Karlsruhe Institute of Technology

Workgroup Inverse Problems
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Inverse scattering problems in inhomogeneous chiral media

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Technical Details

time-independent complex-valued material functions: permittivity ε, magnetic permeability μ, chirality β

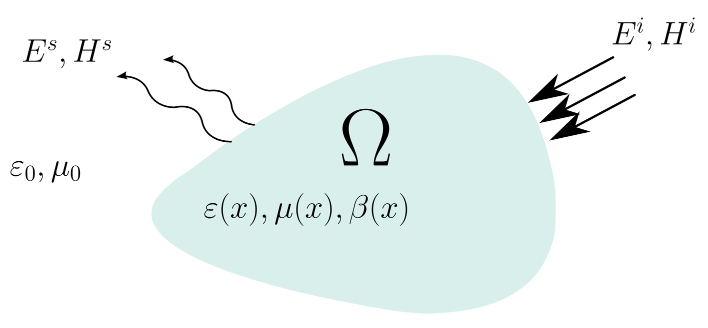

Figure 1: Direct problem setting

wavenumber	$k^2 = \omega^2 \varepsilon_0 \mu_0$
relative permittivity	$\varepsilon_r := \varepsilon / \varepsilon_0$
relative permeability	$\mu_r := \mu / \mu_0$
contrasts	$q_\mu := \mu_r - 1$
	$q_\varepsilon := 1 - \frac{1}{\varepsilon_r}$

Silver–Müller radiation condition:
$\operatorname{curl} H^s(x) \times \frac{x}{|x|} - ikH^s(x) = \mathcal{O}\left(\frac{1}{|x|^2}\right)$ as $|x| \to \infty$

$H(\operatorname{curl}, B) := \{v \in L^2(B, \mathbb{C}^3) : v \text{ possesses } L^2\text{-}\operatorname{curl}\}$

$H_{\text{loc}}(\operatorname{curl}, \mathbb{R}^3) := \{v : v|_B \in H(\operatorname{curl}, B) \text{ f.a. balls } B\}$

Define function f and bounded operators $\mathcal{A}_\kappa, \mathcal{B}_\kappa, \mathcal{C}_\kappa \colon H(\operatorname{curl}, \Omega) \to H(\operatorname{curl}, \Omega)$

$$f(x) := (k^2 + \nabla \operatorname{div}) \int_\Omega g\, \Phi_k(x,\cdot)\, dy + \operatorname{curl} \int_\Omega h\, \Phi_k(x,\cdot)\, dy$$

$$(\mathcal{A}_\kappa v)(x) := (\kappa^2 + \nabla \operatorname{div}) \int_\Omega q_\mu v\, \Phi_\kappa(x,\cdot)\, dy + (\kappa^2 + \nabla \operatorname{div}) \int_\Omega \mu_r \beta \operatorname{curl} v\, \Phi_\kappa(x,\cdot)\, dy$$

$$(\mathcal{B}_\kappa v)(x) := \operatorname{curl} \int_\Omega q_\varepsilon \operatorname{curl} v\, \Phi_\kappa(x,\cdot)\, dy$$

$$(\mathcal{C}_\kappa v)(x) := \operatorname{curl} \int_\Omega [\mu_r \beta(\beta \operatorname{curl} v + v)]\, \Phi_\kappa(x,\cdot)\, dy$$

Assumptions: $k > 0, \exists\, c_1, c_2 > 0$ and $c_3 \in (0,1)$:
$\operatorname{Re} \mu_r \geq c_1$, $\operatorname{Re} \frac{1}{\varepsilon_r} \geq c_2$, $k^2 \beta^2 \frac{|\varepsilon_r|^2 |\mu_r|^2}{\operatorname{Re} \varepsilon_r \operatorname{Re} \mu_r} \leq c_3$

Chirality

In geometry, a figure is CHIRAL if it cannot be mapped to its mirror image by rotations and translations alone. In chemistry, chirality usually refers to molecules. Two mirror images of a chiral molecule are called ENANTIOMERS .

$$\begin{aligned} \operatorname{curl} H &= -i\omega D \\ \operatorname{curl} E &= i\omega B \\ D &= \varepsilon(E + \beta \operatorname{curl} E) \\ B &= \mu(H + \beta \operatorname{curl} H) \end{aligned}$$

Chiral material is optically active: It rotates plane polarized light and left- and right-circularly polarized waves propagate with different phase velocities. Wave propagation in chiral media is governed by Maxwell's equations and the Drude-Born-Fedorov equations (constitutive relations). We treat the time-harmonic case with frequency ω, electric field E, electric induction D, magnetic field H and magnetic induction B.

