_{k_m}(x,z) M(\lambda(\omega), B) E^{\mathrm{in}}(z) + O\Big(\frac{\delta^4}{\mathrm{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))}\Big).$$

- $\mathbf{G}_{k_m}$: fundamental (outgoing) solution to Maxwell's equations in free space.
- Shift in the plasmonic resonances due to the finite size of the nanoparticle.

Plasmonic nanoparticles

- Integral formulation:

$$\begin{pmatrix} I + \mathcal{M}_D^{k_c} - \mathcal{M}_D^{k_m} & \mathcal{L}_D^{k_c} - \mathcal{L}_D^{k_m} \\ \mathcal{L}_D^{k_c} - \mathcal{L}_D^{k_m} & \frac{1}{2}(k_c^2 + k_m^2)I + k_c^2 \mathcal{M}_D^{k_c} - k_m^2 \mathcal{M}_D^{k_m} \end{pmatrix}$$

- Integral operators:

$$\begin{array}{rcl} \mathcal{M}_D^k[\varphi] : H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D) & \longrightarrow & H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D) \qquad (\text{compact}) \\ \varphi & \longmapsto & \displaystyle\int_{\partial D} \nu(x) \times \nabla_x \times \mathbf{G}_k(x,y)\varphi(y) ds(y); \end{array}$$

$$\begin{array}{rcl} \mathcal{L}_D^k[\varphi] : H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D) & \longrightarrow & H_T^{-\frac{1}{2}}(\mathrm{div}, \partial D) \\ \varphi & \longmapsto & \nu(x) \times \left(k^2 \mathcal{S}_D^k[\varphi](x) + \nabla \mathcal{S}_D^k[\nabla_{\partial D} \cdot \varphi](x) \right). \end{array}$$

- Key identities: $\mathcal{M}_D^{k=0}[\mathrm{curl}_{\partial D}\varphi] = \mathrm{curl}_{\partial D}\mathcal{K}_D[\varphi], \quad \forall \varphi \in H^{\frac{1}{2}}(\partial D)$,

$$\mathcal{M}_D^{k=0}[\nabla_{\partial D}\varphi] = -\nabla_{\partial D}\Delta_{\partial D}^{-1}\mathcal{K}_D^*[\Delta_{\partial D}\varphi] + \mathcal{R}_D[\varphi],$$

$\mathcal{R}_D = -\mathrm{curl}_{\partial D}\Delta_{\partial D}^{-1}\mathrm{curl}_{\partial D}\mathcal{M}_D\nabla_{\partial D}, \ \forall \varphi \in H^{\frac{3}{2}}(\partial D).$

Plasmonic nanoparticles

- Quasi-static approximation:

$$\widetilde{\mathcal{M}}_B = \begin{pmatrix} -\Delta_{\partial B}^{-1}\mathcal{K}_B^*\Delta_{\partial B} & 0 \\ \mathcal{R}_B & \mathcal{K}_B \end{pmatrix}.$$

- $H(\partial B) := H_0^{\frac{3}{2}}(\partial B) \times H^{\frac{1}{2}}(\partial B)$, equipped with the inner product

$$(u, v)_{H(\partial B)} = (\Delta_{\partial B} u^{(1)}, \Delta_{\partial B} v^{(1)})_{\mathcal{H}^*} + (u^{(2)}, v^{(2)})_{\mathcal{H}},$$

$$(u, v)_{\mathcal{H}^*} := -(u, \mathcal{S}_D[v])_{-\frac{1}{2},\frac{1}{2}}, \quad (u, v)_{\mathcal{H}} = -(\mathcal{S}_D^{-1}[u], v)_{-\frac{1}{2},\frac{1}{2}}.$$

- The spectrum $\sigma(\widetilde{\mathcal{M}}_B) = \sigma(-\mathcal{K}_B^*) \cup \sigma(\mathcal{K}_B^*) \backslash \{-\frac{1}{2}\}$ in $H(\partial B)$.
- Only $\sigma(\mathcal{K}_B^*)$ can be excited in the quasi-static approximation.

Plasmonic nanoparticles

- System of weakly coupled plasmonic nanoparticles.
- Size of the nanoparticle $\delta \ll$ wavelength $2\pi/k_m$; distance between the nanoparticles of order one.
- $\Im \mathbf{G}^\delta = \Im \mathbf{G}_{k_m} +$ exhibits subwavelength peak with width of order one.
- Break the resolution limit.

Plasmonic nanoparticles

- Effective medium theory: Y: unit cell; $\gamma = \varepsilon_m \chi(Y \setminus \overline{D}) + \varepsilon_c \chi(D)$; $\gamma_\eta(x) = \gamma(\frac{x}{\eta})$: periodic with period η.
- Cell problem:

$$\begin{cases} \nabla \cdot \gamma \nabla u_p = 0 \quad \text{in } Y, \\ u_p - x_p \quad \text{periodic with period } 1, \\ \displaystyle\int_Y u_p(x) = 0. \end{cases}$$

- Effective material parameter γ^*:

$$\gamma^*_{pq} = \int_Y \gamma(x) \nabla u_p(x) \cdot \nabla u_q(x)\, dx, \quad p, q = 1, 2, 3.$$

- As $\eta \to 0$, u_0: valid approximation of u_η,

$$\nabla \cdot \gamma^* \nabla u_0 = 0 \quad \text{in } \Omega.$$

Plasmonic nanoparticles

- Maxwell-Garnett formula: Small volume fraction approximation,

$$\varepsilon_{\mathrm{eff}}(\omega) = \varepsilon_m \big(I + f M(\lambda(\omega), B)(I - \frac{f}{3} M(\lambda(\omega), B))^{-1} \big) + O\big(\frac{f^{8/3}}{\mathrm{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))^2} \big).$$

- f: volume fraction; B: rescaled particle ($D = \eta^\beta B$).
- $\varepsilon_{\mathrm{eff}}(\omega)$: anisotropic.
- Validity of the effective medium theory:

$$f \ll \mathrm{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))^{3/5}.$$

Plasmonic nanoparticles

- High contrast effective medium at plasmonic resonances:

$$\nabla \times \nabla \times E - \omega^2 \Big(\varepsilon_m \chi(\mathbb{R}^d \setminus \bar{\Omega}) + \varepsilon_{\mathrm{eff}}(\omega) \chi(\overline{\Omega}) \Big) E = 0.$$

- $E|_\Omega \mapsto \displaystyle\int_\Omega (\varepsilon_{\mathrm{eff}}(\omega) - \varepsilon_m) E(y) \mathbf{G}_{k_m}(x, y)\, dy, \quad x \in \Omega.$
- Mixing of resonant modes: intrinsic nature of non-hermitian systems.
- Subwavelength resonance modes excited $\Rightarrow$ dominate over the other ones in the expansion of the Green function.
- Imaginary part of the Green function may have sharper peak than the one of G due to the excited sub-wavelength resonant modes.
- Subwavelength modes: determine the superesolution.

Lecture 12: Electromagnetic invisibility

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Electromagnetic invisibility

- Cloaking: make a target invisible when probed by electromagnetic waves.
- Two schemes:
  - Interior cloaking: target interior to the cloaking device;
  - Exterior cloaking: target exterior to the cloaking device.
- Interior cloaking: Polarization tensors/scattering coefficients cancellation technique.
- Exterior cloaking: anomalous resonances.

Electromagnetic invisibility

- Interior cloaking:
  - Small layered object with vanishing first-order polarization tensors (in the quasi-static limit) or scattering coefficients;
  - Transformation optics;
  - Core invisible.

