Inverse problems and quantum mechanics

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Mathematical Challenges in Quantum Mechanics

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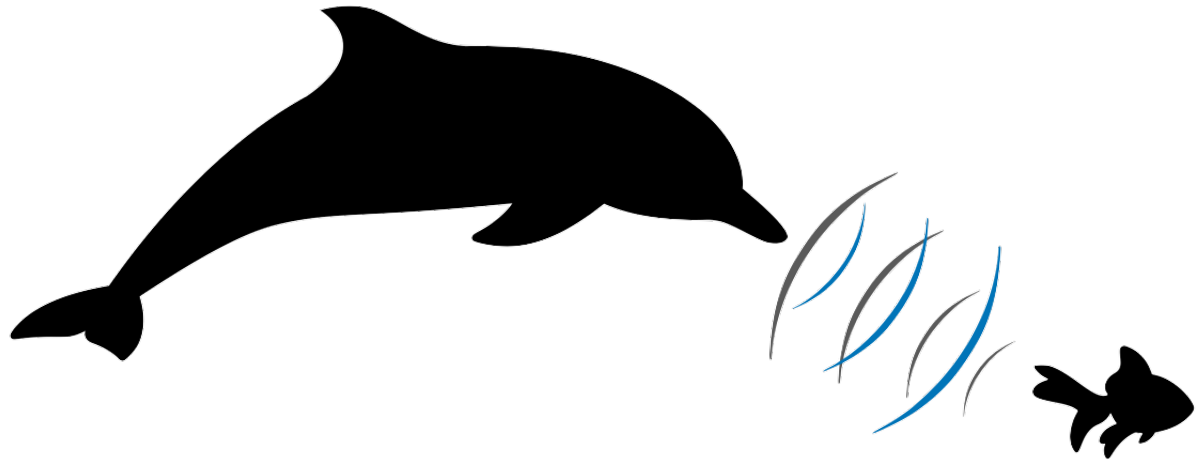
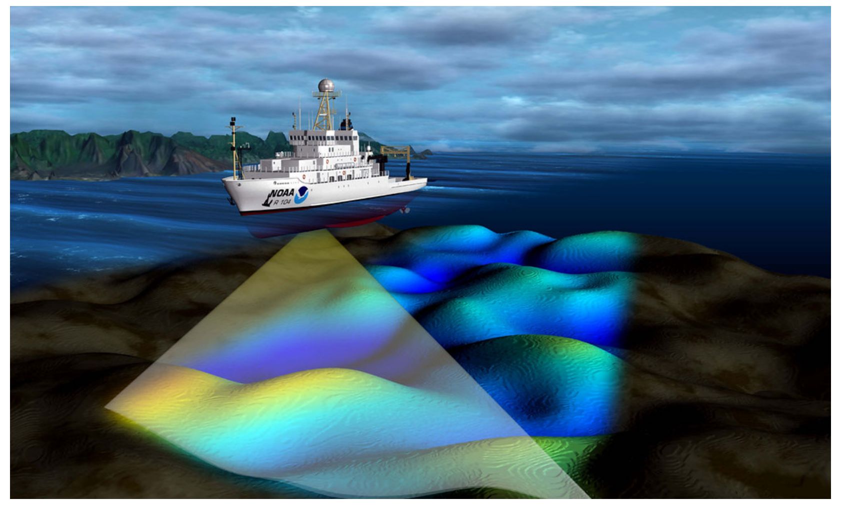
What is an inverse problem?