Direct scattering problem

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with $\varepsilon \equiv \varepsilon_0$, $\mu \equiv \mu_0$, $\beta \equiv 0$ in $\mathbb{R}^3 \setminus \overline{\Omega}$ and $\operatorname{Im} \beta = 0$. The constants ε_0 and μ_0 are the permittivity and the magnetic permeability in vacuum. The total fields E and H are superpositions of the incident and the scattered fields: $E = E^i + E^s$ and $H = H^i + H^s$. Elimination of the fields E, B and D in the above equations leads to a second order equation for H:

$$\operatorname{curl}\left[\left(\tfrac{1}{\varepsilon_r} - k^2\mu_r\beta^2\right) \operatorname{curl} H - k^2\mu_r\beta H\right] - k^2\mu_r\beta \operatorname{curl} H - k^2\mu_r H = 0$$

The incident field H^i satisfies Maxwell's equations in vacuum: $\operatorname{curl}^2 H^i - k^2 H^i = 0$. Subtraction of the equations leads to the scattering equation

$$\begin{aligned} &\operatorname{curl}\left[\left(\tfrac{1}{\varepsilon_r} - k^2\mu_r\beta^2\right) \operatorname{curl} H^s - k^2\mu_r\beta H^s\right] - k^2\mu_r\beta \operatorname{curl} H^s - k^2\mu_r H^s \\ &= k^2 q_\mu H^i + k^2 \mu_r\beta \operatorname{curl} H^i + \operatorname{curl}\left[(q_\varepsilon + k^2\mu_r\beta^2) \operatorname{curl} H^i + k^2\mu_r\beta H^i\right] \end{aligned} \tag{1}$$

Additionally, we need transmission conditions on $\partial\Omega$ and a radiation condition for H^s.

Variational formulation

For $g, h \in L^2(\Omega, \mathbb{C}^3)$ determine radiating $H^s \in H_{\text{loc}}(\operatorname{curl}, \mathbb{R}^3)$ such that

$$\begin{aligned} &\int_{\mathbb{R}^3} \left[\left(\tfrac{1}{\varepsilon_r} - k^2\mu_r\beta^2\right) \operatorname{curl} H^s - k^2\mu_r\beta\, H^s\right] \cdot \operatorname{curl} \psi - k^2\left[\mu_r\beta \operatorname{curl} H^s + \mu_r H^s\right] \cdot \psi \, dx \\ &= \int_\Omega k^2 g \cdot \psi + h \cdot \operatorname{curl} \psi \, dx \end{aligned} \tag{2}$$

for all $\psi \in H(\operatorname{curl}, \mathbb{R}^3)$ with compact support. Denote by $\Phi_k(x,y) := \frac{\exp(ik|x-y|)}{4\pi|x-y|}$, $x \neq y$, the fundamental solution to the scalar Helmholtz equation. Then (2) is equivalent to solving the integro-differential equation [1]

$$\begin{aligned} v(x) = (k^2 + \nabla \operatorname{div}) &\int_\Omega \left[q_\mu v + \mu_r\beta \operatorname{curl} v + g\right] \Phi_k(x,\cdot)\, dy \\ + \operatorname{curl} &\int_\Omega \left[q_\varepsilon \operatorname{curl} v + k^2\mu_r\beta^2 \operatorname{curl} v + k^2\mu_r\beta v + h\right] \Phi_k(x,\cdot)\, dy \end{aligned} \tag{3}$$

Write equation (3) in operator form $\quad (I - \mathcal{A}_k - \mathcal{B}_k - k^2\mathcal{C}_k)v = f.$

Solvability: Fredholm alternative

Lemma 1. *(a) The operator $I - \mathcal{A}_{ik} - \mathcal{B}_{ik} - k^2\mathcal{C}_{ik}$ is boundedly invertible in $H(\operatorname{curl}, \Omega)$.*
(b) The operators $\mathcal{A}_k - \mathcal{A}_{ik}$, $\mathcal{B}_k - \mathcal{B}_{ik}$ and $\mathcal{C}_k - \mathcal{C}_{ik}$ are compact.