Electromagnetic invisibility

For a given entire harmonic function u^{in}, $D \ni 0$, $0 < k \neq 1 < +\infty$, consider

$$\begin{cases} \nabla \cdot \Big(\chi(\mathbb{R}^2 \setminus \overline{D}) + k\chi(D) \Big) \nabla u = 0 \quad \text{in } \mathbb{R}^2, \\ u(x) - u^{\mathrm{in}}(x) = O(1/|x|) \quad \text{as } |x| \to \infty. \end{cases}$$

- Multipolar approximation:

$$u(x) = u^{\mathrm{in}}(x) + \sum_{\alpha} \sum_{\beta} \frac{(-1)^{|\beta|}}{\alpha!\beta!} \partial^\alpha u^{\mathrm{in}}(0) \partial^\beta \Gamma(x) M_{\alpha\beta}, \quad |x| \to \infty.$$

- Multi-indices $\alpha, \beta \in \mathbb{N}^2$ and $|\lambda| > 1/2$:

$$M_{\alpha\beta}(\lambda, D) := \int_{\partial D} x^\beta (\lambda I - \mathcal{K}_D^*)^{-1} [\frac{\partial y^\alpha}{\partial \nu}](x) \, d\sigma(x).$$

- $\{M_{\alpha\beta}\}$: generalized polarization tensors (GPTs) associated with D and $\lambda = (k+1)/(2(k-1))$.

Electromagnetic invisibility

- Cloak a region inside the cloaking device.
- Conductivity problem (quasi-static regime): the Dirichlet-to-Neumann map is nearly the same as the one associated to the constant conductivity distribution.
- Change of variable scheme + structures with vanishing generalized polarization tensors.

Electromagnetic invisibility

- Dirichlet-to-Neumann map $\Lambda[\sigma]$:

$$\Lambda[\sigma](\phi) = \sigma \frac{\partial u}{\partial \nu},$$

$$\begin{cases} \nabla \cdot \sigma \nabla u = 0, & \text{in } \Omega, \\ u = \phi, & \text{on } \partial\Omega. \end{cases}$$

- F: diffeomorphism of Ω which is identity on $\partial\Omega$.
- Push-forward of σ by F to obtain the anisotropic conductivity:

$$F_*\sigma(y) = \frac{DF(x)\sigma(x)DF(x)^t}{\det(DF(x))}, \quad x = F^{-1}(y).$$

-

$$\Lambda[\sigma] = \Lambda[F_*\sigma].$$

Electromagnetic invisibility

- $F : \{x : 0 < |x| < 2\} \to \{x : 1 < |x| < 2\}$ given by

$$F(x) := \left(1 + \frac{|x|}{2}\right) \frac{x}{|x|}.$$

- Perfect cloaking: anything inside the hole $\{|x| < 1\}$ surround by a suitable anisotropic conductivity is invisible by the DtN map.
- Transformation optics for electromagnetic cloaking.
- Physically: selective bending of light rays, i.e., a ray is diverted in the direction of the high conductivity, routed tangentially around $|x| = 1$, and then ejected out the other side to continue on its way.
- Drawback: $F_* 1$ is singular on $|x| = 1$ (0 in the normal direction, ∞ in tangential direction, 2D)

Near cloaking (regularization)

Blowing-up a small ball

- For a small number ρ, let

$$\sigma = \begin{cases} \sigma_1 & \text{if } |x| < \rho, \\ 1 & \text{if } \rho \leq |x| \leq 2. \end{cases}$$

(σ_1 can be 0 (insulating core) or ∞ (perfect conductor).)

Near cloaking

- Let

$$F(x) = \begin{cases} \left(\frac{2-2\rho}{2-\rho} + \frac{1}{2-\rho}|x|\right)\frac{x}{|x|} & \text{if } \rho \leq |x| \leq 2, \\ \frac{x}{\rho} & \text{if } 0 \leq |x| \leq \rho. \end{cases}$$

- F maps B_2 onto B_2 and blows up B_ρ onto B_1.
- Approximate cloaking:

$$\|\Lambda[F_*\sigma] - \Lambda[1]\| \leq C\rho^2.$$

- Conductivity in the inner cloaking region: $O(\rho)$ in the normal direction, $0(1/\rho)$ in tangential direction, 2D (product $= 1$).

Small volume expansions

- $\Lambda[F_*\sigma] = \Lambda[\sigma]$ and

$$\Lambda[\sigma](\phi)(x) = \Lambda[1](\phi)(x) + \nabla U(0) \cdot M \frac{\partial}{\partial \nu_x} \nabla_y G(x,0) + \text{h.o.t}, \quad x \in \partial\Omega,$$

  G: the Dirichlet Green function;

$$\begin{cases} \Delta U = 0 & \text{in } \Omega, \\ U = \phi & \text{on } \partial\Omega, \end{cases}$$

  M: polarization tensor of B_ρ.

- PT for B_ρ with conductivity σ_1 (proportional to the volume):

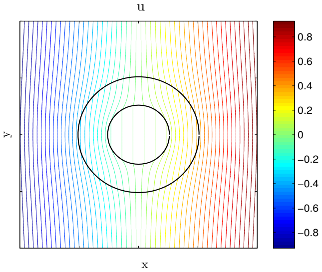
$$M = \frac{2(\sigma_1 - 1)}{\sigma_1 + 1} |B_\rho| I.$$

Polarization tensor of a two-phase structure

- Make PT vanish enhances the cloaking.
- Not possible to make PT vanish with two phases.
- Multi-phase structures.

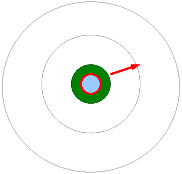
Hashin's neutral inclusion

$M = 0$ (GPTs vanishing structure of order 1; a disc with a single coating)



Enhanced near cloaking

σ^N (GPTs vanishing structure of order N)



Blow-up of a layered small inclusion

- Estimate:

$$\|\Lambda[F_*\sigma^N] - \Lambda[1]\| = \|\Lambda[\sigma^N] - \Lambda[1]\| \leq C\rho^{2N+2}$$

  for some C independent of ρ and N.
- Keep the conductivity in the inner cloaking $O(\rho)$ in the normal direction, $0(1/\rho)$ in tangential direction, 2D.
- Make the h.o.t. vanish in the asymptotic expansion of the Dirichlet-to-Neumann map.

Multiply layered structure

- Let u be the solution to

$$\begin{cases} \nabla \cdot \big(\sigma\chi(D) + \chi(\mathbb{R}^2 \setminus \overline{D})\big) \nabla u = 0 & \text{in } \mathbb{R}^2, \\ u(x) - u^{\rm in}(x) = O(|x|^{-1}) & \text{as } |x| \to \infty. \end{cases}$$

- **Theorem**: The far-field expansion holds as $|x| \to \infty$:

$$(u - u^{\rm in})(x) = -\sum_{m,n=1}^{\infty} \left[\frac{\cos m\theta}{2\pi m r^m} (M^{cc}_{mn} a^c_n + M^{cs}_{mn} a^s_n) + \frac{\sin m\theta}{2\pi m r^m} (M^{sc}_{mn} a^c_n + M^{ss}_{mn} a^s_n) \right]$$

where $u^{\rm in}(x) = u^{\rm in}(0) + \sum_{n=1}^{\infty} r^n (a^c_n \cos n\theta + a^s_n \sin n\theta)$.

- $M^{cc}_{mn}, M^{cs}_{mn}, M^{sc}_{mn}, M^{ss}_{mn}$: contracted GPTs.

Multiply layered structure

Disc with multiple coatings:

- For a positive integer N, let $1 = r_{N+1} < r_N < \ldots < r_1 = 2$ and define

$$A_j := \{r_{j+1} < r \leq r_j\}, \quad j = 1, 2, \ldots, N.$$

- $A_0 = \mathbb{R}^2 \setminus B_2$, $A_{N+1} = B_1$.
- Set σ_j to be the conductivity of A_j for $j = 1, 2, \ldots, N+1$, and $\sigma_0 = 1$. Let

$$\sigma = \sum_{j=0}^{N+1} \sigma_j \chi(A_j).$$

(σ_{N+1} may (or may not) be fixed: σ_{N+1} is fixed to be 0 if the core is insulated.)

GPTs vanishing structure

- Let $M_{mn}^{cc}[\sigma]$, etc, denote the GPTs associated with σ. Because of the symmetry of the disc,

$$M_{mn}^{cs}[\sigma] = M_{mn}^{sc}[\sigma] = 0 \quad \text{for all } m, n,$$

$$M_{mn}^{cc}[\sigma] = M_{mn}^{ss}[\sigma] = 0 \quad \text{if } m \neq n,$$

and

$$M_{nn}^{cc}[\sigma] = M_{nn}^{ss}[\sigma] \quad \text{for all } n.$$

- Let $M_n = M_{nn}^{cc}$, $n = 1, 2, \ldots$.