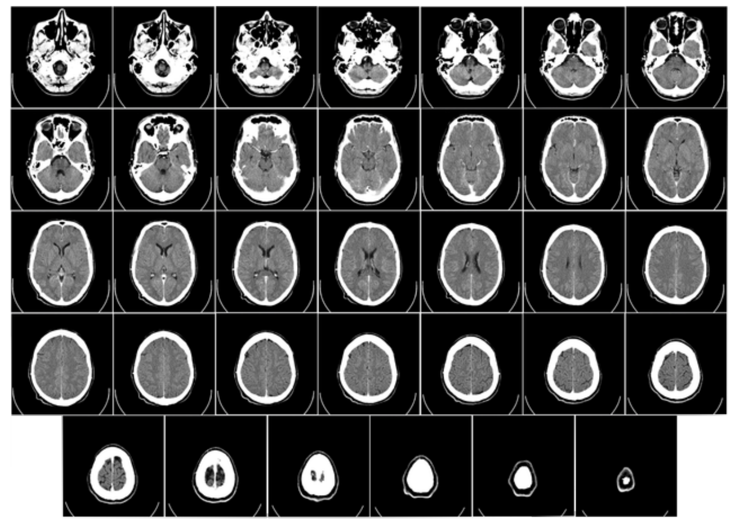


Dolphin echolocation



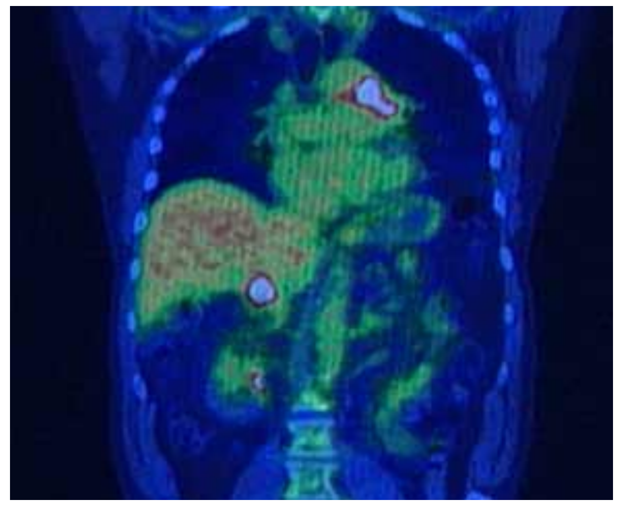
Sonar

Ultrasonography



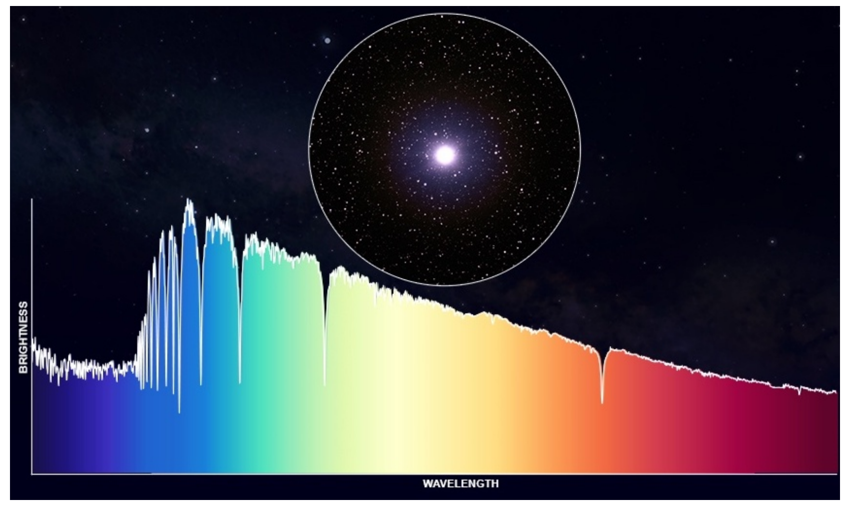
X-ray tomography
(CAT scan)

Magnetic resonance
imaging (MRI)

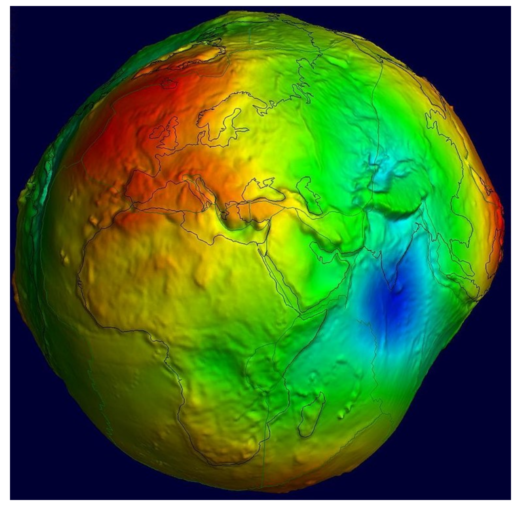


Positron emission
tomography (PET)

Image deblurring



Astronomical spectroscopy



Gravimetry

What is an inverse problem (in mathematical terms)?