Theorem 1. *The variational problem (2) satisfies the Fredholm alternative, i.e. there exists a unique radiating solution provided uniqueness holds.*

Inverse problem

Every radiating solution H^s of (2) has the asymptotic form uniformly in all directions $\hat{x} = x/|x|$

$$H^s(x) = \frac{e^{ik|x|}}{4\pi|x|}\left\{H^\infty(\hat{x}) + \mathcal{O}\left(\frac{1}{|x|}\right)\right\}, \qquad |x| \to \infty.$$

The function H^∞ defined on the unit sphere S^2 is called MAGNETIC FAR FIELD PATTERN. Denote by $H^\infty(\hat{x}; d, p)$ the far field pattern of the scattered field caused by the incident field $H^i(x; d, p) := pe^{ik\, d\cdot x}$ for a direction of incidence d and a polarization vector p with $d \cdot p = 0$.

Inverse Problem. *Given $H^\infty(\hat{x}; d, p)$ for all $\hat{x}, d \in S^2$ and $p \in \mathbb{C}^3$ with $d \cdot p = 0$ localize Ω.*

Far field operator. $\mathcal{F} \colon L^2_t(S^2) \to L^2_t(S^2)$, $p \mapsto \int_{S^2} H^\infty(\cdot; d, p(d))\, ds(d)$

Factorization method

Assume (2) is uniquely solvable (e.g. $\operatorname{Im} \varepsilon > 0$). $\mathcal{F}$ can be factorized as $\mathcal{F} = \mathcal{H}^*\mathcal{T}\mathcal{H}$ with operators $\mathcal{H}p = (\mathcal{H}_1 p, \mathcal{H}_2 p)^\top$, its adjoint $\mathcal{H}^* f = \sum_j \mathcal{H}_j^* f_j$ and $\mathcal{T}$. $\mathcal{T}$ involves a solution of an equation similar to (1).

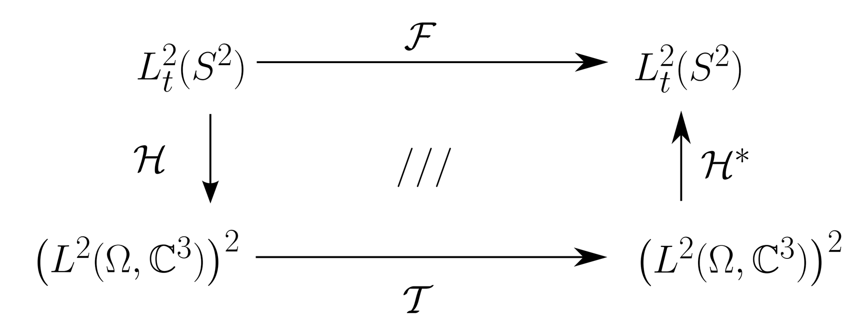

Figure 2: Factorization of $\mathcal{F}$

Localization of the scatterer

For any $z \in \mathbb{R}^3$ we define an explicite function $\phi_z \in L^2_t(S^2)$ such that the following equivalence holds:

$$z \in \Omega \iff \phi_z \in \mathcal{R}(\mathcal{H}^*)$$

Theorem 2. *Assume $\exists\, c_3, c_4 > 0 : \operatorname{Im} q_\varepsilon > c_3|q_\varepsilon|$ and $\operatorname{Im} q_\mu > c_4|q_\mu|$. Then*
(a) The operator $\operatorname{Im} \mathcal{T} = \frac{1}{2i}(\mathcal{T} - \mathcal{T}^*)$ is coercive on $\mathcal{R}(\mathcal{H})$.
(b) The ranges of $\mathcal{H}^*$ and $(\operatorname{Im} \mathcal{F})^{1/2}$ coincide [2].

References

[1] A. KIRSCH, *An integral equation approach and the interior transmission problem for Maxwell's equations*, Inverse Problems and Imaging, 1 (2007), pp. 159–180.
[2] A. KIRSCH AND N.I. GRINBERG, *The Factorization Method for Inverse Problems*, Oxford Lecture Series in Mathematics and its Applications 36, Oxford University Press, 2008.