GPTs vanishing structure

- To compute M_k, we look for solutions u_k to

$$\nabla \cdot \sigma \nabla u = 0 \quad \text{in } \mathbb{R}^2$$

of the form

$$u_k(\mathbf{x}) = a_j^{(k)} r^k \cos k\theta + \frac{b_j^{(k)}}{r^k} \cos k\theta \quad \text{in } A_j, \quad j = 0, 1, \ldots, N+1,$$

with $a_0^{(k)} = 1$ and $b_{N+1}^{(k)} = 0$.

- Then u_k satisfies

$$(u_k - u^{\mathrm{in}})(x) = \frac{b_0^{(k)}}{r^k} \cos k\theta \quad \text{as } |\mathbf{x}| \to \infty.$$

with $u^{\mathrm{in}}(x) = r^k \cos k\theta$.

- Hence, $M_k = -2\pi k b_0^{(k)}$.

GPTs vanishing structure

- The transmission conditions on the interface $\{r = r_j\}$:

$$\begin{bmatrix} a_j^{(k)} \\ b_j^{(k)} \end{bmatrix} = \frac{1}{2\sigma_j} \begin{bmatrix} \sigma_j + \sigma_{j-1} & (\sigma_j - \sigma_{j-1}) r_j^{-2k} \\ (\sigma_j - \sigma_{j-1}) r_j^{2k} & \sigma_j + \sigma_{j-1} \end{bmatrix} \begin{bmatrix} a_{j-1}^{(k)} \\ b_{j-1}^{(k)} \end{bmatrix},$$

and hence

$$\begin{bmatrix} a_{N+1}^{(k)} \\ 0 \end{bmatrix} = \prod_{j=1}^{N+1} \frac{1}{2\sigma_j} \begin{bmatrix} \sigma_j + \sigma_{j-1} & (\sigma_j - \sigma_{j-1}) r_j^{-2k} \\ (\sigma_j - \sigma_{j-1}) r_j^{2k} & \sigma_j + \sigma_{j-1} \end{bmatrix} \begin{bmatrix} 1 \\ b_0^{(k)} \end{bmatrix}.$$

- Let

$$P^{(k)} = \begin{bmatrix} p_{11}^{(k)} & p_{12}^{(k)} \\ p_{21}^{(k)} & p_{22}^{(k)} \end{bmatrix} := \prod_{j=1}^{N+1} \frac{1}{2\sigma_j} \begin{bmatrix} \sigma_j + \sigma_{j-1} & (\sigma_j - \sigma_{j-1}) r_j^{-2k} \\ (\sigma_j - \sigma_{j-1}) r_j^{2k} & \sigma_j + \sigma_{j-1} \end{bmatrix}.$$

Then,

$$b_0^{(k)} = -\frac{p_{21}^{(k)}}{p_{22}^{(k)}}.$$

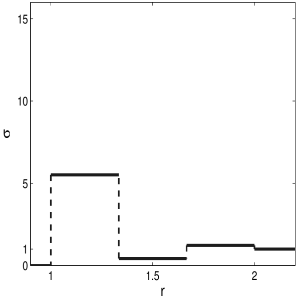
GPTs vanishing structure

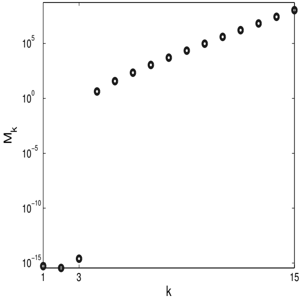
- GPTs vanishing structure of order N: $M_k = 0$ for $k = 1, \ldots, N$, or

$$p_{21}^{(k)} = 0, \quad k = 1, \ldots, N.$$

- Solve the equations for $r_N < \ldots < r_2$ and $\sigma_N, \ldots, \sigma_1$.
- If $N = 1$, Hashin's neutral inclusion.
- For $N = 2, 3, \ldots$, can be solved by hand.
- For arbitrary N, the equation is nonlinear algebraic equation: numerical optimization.

GPTs vanishing structure





The conductivity of the core is fixed to be 0. $N = 3$.

Enhancement of near cloaking

- σ: multi-layered structure with $r_1 = 2$ and $r_{N+1} = 1$; $f = \sum_{k=-\infty}^{\infty} f_k e^{ik\theta}$,

$$\Big(\Lambda[\sigma(\frac{1}{\rho}\mathbf{x})] - \Lambda[1]\Big)(f) = \sum_{k=-\infty}^{\infty} \frac{2|k|\rho^{2|k|} M_{|k|}[\sigma]}{2\pi|k| - \rho^{2|k|} M_{|k|}[\sigma]} f_k e^{ik\theta}.$$

- σ: a GPTs vanishing structure of order N, $\sigma^N(\mathbf{x}) = \sigma(\frac{1}{\rho}\mathbf{x})$,

$$\Big(\Lambda[\sigma^N] - \Lambda[1]\Big)(f) = \sum_{|k|>N} \frac{2|k|\rho^{2|k|} M_{|k|}[\sigma]}{2\pi|k| - \rho^{2|k|} M_{|k|}[\sigma]} f_k e^{ik\theta}.$$

- $|M_k[\sigma]| \leq 2\pi k 2^{2k}$ for all k.
- Using the transformation blowing up a small ball, we can get a near-cloaking structure s.t.

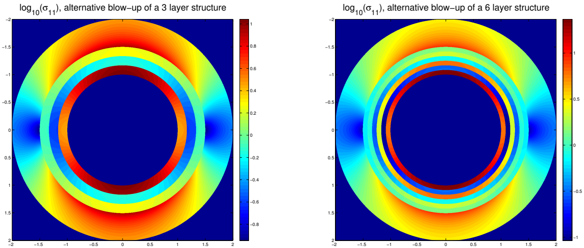
$$\| \Lambda[\sigma^N] - \Lambda[1] \| = \| \Lambda[F_* \sigma^N] - \Lambda[1] \| \leq C\rho^{2N+2}.$$

Enhancement of near cloaking

Change of variables (sends the annulus $[\rho, 2\rho]$ onto a fixed annulus):

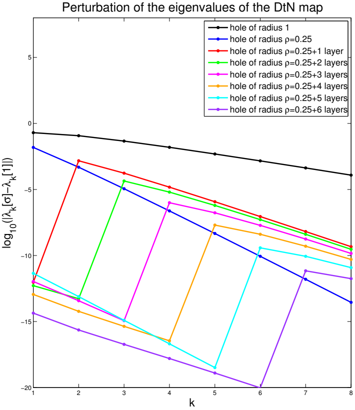
$$F_\rho(\mathbf{x}) := \begin{cases} \left(\dfrac{3-4\rho}{2(1-\rho)} + \dfrac{1}{4(1-\rho)} |\mathbf{x}| \right) \dfrac{\mathbf{x}}{|\mathbf{x}|} & \text{for } 2\rho \leq |\mathbf{x}| \leq 2, \\ \left(\dfrac{1}{2} + \dfrac{1}{2\rho} |\mathbf{x}| \right) \dfrac{\mathbf{x}}{|\mathbf{x}|} & \text{for } \rho \leq |\mathbf{x}| \leq 2\rho, \\ \dfrac{\mathbf{x}}{\rho} & \text{for } |\mathbf{x}| \leq \rho. \end{cases}$$

Anisotropic conductivity distributions:



Enhancement of near cloaking

$\log_{10}$ of the eigenvalues of $\Lambda[\sigma(\frac{1}{\rho}\mathbf{x})] - \Lambda[1]$ for different values of N:



N-layer vanishing GPTs structure: same first N DtN eigenvalues as $\Lambda[1]$.

Electromagnetic invisibility

- Helmholtz equation:

$$\begin{cases} \nabla\cdot\Big(\varepsilon_m\chi(\mathbb{R}^d \setminus \bar{D}) + \varepsilon_c\chi(\overline{D})\Big)\nabla u + \omega^2 u = 0, \\ u^s := u - u^i \text{ satisfies the outgoing radiation condition.} \end{cases}$$

  u^i: incident plane wave; $k_m := \omega\sqrt{\varepsilon_m}, k_c := \omega\sqrt{\varepsilon_c}$.