Let X and Y be subsets of Banach spaces.

Forward problem

$$\begin{aligned} \Lambda : \ & X \to Y \\ & \mathrm{x} \mapsto \mathrm{y} = \Lambda(\mathrm{x}) \end{aligned}$$

We assume it is well-posed (in the sense of Hadamard):

- existence: for any $\mathrm{x} \in X$, there is $\mathrm{y} \in Y$,
- uniqueness: for each x, y is unique,
- continuous: if $\|\mathrm{x}_1 - \mathrm{x}_2\| \to 0$, then $\|\mathrm{y}_1 - \mathrm{y}_2\| \to 0$.

Inverse problem (IP)

Given $\mathrm{y} = \Lambda(\mathrm{x})$, find x.

The inverse problem is well-posed (in the sense of Hadamard) if $\Lambda^{-1} : Y \to X$ is well-posed, i.e.

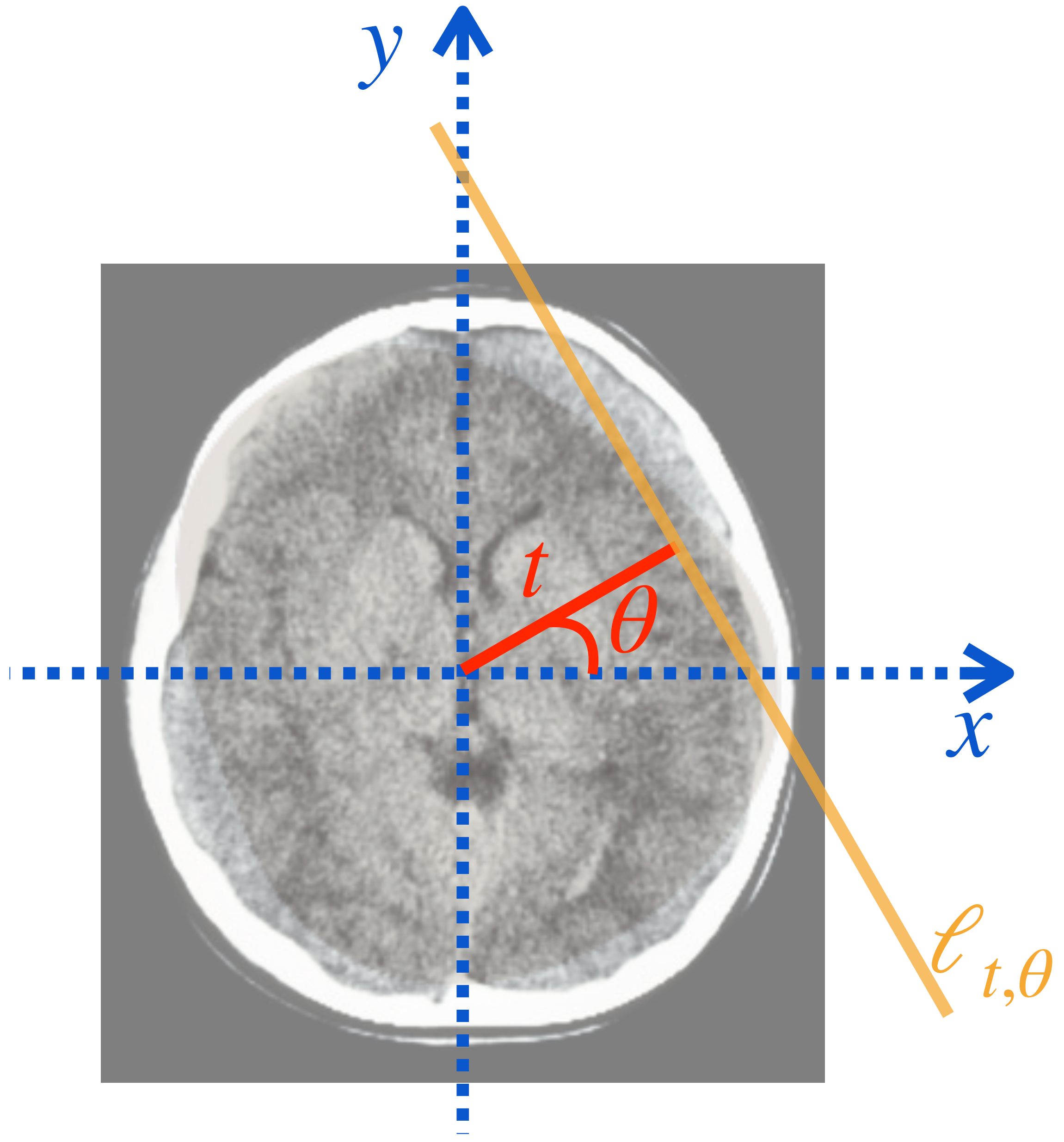
- Λ is surjective ($Y = \Lambda(X)$),
- Λ is injective (uniqueness),
- Λ^{-1} is continuous (stability).