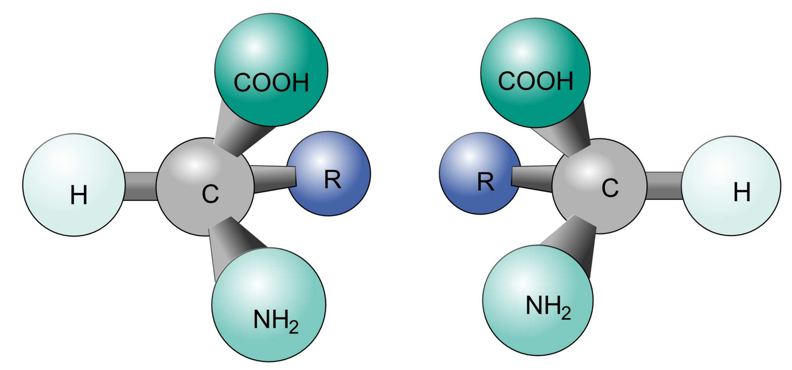

Figure 3: The two enantiomers of a generic amino acid

Technical Details

subspace of tangential fields:
$L^2_t(S^2) := \{p \in L^2(S^2, \mathbb{C}^3) : p(d) \cdot d = 0, d \in S^2\}$

Define 2 modified Herglotz operators $\mathcal{H}_j \colon L^2_t(S^2) \to L^2(\Omega, \mathbb{C}^3)$

$$(\mathcal{H}_1 p)(y) := \sqrt{|q_\mu(y)|} \int_{S^2} p(d) e^{ik\, d\cdot y} ds(d)$$

$$(\mathcal{H}_2 p)(y) := \sqrt{|q_\varepsilon(y)|} \operatorname{curl} \int_{S^2} p(d) e^{ik\, d\cdot y} ds(d)$$

and their adjoints $\mathcal{H}_j^* \colon L^2(\Omega, \mathbb{C}^3) \to L^2_t(S^2)$

$$(\mathcal{H}_1^*\varphi_1)(d) = d \times \int_\Omega \varphi_1(y) \sqrt{|q_\mu(y)|} e^{-ik\, d\cdot y}\, dy \times d$$

$$(\mathcal{H}_2^*\varphi_2)(d) = ik\, d \times \int_\Omega \varphi_2(y) \sqrt{|q_\varepsilon(y)|} e^{-ik\, d\cdot y}\, dy$$

operator $\mathcal{T} \colon \left(L^2(\Omega, \mathbb{C}^3)\right)^2 \to \left(L^2(\Omega, \mathbb{C}^3)\right)^2$

$$\mathcal{T}(f_1, f_2) := \begin{pmatrix} k^2 \operatorname{sgn} q_\mu (f_1 + \sqrt{|q_\mu|} v) \\ (k^2 \frac{\mu_r\beta^2}{|q_\varepsilon|} + \operatorname{sgn} q_\varepsilon)(f_2 + \sqrt{|q_\varepsilon|} \operatorname{curl} v) \end{pmatrix} + k^2 \frac{\mu_r\beta}{\sqrt{|q_\mu||q_\varepsilon|}} \begin{pmatrix} f_2 + \sqrt{|q_\varepsilon|} \operatorname{curl} v \\ f_1 + \sqrt{|q_\mu|} v \end{pmatrix}$$

v is a solution of

$$\begin{aligned} &\operatorname{curl}\left[\left(\tfrac{1}{\varepsilon_r} - k^2\mu_r\beta^2\right) \operatorname{curl} v - k^2\mu_r\beta v\right] - k^2\left[\mu_r\beta \operatorname{curl} v + \mu_r v\right] \\ &= k^2\left[\frac{q_\mu}{\sqrt{|q_\mu|}} f_1 + \frac{\mu_r\beta}{\sqrt{|q_\varepsilon|}} f_2\right] + \operatorname{curl}\left[\frac{q_\varepsilon + k^2\mu_r\beta^2}{\sqrt{|q_\varepsilon|}} f_2 + k^2 \frac{\mu_r\beta}{\sqrt{|q_\mu|}} f_1\right] \end{aligned}$$

$\phi_z(d) := \{-d \times (d \times p_1) + ik\, d \times p_2\} e^{-ik\, d\cdot z}, \quad d \in S^2.$
for fixed $p_1, p_2 \in \mathbb{C}$.