- Scattering coefficients:

$$W_{ll'}(D, \varepsilon_c, \varepsilon_m, \omega) = \int_{\partial D} \psi_l(y) J_{l'}(\omega|y|) e^{-il'\theta_y}\, ds(y).$$

- ψ_l: electric current density on ∂D induced by the cylindrical wave $J_l(\omega|x|)e^{il\theta_x}$.
- J_l: Bessel function.

Electromagnetic invisibility

- $$\begin{cases} \mathcal{S}_D^{k_c}[\phi_l] - \mathcal{S}_D^{k_m}[\psi_l] = J_l(\omega|x|)e^{il\theta_x}, \\ \varepsilon_c\left(\frac{I}{2} - (\mathcal{K}_D^{k_c})^*\right)[\phi_l] - \varepsilon_m\left(\frac{I}{2} + (\mathcal{K}_D^{k_m})^*\right)[\psi_l] = \varepsilon_m \frac{\partial (J_l(\omega|x|)e^{il\theta_x})}{\partial \nu}. \end{cases}$$

- Properties of the scattering coefficients:
  - $W_{ll'}$ decays rapidly:

$$|W_{ll'}| \leq O(\omega^{|l|+|l|'})\frac{C^{|l|+|l|'}}{|l|^{|l|}|l'|^{|l|'}}, \ \ l, l' \in \mathbb{Z};$$

C: independent of ω.

Electromagnetic invisibility

- Scattering amplitude:

$$u^s(x) = -ie^{-\frac{\pi i}{4}} \frac{e^{ik_m|x|}}{\sqrt{8\pi k_m|x|}} A_\infty[D, \varepsilon_c, \varepsilon_m, \omega](\theta, \theta') + o(|x|^{-\frac{1}{2}}),$$

$|x| \to \infty$; θ, θ': incident and scattered directions.

- Graf's formula:

$$A_\infty[D, \varepsilon_c, \varepsilon_m, \omega](\theta, \theta') = \sum_{l,l' \in \mathbb{Z}} (-i)^l i^{l'} e^{il\theta} W_{ll'}(D, \varepsilon_c, \varepsilon_m, \omega) e^{-il'\theta'}.$$

- Scattering cross-section:

$$Q^s[D, \varepsilon_c, \varepsilon_m, \omega](\theta') := \int_0^{2\pi} \left| A_\infty[D, \varepsilon_c, \varepsilon_m, \omega](\theta, \theta') \right|^2 d\theta.$$

Electromagnetic invisibility

- Scattering coefficient cancellation technique:
  - Small layered object with vanishing first-order scattering coefficients.
  - Transformation optics:

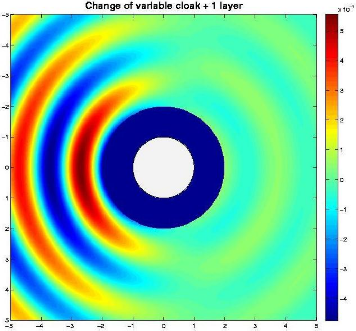
$$(F_\rho)_*[\phi](y) = \frac{DF_\rho(x)\phi(x)DF_\rho(x)^t}{\det(DF_\rho(x))}, \quad x = F_\rho^{-1}(y).$$

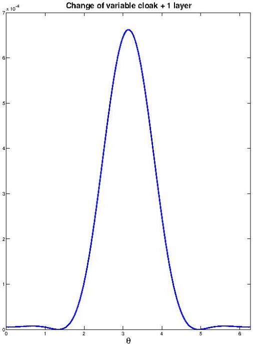
  - Change of variables F_ρ sends the annulus $[\rho, 2\rho]$ onto a fixed annulus.
- Scattering coefficients vanishing structures of order N:

$$Q^s\left[D, (F_\rho)_*(\varepsilon \circ \Psi_{\frac{1}{\rho}}), \varepsilon_m, \omega\right](\theta') = o(\rho^{4N}), \quad \Psi_{1/\rho}(x) = (1/\rho)x.$$

ρ: size of the small object; N: number of layers.
- Anisotropic permittivity distribution.
- Invisibility at $\omega \Rightarrow$ invisibility at all frequencies $\leq \omega$.

Electromagnetic invisibility





Cancellation of the scattered field and the scattering cross-section: 4 orders of magnitude (with wavelength of order 1, $\rho = 10^{-1}$, and $N = 1$).

Anomalous resonance

- Ω: bounded domain in $\mathbb{R}^2$; $D \Subset \Omega$. Ω and D of class $\mathcal{C}^{1,\mu}$, $0 < \mu < 1$. For a given loss parameter $\delta > 0$, the permittivity distribution in $\mathbb{R}^2$ is given by

$$\varepsilon_\delta = \begin{cases} 1 & \text{in } \mathbb{R}^2 \setminus \overline{\Omega}, \\ -1 + i\delta & \text{in } \Omega \setminus \overline{D}, \\ 1 & \text{in } D. \end{cases}$$

- Configuration (plasmonic structure): core with permittivity 1 coated by the shell $\Omega \setminus \overline{D}$ with permittivity $-1 + i\delta$.

Anomalous resonance

- For a given function f compactly supported in $\mathbb{R}^2$ satisfying $\int_{\mathbb{R}^2} f dx = 0$ (conservation of charge), consider the following dielectric problem:

$$\nabla \cdot \varepsilon_\delta \nabla V_\delta = \alpha f \quad \text{in } \mathbb{R}^2,$$

with the decay condition $V_\delta(x) \to 0$ as $|x| \to \infty$.

- Dielectric problems: models the quasi-static (zero-frequency) transverse magnetic regime.

Anomalous resonance

- Fundamental problem: identify f s.t. when $\alpha = 1$

$$E_\delta := \int_{\Omega \setminus \overline{D}} \delta |\nabla V_\delta|^2 dx \to \infty \quad \text{as } \delta \to 0.$$

$$|V_\delta(x)| < C, \quad \text{when} \quad |x| > a$$

  for some constants C and a independent of δ.

- E_δ: proportional to the electromagnetic power dissipated into heat by the time harmonic electrical field averaged over time.
- Infinite amount of energy dissipated per unit time in the limit $\delta \to 0$: unphysical.
- Choose $\alpha = 1/\sqrt{E_\delta}$: αf produces the same power independent of δ and the new associated solution V_δ approaches zero outside the radius a.
- Necessary and sufficient condition for CALR (with $\alpha = 1$) $V_\delta/\sqrt{E_\delta}$ goes to zero outside some radius as $\delta \to 0$.

Anomalous resonance

- Using layer potential techniques: we reduce the problem to a singularly perturbed system of integral equations.
- The system is non-self-adjoint $\Rightarrow$ we introduce a symmetrization technique in order to express the solution in terms of the eigenfunctions of a self-adjoint compact operator.
- Symmetrization technique: based on a generalization of a Calderón identity to the system of integral equations.
- Necessary and sufficient condition on the source term under which the blowup of the power dissipation takes place given in terms of the Newtonian potential of the source

$$\frac{1}{2\pi}\int_{\mathbb{R}^2} \ln|x-y| f(y) dy, \quad x \in \mathbb{R}^2,$$

  which is the solution for the potential in the absence of the plasmonic structure.

Anomalous resonance

- In the case of an annulus (D is the disk of radius r_i and $\Omega =: B_e$ is the concentric disk of radius r_e), it is known (Milton et al.) that there exists a critical radius (the cloaking radius)

$$r_* = \sqrt{r_e^3 r_i^{-1}}.$$

  s.t. any finite collection of dipole sources located at fixed positions within the annulus $B_{r_*} \setminus \overline{B}_e$ is cloaked.
- Sufficient conditions for a source αf supported in E to be cloaked. (In particular, quadrupole source inside the annulus $B_{r_*} \setminus \overline{B}_e$: cloaked).
- Conversely, if the source function f is supported outside B_{r_*} then no cloaking occurs.