Disclaimer: Often, inverse problems are ill-posed.

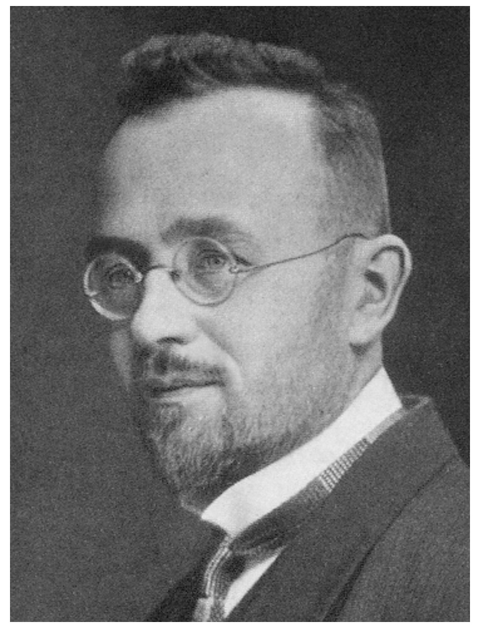
In the context of PDEs: x refers to the model (coefficients of the PDE, domains involved,...) and y represents properties of the solutions to the model.

$$\Lambda : \mu(x,y) \mapsto \Lambda\mu(t,\theta) = \int_{\ell_{t,\theta}} \mu \qquad \ell_{t,\theta} = \{(x,y) : x\cos\theta + y\sin\theta = t\}$$

Λ = Radon transform

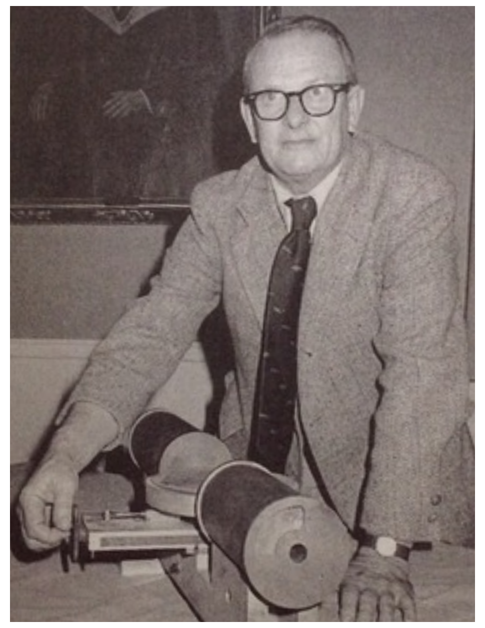


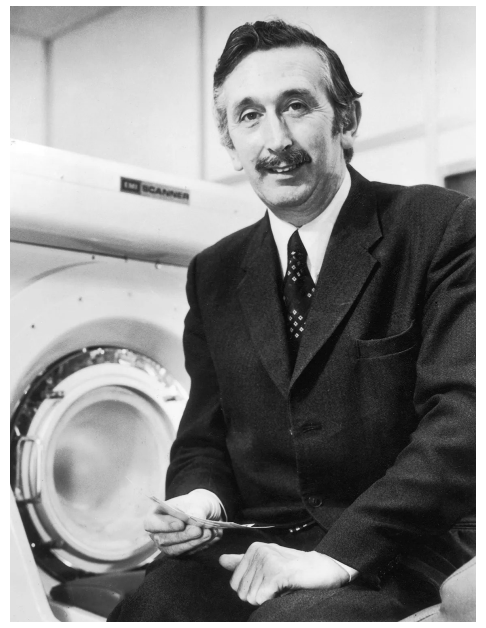
The IP is ill-posed due to the lack of continuity of the inverse of the Radon transform: $\mu(x,y) \simeq \int_0^{\pi} \big(\Lambda\mu(\,\cdot\,,\theta) * h\big)(x\cos\theta + y\sin\theta)d\theta,\ \hat{h}(\xi) = |\xi|.$