Anomalous resonance

- Notation: $\Gamma_i := \partial D$ $\Gamma_e := \partial\Omega$, F Newtonian potential of f; $\mathcal{H} = L^2(\Gamma_i) \times L^2(\Gamma_e)$; $z_\delta = \frac{i\delta}{2(2-i\delta)}$.
- Representation formula:

$$V_\delta(x) = F(x) + \mathcal{S}_{\Gamma_i}[\varphi_i](x) + \mathcal{S}_{\Gamma_e}[\varphi_e](x).$$

- Introduce:

$$\Phi := \begin{bmatrix} \varphi_i \\ \varphi_e \end{bmatrix}, \quad g := \begin{bmatrix} \dfrac{\partial F}{\partial \nu_i} \\ -\dfrac{\partial F}{\partial \nu_e} \end{bmatrix}.$$

- Singularly perturbed equation:

$$(z_\delta \mathbb{I}_2 + \mathbb{K}^*)\Phi = g.$$

- $\mathbb{K}^* : \mathcal{H} \to \mathcal{H}$ Neumann-Poincaré-type operator (compact non-self-adjoint in general):

$$\mathbb{K}^* := \begin{bmatrix} -\mathcal{K}^*_{\Gamma_i} & -\dfrac{\partial}{\partial \nu_i}\mathcal{S}_{\Gamma_e} \\ \dfrac{\partial}{\partial \nu_e}\mathcal{S}_{\Gamma_i} & \mathcal{K}^*_{\Gamma_e} \end{bmatrix}.$$

Anomalous resonance

- Spectrum of $\mathbb{K}^* \subset [-1/2, 1/2]$.
- The operator
$$\mathbb{S} = \begin{bmatrix} \mathcal{S}_{\Gamma_i} & \mathcal{S}_{\Gamma_e} \\ \mathcal{S}_{\Gamma_i} & \mathcal{S}_{\Gamma_e} \end{bmatrix}$$
is self-adjoint and $-\mathbb{S} \geq 0$ on $\mathcal{H}$.
- Calderón's-type identity: $\mathbb{S}\mathbb{K}^* = \mathbb{K}\mathbb{S}$.
- $\mathbb{K}^*$: Hilbert-Schmidt (in 2D; Schatten-von Neumann in 3D).
- $\mathbb{K}^*$: symmetrizable $\Leftarrow$ there is a bounded self-adjoint operator $\mathbb{A}$ on $\mathrm{Range}(\mathbb{S})$ such that $\mathbb{A}\sqrt{-\mathbb{S}} = \sqrt{-\mathbb{S}}\mathbb{K}^*$.

Anomalous resonance

- $\mathbb{A}$ self-adjoint $\Rightarrow$ an orthogonal decomposition: $\mathcal{H} = \text{Ker}\,\mathbb{A} \oplus (\text{Ker}\,\mathbb{A})^\perp$, and $(\text{Ker}\,\mathbb{A})^\perp = \overline{\text{Range}\mathbb{A}}$.
- P and $Q = I - P$: the orthogonal projections from $\mathcal{H}$ onto $\text{Ker}\,\mathbb{A}$ and $(\text{Ker}\,\mathbb{A})^\perp$, respectively. Let $\lambda_1, \lambda_2, \ldots$ with $|\lambda_1| \geq |\lambda_2| \geq \ldots$ be the nonzero eigenvalues of $\mathbb{A}$ and Ψ_n be the corresponding (normalized) eigenfunctions. $\mathbb{A} \in \mathcal{C}_2(\mathcal{H}) \Rightarrow$

$$\sum_{n=1}^{\infty} \lambda_n^2 < \infty,$$

and

$$\mathbb{A}\Phi = \sum_{n=1}^{\infty} \lambda_n \langle \Phi, \Psi_n \rangle \Psi_n, \quad \Phi \in \mathcal{H}.$$

- If $P\sqrt{-\mathbb{S}}g \neq 0$, then CALR takes place. If $\text{Ker}(\mathbb{K}^*) = \{0\}$, then CALR takes place iff

$$\delta \sum_n \frac{|\langle \sqrt{-\mathbb{S}}g, \Psi_n \rangle|^2}{\lambda_n^2 + \delta^2} \to \infty \quad \text{as } \delta \to 0.$$

Anomalous resonance

Anomalous resonance in an annulus:

- Eigenvalues λ of $\mathbb{A} = \{\pm\rho^{|n|}\}$, $\rho = \frac{r_i}{r_e}$.
- (Blow-up of power dissipation criterion) For a given source f supported outside $\overline{B}_e$ (with $\alpha = 1$). If the Fourier coefficients of $-\frac{\partial F}{\partial \nu_e}$ on Γ_e, where F is the Newton potential of f satisfies a Gap condition (mild condition), then
$$\int_{B_e \setminus B_i} \delta |\nabla V_\delta|^2 \to \infty \quad \text{as } \delta \to 0,$$
and CALR occurs.
- Quadrupole satisfies the Gap condition.

Anomalous resonance

Anomalous resonance in an annulus:

- Any source supported outside B_{r_*} cannot make the blow-up of the power dissipation happen and is not cloaked. Indeed, in the limit $\delta \to 0$ the annulus itself becomes invisible to sources that are sufficiently far away.
- If f is supported in $\mathbb{R}^2 \setminus \overline{B}_{r_*}$, then

$$\int_{B_e \setminus B_i} \delta |\nabla V_\delta|^2 < C$$

holds for some constant C independent of δ (with $\alpha = 1$). Moreover,

$$\sup_{|x| \geq r_*} |V_\delta(x) - F(x)| \to 0 \quad \text{as} \quad \delta \to 0.$$

- Annulus itself becomes invisible to sources that are sufficiently far away.

Lecture 13: Helmholtz resonators

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Helmholtz resonators

- Photonics: ubwavelength resonator (plasmonic nanoparticle): low-frequency resonance $\Rightarrow$ metamaterials/cloaking/super-resolution/high-contrast materials/metasurfaces.
- Analogue in phononics: Helmholtz resonators/Minnaert bubbles.

Helmholtz resonators

- Helmholtz resonator:

Helmholtz resonators

- Finite Hilbert transform
- $\mathcal{X}^\epsilon$, for small $\epsilon > 0$,

$$\mathcal{X}^\epsilon = \left\{ \varphi : \int_{-\varepsilon}^{\varepsilon} \sqrt{\epsilon^2 - x^2} \, |\varphi(x)|^2 \, dx < +\infty \right\}.$$

- $\mathcal{X}^\epsilon$: Hilbert space equipped with the norm

$$\|\varphi\|_{\mathcal{X}^\epsilon} = \left(\int_{-\varepsilon}^{\varepsilon} \sqrt{\epsilon^2 - x^2} \, |\varphi(x)|^2 \, dx \right)^{1/2}.$$

- Introduce

$$\mathcal{Y}^\epsilon = \left\{ \psi \in \mathcal{C}^0 \left([-\epsilon, \epsilon] \right) : \psi' \in \mathcal{X}^\epsilon \right\}.$$

- ψ': distribution derivative of ψ.
- $\mathcal{Y}^\epsilon$: Hilbert space with the norm

$$\|\psi\|_{\mathcal{Y}^\epsilon} = \left(||\psi||^2_{\mathcal{X}^\epsilon} + ||\psi'||^2_{\mathcal{X}^\epsilon} \right)^{1/2}.$$

Helmholtz resonators

- $\mathcal{L}_\varepsilon : \mathcal{X}^\epsilon \rightarrow \mathcal{Y}^\epsilon$:
$$\mathcal{L}_\varepsilon[\varphi](x) = \int_{-\epsilon}^{\epsilon} \ln|x-y|\,\varphi(y)\,dy.$$
- For all $0 < \epsilon < 2$, the integral operator $\mathcal{L}_\varepsilon : \mathcal{X}^\epsilon \mapsto \mathcal{Y}^\epsilon$: invertible.
- For $\varphi \in \mathcal{X}^\epsilon$, $\psi(x) = \int_{-\epsilon}^{\epsilon} \ln|x-y|\,\varphi(y)\,dy$: differentiable;
- Derivative on $(-\epsilon, \epsilon)$:
$$\psi'(x) = \mathcal{H}_\varepsilon[\varphi](x).$$
- $\mathcal{H}_\varepsilon$: the finite Hilbert transform
$$\mathcal{H}_\varepsilon[\varphi](x) = \int_{-\epsilon}^{\epsilon} \frac{\varphi(y)}{x-y}\,dy \quad \text{for } x \in (-\epsilon, \epsilon)\,.$$