Math. theory published in 1917

J. Radon (Austria 1887-1956)



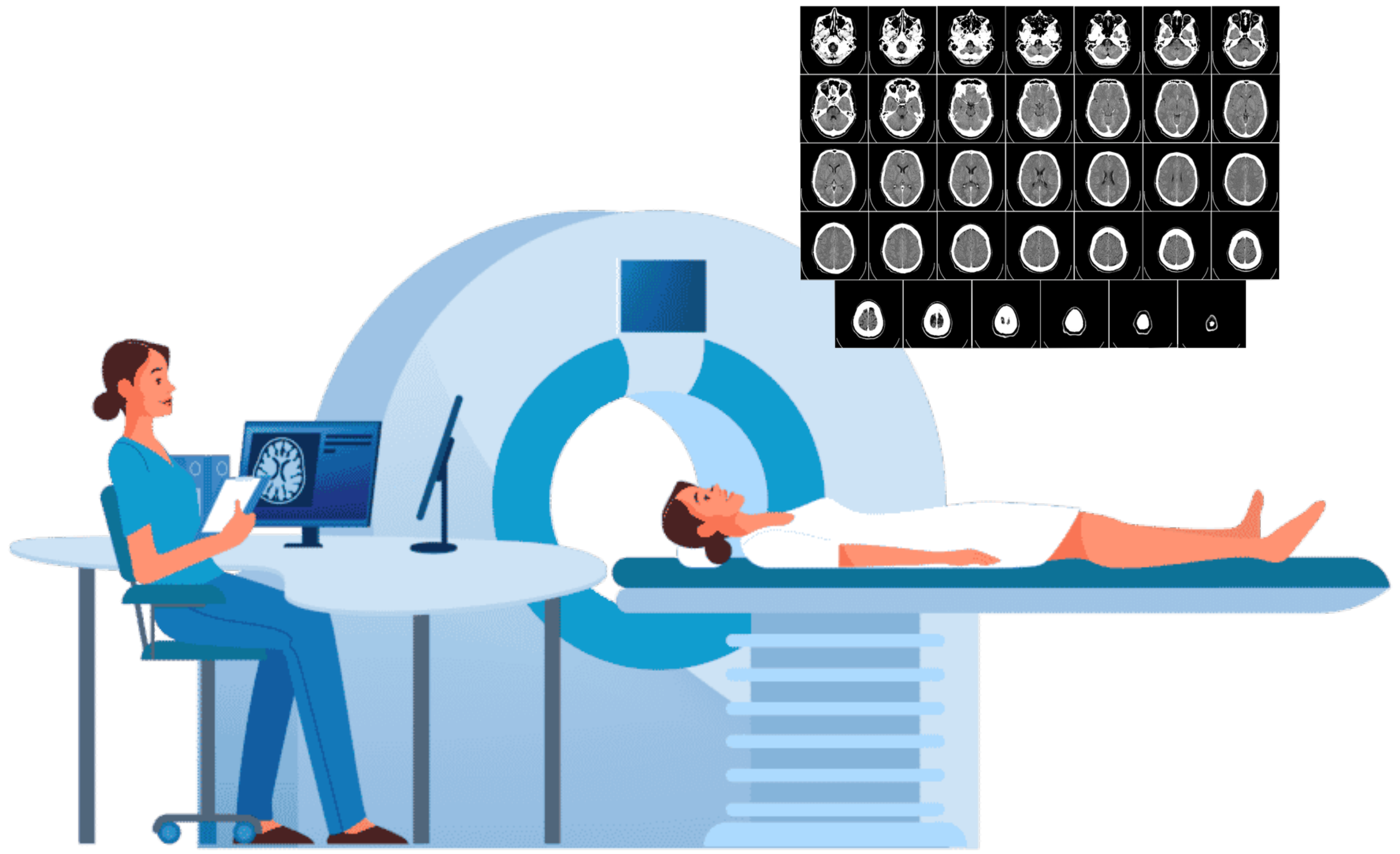


TAC development in the 60's -70's

A. McL. Cormack(Sudáfrica 1924-EEUU 1998)

G. Hounsfield (Reino Unido 1919-2004)

Nobel Prize in Physiology or Medicine in 1979



Questions about an inverse problem

IP: Can we find x from measurements $\mathrm{y} = \Lambda(\mathrm{x})$?

Main questions

- Uniqueness: $\Lambda(\mathrm{x}_1) = \Lambda(\mathrm{x}_2) \Rightarrow \mathrm{x}_1 = \mathrm{x}_2$?
- Stability: $\|\Lambda(\mathrm{x}_1) - \Lambda(\mathrm{x}_2)\|_* \to 0 \Rightarrow \|\mathrm{x}_1 - \mathrm{x}_2\|_X \to 0$? (and if so, how fast?)
- Reconstruction: given $\Lambda(\mathrm{x})$, is there a convergent algorithm to obtain x?

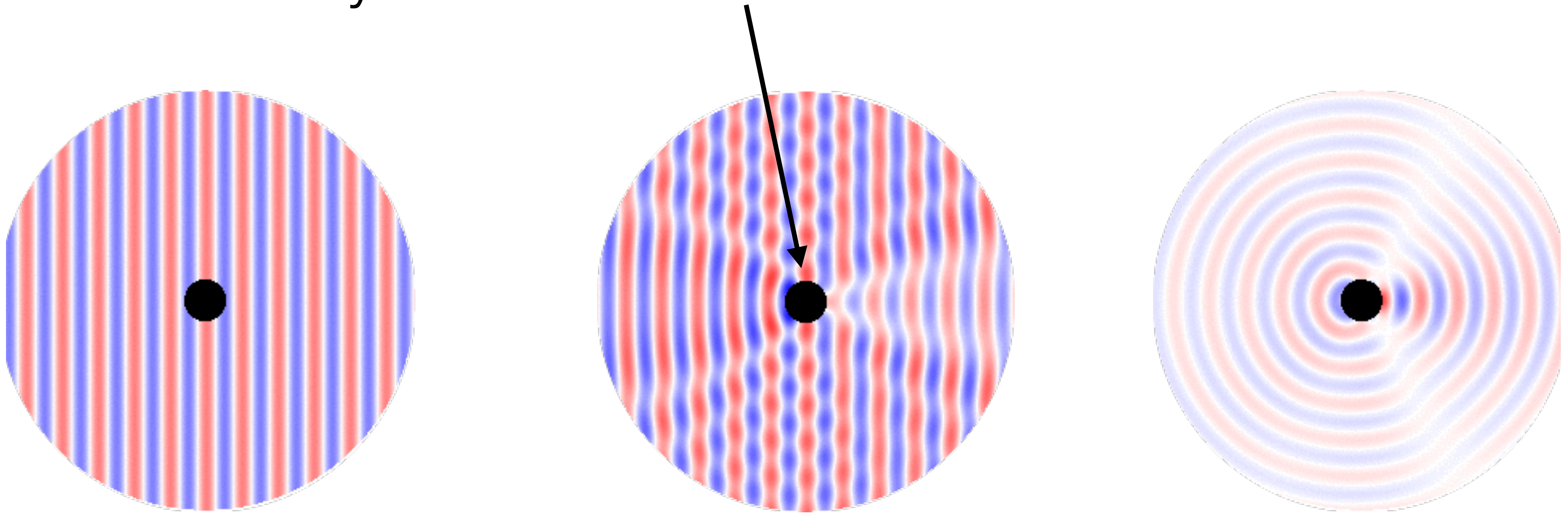
Other scenarios

- Partial data: we know $\Lambda(\mathrm{x})$ only partially.

  E.g.: the Radon transform only for angles θ in some interval.
- Finite data: we know only a finite set of measurements of $\Lambda(\mathrm{x})$.

  E.g.: the Radon transform only for some (t_j, θ_j), $j \in \{1, \ldots, J\}$.

Idea: (acoustic) waves are scattered by some obstacle.