Helmholtz resonators

- For any $x \in (-\varepsilon, \varepsilon)$,

$$\mathcal{H}_\varepsilon[\frac{1}{\sqrt{\varepsilon^2 - y^2}}](x) = 0, \quad \mathcal{H}_\varepsilon[\sqrt{\varepsilon^2 - y^2}](x) = \pi x, \quad \mathcal{H}_\varepsilon[\frac{y}{\sqrt{\varepsilon^2 - y^2}}](x) = -\pi.$$

- No smoothness preserving property:

$$\mathcal{H}_\varepsilon[1](x) = \ln \frac{\varepsilon + x}{\varepsilon - x}$$

and

$$\mathcal{H}_\varepsilon'[\varphi](x) - \frac{\varphi(-\varepsilon)}{\varepsilon + x} + \frac{\varphi(\varepsilon)}{\varepsilon - x} + \mathcal{H}_\varepsilon[\varphi'](x).$$

- $\mathcal{H}_\varepsilon : \mathcal{X}^\epsilon \to \mathcal{X}^\epsilon$ satisfies $\dim \ker(\mathcal{H}_\varepsilon) = 1$ and $\mathrm{Im}\ \mathcal{H}_\varepsilon = \mathcal{X}^\epsilon$.
- $\ker(\mathcal{H}_\varepsilon)$: spanned by $1/\sqrt{\varepsilon^2 - y^2}$.
- Hölder estimate: for $\varphi \in \mathcal{C}^{0,\eta}([-1,1])$ with $\eta > 0$,

$$\left\| \int_{-1}^{1} \frac{\varphi(y)}{x - y}\, dy \right\|_{L^\infty([-1,1])} \leq C \left\| \varphi \right\|_{\mathcal{C}^{0,\eta}([-1,1])}.$$

Helmholtz resonators

- Explicit solution to

$$\mathcal{L}_\varepsilon[\varphi](x) = \psi(x) \in \mathcal{Y}^\epsilon, \quad \forall\, x \in (-\epsilon, \epsilon)\,.$$

- $\Rightarrow$

$$\psi'(x) = \mathcal{H}_\varepsilon[\varphi](x).$$

- General solution:

$$\varphi_\lambda(x) = -\frac{1}{\pi^2\sqrt{\epsilon^2 - x^2}} \int_{-\epsilon}^{\epsilon} \frac{\sqrt{\epsilon^2 - y^2}\psi'(y)}{x - y}\, dy + \frac{\lambda}{\sqrt{\epsilon^2 - x^2}};$$

- λ: complex constant.
-

$$a(\psi) = \psi(x) - \mathcal{L}_\varepsilon[\varphi_{\lambda=0}](x).$$

- $a(\psi)$: constant.

Helmholtz resonators

- $$\lambda(\psi)\,\mathcal{L}_\varepsilon\left[y\mapsto\frac{1}{\sqrt{\epsilon^2-y^2}}\right] = a(\psi).$$
- $\Rightarrow$ $$\mathcal{L}_\varepsilon\left[y\mapsto\frac{1}{\sqrt{\epsilon^2-y^2}}\right](x)=\pi\ln\frac{\epsilon}{2}\quad\text{for all } x\in\ (-\epsilon,\epsilon)\,.$$
- $\Rightarrow$ $$\lambda(\psi) = \frac{a(\psi)}{\pi\ln(\epsilon/2)}.$$
- $\Rightarrow$ $$\mathcal{L}_\varepsilon^{-1}[\psi](x) = -\frac{1}{\pi^2\sqrt{\epsilon^2-x^2}}\int_{-\epsilon}^{\epsilon}\frac{\sqrt{\epsilon^2-y^2}\psi'(y)}{x-y}\,dy+\frac{a(\psi)}{(\pi\ln(\epsilon/2))\,\sqrt{\epsilon^2-x^2}}.$$
- For $\varepsilon=2$, $\mathcal{L}_2$: nontrivial kernel.
- For $0<\varepsilon<2$, unique solution: $\psi\equiv 0\Rightarrow\mathcal{L}_\varepsilon^{-1}[\psi]\equiv 0$.

Helmholtz resonators

- $R(x,y) \in \mathcal{C}^{1,\eta}$ in x and y, for $\eta > 0$.
- $\mathcal{R}_\varepsilon : \mathcal{X}^\epsilon \to \mathcal{Y}^\epsilon$

$$\mathcal{R}_\varepsilon[\varphi](x) = \int_{-\epsilon}^{\epsilon} R(x,y)\,\varphi(y)\,dy,$$

- There exists a positive constant C, independent of ϵ, s.t.

$$\|\mathcal{L}_\varepsilon^{-1}\mathcal{R}_\varepsilon\|_{\mathcal{L}(\mathcal{X}^\epsilon,\mathcal{X}^\epsilon)} \leq \frac{C}{|\ln \epsilon|};$$

- $$\|\mathcal{L}_\varepsilon^{-1}\mathcal{R}_\varepsilon\|_{\mathcal{L}(\mathcal{X}^\epsilon,\mathcal{X}^\epsilon)} = \sup_{\varphi\in\mathcal{X}^\epsilon, \|\varphi\|_{\mathcal{X}^\epsilon}=1} \|\mathcal{L}_\varepsilon^{-1}\mathcal{R}_\varepsilon[\varphi]\|_{\mathcal{X}^\epsilon}.$$

Helmholtz resonators

- Perturbations of scattering frequencies.
- $\Omega \subset \mathbb{R}^2$: bounded simply connected domain with boundary $\partial\Omega \in \mathcal{C}^2$.
- μ_0: simple eigenvalues of $-\Delta$ in Ω with Neumann conditions.
- V: neighborhood of μ_0 in $\mathbb{C}$ s.t. μ_0: the only eigenvalue in V of $-\Delta$ in Ω with Neumann boundary condition on $\partial\Omega$.
- Acoustic Helmholtz resonator: surface $\partial\Omega_\varepsilon = \partial\Omega \setminus \Sigma_\varepsilon$, where $\partial\Omega_\varepsilon$: obtained from $\partial\Omega$ by making a small opening Σ_ε in the boundary with diameter tending to zero as $\varepsilon \to 0$.
- Opening connects the interior and the exterior parts of the resonator.

Helmholtz resonators

- μ_0: Neumann eigenvalue of $-\Delta$ in Ω, the corresponding scattering problem is to find μ^ε (with $\Im m\, \mu^\varepsilon \geq 0$) close to μ_0 s.t. that there exists a nontrivial solution to

$$\begin{cases} (\Delta + \mu^\varepsilon) u^\varepsilon = 0 \quad \text{in } \Omega \cup (\mathbb{R}^2 \setminus \overline{\Omega}), \\ \dfrac{\partial u^\varepsilon}{\partial \nu} = 0 \quad \text{on } \partial \Omega_\varepsilon, \\ \left| \dfrac{\partial u^\varepsilon}{\partial r} - \sqrt{-1 \mu^\varepsilon} u^\varepsilon \right| = O(r^{-1}) \quad \text{as } r = |x| \to +\infty. \end{cases}$$

- Reduce the scattering problem to the study of characteristic values of a certain operator-valued function, and by means of the generalized Rouché theorem:
    - prove the existence of a scattering frequency μ^ε with small imaginary part which converges to μ_0 as $\varepsilon \to 0$;
    - Construct the leading-order term in its asymptotic expansion.
- Assume 0: the center to which the opening can be contracted and the opening Σ_ε flat: $\Sigma_\varepsilon = (-\varepsilon, \varepsilon)$.

Helmholtz resonators

- $\mu \in \mathbb{C}$ (with $\Im m\, \mu \geq 0$): scattering pole if there exists a nontrivial solution to the exterior problem

$$\begin{cases} (\Delta + \mu) v = 0 \quad \text{in } \mathbb{R}^2 \setminus \overline{\Omega}, \\ \dfrac{\partial v}{\partial \nu} = 0 \quad \text{on } \partial\Omega, \\ \displaystyle\int_{\mathbb{R}^2 \setminus \overline{\Omega}} |v|^2 < +\infty. \end{cases}$$

- Exterior Neumann function $N^{\sqrt{\mu}}_{\mathbb{R}^2 \setminus \overline{\Omega}}$: unique solution to

$$\begin{cases} (\Delta_x + \mu) N^{\sqrt{\mu}}_{\mathbb{R}^2 \setminus \overline{\Omega}}(x, z) = -\delta_z & \text{in } \mathbb{R}^2 \setminus \overline{\Omega}, \\ \dfrac{\partial N^{\sqrt{\mu}}_{\mathbb{R}^2 \setminus \overline{\Omega}}}{\partial \nu}\Big|_{\partial\Omega} = 0 & \text{on } \partial\Omega, \\ \left| \dfrac{\partial N^{\sqrt{\mu}}_{\mathbb{R}^2 \setminus \overline{\Omega}}}{\partial r} - \sqrt{-1\mu} N^{\sqrt{\mu}}_{\mathbb{R}^2 \setminus \overline{\Omega}} \right| = O(r^{-1}) \quad \text{as } r = |x| \to +\infty. \end{cases}$$

Helmholtz resonators

- $N_{\Omega}^{\sqrt{\mu^{\varepsilon}}}$: interior Neumann function.
- $$\varphi^{\varepsilon} = \frac{\partial u^{\varepsilon}}{\partial \nu} \quad \text{on } \Sigma_{\varepsilon}.$$
- Green's formula $\Rightarrow \varphi^{\varepsilon}$ satisfies the integral equation:
$$\int_{\Sigma_{\varepsilon}} \left(N_{\mathbb{R}^2 \setminus \overline{\Omega}}^{\sqrt{\mu^{\varepsilon}}} + N_{\Omega}^{\sqrt{\mu^{\varepsilon}}} \right)(x, y)\, \varphi^{\varepsilon}(y)\, dy = 0 \quad \text{on } \Sigma_{\varepsilon}.$$
- Define $\mu \mapsto \mathcal{A}_{\varepsilon}(\mu)$ by
$$\mathcal{A}_{\varepsilon}(\mu)[\varphi](x) := \int_{-\epsilon}^{\epsilon} \left(N_{\mathbb{R}^2 \setminus \overline{\Omega}}^{\sqrt{\mu^{\varepsilon}}} + N_{\Omega}^{\sqrt{\mu^{\varepsilon}}} \right)(x, y)\, \varphi(y)\, dy.$$
- The problem of finding the scattering frequencies: reduced to that of finding the characteristic values of $\mathcal{A}_{\varepsilon}(\mu)$.

Helmholtz resonators

- Asymptotic formula for perturbations in scattering frequencies.
- Assumptions:
  - μ_0: simple Neumann eigenvalue of of $-\Delta$ in Ω associated with the normalized eigenfunction u_{j_0}
  - V: complex neighborhood of μ_0 s.t. (i) μ_0: the only Neumann eigenvalue in V of $-\Delta$ in Ω and (ii) there is no scattering pole of in V.
- $$N^{\sqrt{\mu}}_{\mathbb{R}^2\setminus\overline{\Omega}}(x,z) = -\frac{1}{2\pi}\ln|x-z| + r(x,z,\mu);$$
- $r(x,z,\mu)$: holomorphic with respect to μ in V and smooth in x and z.

Helmholtz resonators

- Pole-pencil decomposition of $\mathcal{A}_\varepsilon : \mathcal{X}^\epsilon \to \mathcal{Y}^\epsilon$ in $V \setminus \{\mu_0\}$:

$$\mathcal{A}_\varepsilon(\mu) = -\frac{1}{\pi}\mathcal{L}_\varepsilon + \frac{\mathcal{K}_\varepsilon}{\mu_0 - \mu} + \mathcal{R}_\varepsilon(\mu);$$

- $$\mathcal{L}_\varepsilon[\varphi](x) = \int_{-\epsilon}^{\epsilon} \ln|x-y|\,\varphi(y)\,dy;$$

- $\mathcal{K}_\varepsilon$: one-dimensional operator

$$\mathcal{K}_\varepsilon[\varphi](x) = \langle \varphi, u_{j_0} \rangle_{L^2(\Sigma_\varepsilon)}\, u_{j_0};$$

- $$\mathcal{R}_\varepsilon(\mu)[\varphi](x) = \int_{-\epsilon}^{\epsilon} R(\mu,x,y)\,\varphi(y)\,dy;$$

- $(\mu, x, y) \mapsto R(\mu, x, y)$: holomorphic in μ and smooth in x and y.

Helmholtz resonators

- Set of characteristic values of $\mu \mapsto \mathcal{A}_\varepsilon$: discrete.
- Proof:
  - $\mathcal{L}_\varepsilon : \mathcal{X}^\epsilon \to \mathcal{Y}^\epsilon$: invertible; $\|\mathcal{L}_\varepsilon^{-1}\mathcal{R}_\varepsilon\|_{\mathcal{L}(\mathcal{X}^\epsilon,\mathcal{X}^\epsilon)} \to 0$ as $\varepsilon \to 0$.
  - $\Rightarrow -(1/(\pi))\,\mathcal{L}_\varepsilon + \mathcal{R}_\varepsilon : \mathcal{X}^\epsilon \to \mathcal{Y}^\epsilon$: invertible for ε small enough.
  - Pole-pencil decomposition $\Rightarrow \mathcal{A}_\varepsilon$: finitely meromorphic and of Fredholm type in V.
  - $\mathcal{K}_\varepsilon$: of finite-dimension $\Rightarrow \exists\ \mu^* \in V$ s.t. $\mathcal{A}_\varepsilon(\mu^*)$: invertible.
  - Generalized Steinberg's theorem $\Rightarrow$ the discreteness of the set of characteristic values of $\mathcal{A}_\varepsilon$ in V.

Helmholtz resonators

- $\exists$ only one characteristic value of $\mathcal{A}_\varepsilon$ in V of μ_0.
- Proof:
  - Define
$$\mathcal{N}_\varepsilon : \mu \mapsto \mathcal{N}_\varepsilon(\mu) = -\frac{1}{\pi}\mathcal{L}_\varepsilon + \frac{\mathcal{K}_\varepsilon}{\mu_0 - \mu}.$$
  - Show that the multiplicity of $\mathcal{N}_\varepsilon$ in V is equal to zero.
  - Find the characteristic values of $\mathcal{N}_\varepsilon$ in V: $\hat{\mu}$ s.t. $\exists\ \hat{\varphi} \not\equiv 0$ satisfying $\mathcal{N}_\varepsilon(\hat{\mu})[\hat{\varphi}] \equiv 0$ on $(-\varepsilon, \varepsilon)$.
  - $\Rightarrow$
$$\frac{1}{\pi}\mathcal{L}_\varepsilon[\hat{\varphi}] + \frac{\langle \hat{\varphi}, u_{j_0}\rangle}{\hat{\mu} - \mu_0}\ u_{j_0} = 0.$$
  - $\mathcal{L}_\varepsilon$: invertible $\Rightarrow$
$$\frac{1}{\pi}\hat{\varphi} + \frac{\langle \hat{\varphi}, u_{j_0}\rangle}{\hat{\mu} - \mu_0}\mathcal{L}_\varepsilon^{-1}[u_{j_0}] = 0.$$

Helmholtz resonators

- Multiply by u_{j_0},

$$\langle \hat{\varphi}, u_{j_0} \rangle \left(\frac{1}{\pi} + \frac{\langle \mathcal{L}_\varepsilon^{-1}[u_{j_0}], u_{j_0} \rangle}{\hat{\mu} - \mu_0} \right) = 0.$$

- $\Rightarrow$

$$\hat{\mu} = \mu_0 - \pi \langle \mathcal{L}_\varepsilon^{-1}[u_{j_0}], u_{j_0} \rangle.$$

- $\Leftarrow \langle \hat{\varphi}, u_{j_0} \rangle = 0$ would imply that $\hat{\varphi} \equiv 0$.
-

$$|\langle \mathcal{L}_\varepsilon^{-1}[u_{j_0}], u_{j_0} \rangle| \longrightarrow 0 \quad \text{as } \varepsilon \to 0.$$