Incoming wave (plane) *Resulting wave (total)* *Scattered wave (difference)*

- The pressure, $p(t,x)$, satisfies the wave equation $\partial_t^2 p = c^2 \Delta p$, where c is the sound speed.
- We assume that $c = c_0$ outside the object ($D \subset \mathbb{R}^n$ compact) and that p has fixed frequency ω, i.e. $p(t,x) = \mathrm{Re}\left(e^{i\omega t} u(x)\right)$. Therefore $(\Delta + k^2)u(x) = 0 \text{ in } \mathbb{R}^n \backslash D$, where $k = \dfrac{\omega}{c_0}$, and u satisfies some boundary condition on ∂D, e.g. $u = 0 \text{ on } \partial\Omega$ (soft obstacle).
- u is the superposition of the incident plane wave, $u^i(x) = e^{ik\theta\cdot x}$, $\theta \in \mathbb{S}^{n-1}$, and the scattered wave, $u^s(x)$, which obeys the Sommerfeld radiation condition (so it is outgoing): $r^{\frac{n-1}{2}}(\partial_r - ik)u^s \to 0$ as $r \to \infty$.

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Idea: particles/waves are scattered off by a potential.

- The wave function, $\Psi(t,x)$, satisfies the Schrödinger equation $i\hbar\partial_t\Psi = \left(-\frac{\hbar}{2m}\Delta + V\right)\Psi$.
- We assume that $V = V(x)$ and that Ψ has fixed energy $E > 0$, i.e. $\Psi(t,x) = e^{-iEt/\hbar}u(x)$. Therefore $\left(\Delta + k^2 - q(x)\right)u(x) = 0 \text{ in } \mathbb{R}^n$, where $k = \frac{\sqrt{2mE}}{\hbar}$ and $q = \frac{2m}{\hbar^2}V$.
- We assume q is bounded and $\operatorname{supp} q \subset B_R$ and consider that u is the superposition of a free wave function $u^i(x) = e^{ik\theta\cdot x}$, $\theta \in \mathbb{S}^{n-1}$, and an outgoing wave function, $u^s(x)$, obeying the Sommerfeld radiation condition: $r^{\frac{n-1}{2}}(\partial_r - ik)u^s \to 0$ as $r \to \infty$.
- Under the previous assumptions u is unique (in suitable space) and

$$u^s(re^{i\alpha}) = \frac{e^{ikr}}{r^{\frac{n-1}{2}}}\left(a_q(k,\theta;\alpha) + O(r^{-1})\right) \text{as } r \to \infty \quad (\alpha \in \mathbb{S}^{n-1}).$$

scattering amplitude / far-field pattern

$$\Lambda:\ q(x) \mapsto a_q(k,\theta;\alpha)$$ (for fixed k, fixed θ, $\alpha = -\theta, \dots$)

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IP: Can we find q from the scattering amplitude at fixed energy, $a_q(k,\cdot\,;\cdot\,)$?

Uniqueness: [Novikov 1994] / Reduction to an inverse boundary value problem.

Let $n \geq 3$, $k \neq 0$, $q_1, q_2 \in L^\infty(\mathbb{R}^n)$ with $\operatorname{supp} q_j \subset B_R$.

1. If $a_{q_1}(k,\cdot\,;\cdot\,) = a_{q_2}(k,\cdot\,;\cdot\,)$, then $\int_{B_R} (q_1 - q_2) u_1 \overline{u_2}\, dx = 0$ for all $u_j \in H^2(B_R)$ such that $(-\Delta - k^2 + q_j)u_j = 0$.

Ingredients: "integration by parts", Rellich uniqueness theorem, density of "$u^i + u^s$" solutions in $H^2(B_R)$.

Equivalently, $a_{q_1}(k,\cdot\,;\cdot\,) = a_{q_2}(k,\cdot\,;\cdot\,)$ implies $\Lambda_{q_1-k^2} = \Lambda_{q_2-k^2}$, where Λ_q denotes the Dirichlet-to-Neumann map $\Lambda_q : f \mapsto \partial_\nu u|_{\partial\Omega}$, with

$$\big(-\Delta + q(x)\big)u = 0 \text{ in } \Omega,$$
$$u = f \text{ on } \partial\Omega\,.$$