- $\Rightarrow$

$$|\hat{\mu} - \mu_0| \longrightarrow 0 \quad \text{as } \varepsilon \to 0.$$

- Normalization condition: $\langle \hat{\varphi}, u_{j_0} \rangle = 1 \Rightarrow$ the root function associated to this characteristic value $\hat{\mu}$:

$$\hat{\varphi} = \frac{\mathcal{L}_\varepsilon^{-1}[u_{j_0}]}{\langle \mathcal{L}_\varepsilon^{-1}[u_{j_0}], u_{j_0} \rangle}.$$

Helmholtz resonators

- Multiplicity of $\hat{\mu}$ as a characteristic value of $\mathcal{N}_\varepsilon$ (the order of $\hat{\mu}$ as a pole of $\mathcal{N}_\varepsilon^{-1}$).
- $\mathcal{N}_\varepsilon(\mu)[\varphi] = f$: equivalent to

$$-\frac{1}{\pi}\varphi + \frac{\langle \varphi, u_{j_0}\rangle \mathcal{L}_\varepsilon^{-1}[u_{j_0}]}{\mu_0 - \mu} = \mathcal{L}_\varepsilon^{-1}[f].$$

- $$\langle \varphi, u_{j_0}\rangle \left[-\frac{1}{\pi} + \frac{\langle \mathcal{L}_\varepsilon^{-1}[u_{j_0}], u_{j_0}\rangle}{\mu_0 - \mu} \right] = \langle \mathcal{L}_\varepsilon^{-1}[f], u_{j_0}\rangle.$$
- $\Rightarrow$

$$\langle \varphi, u_{j_0}\rangle = \frac{\pi(\mu_0 - \mu)}{\mu - \hat{\mu}} \langle \mathcal{L}_\varepsilon^{-1}[f], u_{j_0}\rangle.$$

- $\Rightarrow$

$$\mathcal{N}_\varepsilon(\mu)[\varphi] = f \quad \text{iff} \quad \varphi = -\pi\, \mathcal{L}_\varepsilon^{-1}[f] + \frac{\pi^2 \langle \mathcal{L}_\varepsilon^{-1}[f], u_{j_0}\rangle}{\mu - \hat{\mu}} \mathcal{L}_\varepsilon^{-1}[u_{j_0}].$$

- $\hat{\mu}$: characteristic value of order one of $\mathcal{N}_\varepsilon$.
- $\mathcal{N}_\varepsilon$ has exactly one pole μ_0 and one characteristic value $\hat{\mu}$ in V, each of order one, and its full multiplicity is equal to zero.

Helmholtz resonators

- Multiplicity of $\mathcal{A}_\varepsilon$ in V.
- $\mu \mapsto \mathcal{N}_\varepsilon(\mu)$: finitely meromorphic and of Fredholm type at $\mu = \mu_0$.
- For all $\mu \in V \setminus \{\mu_0, \hat{\mu}\}$, $\mathcal{N}_\varepsilon$: invertible.
- $\Rightarrow \mathcal{N}_\varepsilon$: normal in V.
- $\mathcal{A}_\varepsilon(\mu) - \mathcal{N}_\varepsilon(\mu) = \mathcal{R}_\varepsilon(\mu)$: analytic in V.
- $$\lim_{\varepsilon \to 0} \|\mathcal{N}_\varepsilon^{-1}(\mu)\,\mathcal{R}_\varepsilon(\mu)\|_{\mathcal{L}(\mathcal{X}^\varepsilon,\mathcal{X}^\varepsilon)} = 0, \quad \forall\, \mu \in \partial V.$$
- $\Rightarrow \mu \mapsto \mathcal{A}_\varepsilon(\mu)$ has, by the generalized Rouché's theorem, the same full multiplicity as $\mathcal{N}_\varepsilon$ in V.
- μ_0: pole $\Rightarrow \mu \mapsto \mathcal{A}_\varepsilon(\mu)$ admits in V exactly one characteristic value μ^ε.

Helmholtz resonators

- $\mathcal{A}_\varepsilon(\mu)$ has exactly one characteristic value μ^ε in V. Moreover, the following asymptotic expansion of μ^ε holds:

$$\mu^\varepsilon \approx \mu_0 - \pi\langle \mathcal{L}_\varepsilon^{-1}[u_{j_0}], u_{j_0}\rangle + \pi^2\langle \mathcal{L}_\varepsilon^{-1}\mathcal{R}_\varepsilon(\mu_0)\mathcal{L}_\varepsilon^{-1}[u_{j_0}], u_{j_0}\rangle.$$

- $\Rightarrow$

$$\mu^\varepsilon \approx \mu_0 - \frac{\pi}{\ln \varepsilon}|u_{j_0}(0)|^2.$$

- Proof:
  - μ^ε: eigenvalue in $V \Rightarrow \mu^\varepsilon$: characteristic value of $\mathcal{A}_\varepsilon$ in V.
  - φ^ε: associated root function to μ^ε.
  - $I + \mathcal{L}_\varepsilon^{-1}\mathcal{R}_\varepsilon$: invertible for ε small enough $\Rightarrow \langle \varphi^\varepsilon, u_{j_0}\rangle \neq 0 \Rightarrow$ choose φ^ε s.t. $\langle \varphi^\varepsilon, u_{j_0}\rangle = 1$.

Helmholtz resonators

- With this choice,

$$\frac{1}{2\pi} + \frac{\langle \mathcal{L}_\varepsilon^{-1}[u_{j_0}], u_{j_0} \rangle}{\mu^\varepsilon - \mu_0} - \langle \mathcal{L}_\varepsilon^{-1} \mathcal{R}_\varepsilon(\mu^\varepsilon)[\varphi^\varepsilon], u_{j_0} \rangle = 0.$$

- $\Rightarrow$

$$\mu^\varepsilon = \mu_0 - 2\pi \langle \mathcal{L}_\varepsilon^{-1}[u_{j_0}], u_{j_0} \rangle + O(|\ln \varepsilon|^{-2}).$$

- But

$$(-\frac{1}{2\pi} I + \mathcal{L}_\varepsilon^{-1} \mathcal{R}_\varepsilon(\mu^\varepsilon))[\varphi^\varepsilon] + \frac{\mathcal{L}_\varepsilon^{-1}[u_{j_0}]}{\mu_0 - \mu^\varepsilon} = 0.$$

- $\Rightarrow$

$$\varphi^\varepsilon \approx \frac{\mathcal{L}_\varepsilon^{-1}[u_{j_0}]}{\langle \mathcal{L}_\varepsilon^{-1}[u_{j_0}], u_{j_0} \rangle}.$$

Helmholtz resonators

- In the three-dimensional case, for $\mu_0 = 0$,

$$\mu^\epsilon \approx \frac{1}{|\Omega|} \epsilon \mathrm{cap}(\Sigma).$$

- Capacity of Σ in the rescaled opening (of arbitrary smooth shape):

$$\mathrm{cap}(\Sigma) := -\langle \mathcal{L}_1^{-1}[1], 1 \rangle_{L^2(\Sigma)}.$$

- $\mathcal{L}_1$: three-dimensional analog to $\mathcal{L}_\epsilon$ with $\epsilon = 1$:

$$\mathcal{L}_1 : \varphi \mapsto \frac{1}{\pi} \int_\Sigma \frac{\varphi(y)}{|x-y|} dy, \quad x \in \mathbb{R}^3 \setminus \overline{\Sigma}.$$

Helmholtz resonators

- Sub-wavelength resonance of a system of weakly coupled Helmholtz resonators:

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- Asymptotic expansion of the Green function (δ: size of the resonator openings; z_j: center of aperture for jth resonator; J: number of resonators; $\omega = O(\sqrt{\delta})$):

$$\Im G^{\delta}(x, x_0, \omega) \approx \frac{\sin \omega |x - x_0|}{2\pi |x - x_0|} + \sqrt{\delta} \sum_{j=1}^{J} \frac{c_j}{|x - z_j| \, |x_0 - z_j|}.$$