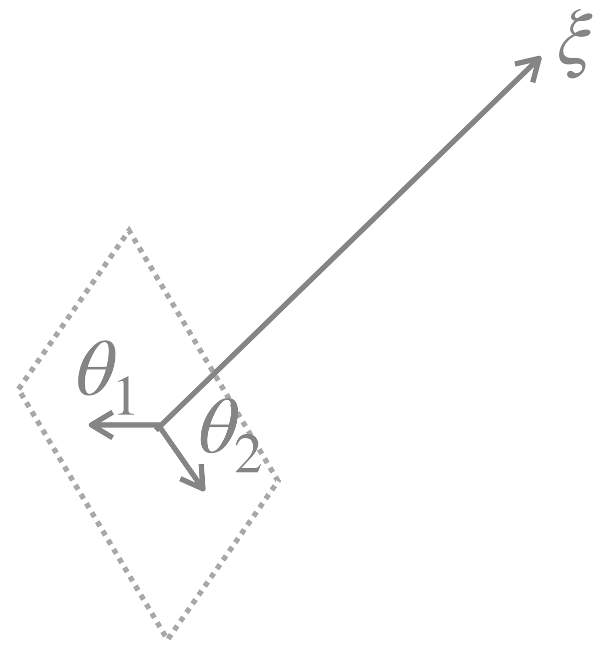
($\Lambda : q \to \Lambda_q$ is well-posed provided 0 is not an eigenvalue.)

2. CGO solutions: Given q and $\zeta \in \mathbb{C}^n$ such that $\zeta \cdot \zeta = 0$ $(|Re\ \zeta| = |Im\ \zeta|\ \&\ Re\ \zeta \cdot Im\ \zeta = 0)$ there exists a solution to $(-\Delta + q)u = 0$ such that $u(x) = e^{\zeta \cdot x}\big(1 + r_{q,\zeta}(x)\big)$, where "$r_{q,\zeta} \to 0$" as $|\zeta| \to \infty$.

Key point: to solve $(\Delta + 2\zeta \cdot \nabla - q)r_{q,\zeta} = q \;\Rightarrow\; r_{q,\zeta} = \Delta_\zeta^{-1}(I - q\Delta_\zeta^{-1})^{-1}(q)$ with $\Delta_\zeta^{-1} = (\Delta + 2\zeta \cdot \nabla)^{-1}$ between suitable spaces so $\|\Delta_\zeta^{-1}\|_* \lesssim |\zeta|^{-1}$.

[Sylvester, Uhlmann 1987] [Nachman, Sylvester, Uhlmann 1988]

For any $\xi \in \mathbb{R}^n$ and $\tau > 0$, let $\zeta_1, \zeta_2 \in \mathbb{C}^n$ such that $\zeta_j \cdot \zeta_j = 0$, $\zeta_1 + \overline{\zeta_2} = -i\xi$ and $|\zeta_j| \geq \tau$



$$\zeta_1 = -i\frac{\xi}{2} + \sqrt{\tau^2 + \frac{|\xi|^2}{4}}\,\theta_1 + i\tau\theta_2\,, \quad \zeta_2 = i\frac{\xi}{2} - \sqrt{\tau^2 + \frac{|\xi|^2}{4}}\,\theta_1 + i\tau\theta_2\,, \quad \theta_1, \theta_2 \in \mathbb{R}^n\text{: } |\theta_j| = 1,\ \theta_j \cdot \xi = 0,\ \theta_1 \cdot \theta_2 = 0$$

Taking the CGO solutions* $u_j = e^{\zeta_j \cdot x}(1 + r_{q_j - k^2, \zeta_j})$, we get

$$0 \overset{\mathbf{1.}}{=} \int_{B_R} (q_1 - q_2)u_1\overline{u_2}dx = \int_{B_R} (q_1 - q_2)e^{-i\xi \cdot x}(1 + r_{q_1 - k^2, \zeta_1})(1 + \overline{r_{q_2 - k^2, \zeta_2}})dx \xrightarrow[\tau \to \infty]{} \int_{B_R} (q_1 - q_2)e^{-i\xi \cdot x}dx = \mathcal{F}(\tilde{q}_1 - \tilde{q}_2)(\xi).$$

extension by 0 outside B_R

Since this holds for any $\xi \in \mathbb{R}^n$, we conclude $q_1 = q_2$.

The inverse conductivity problem

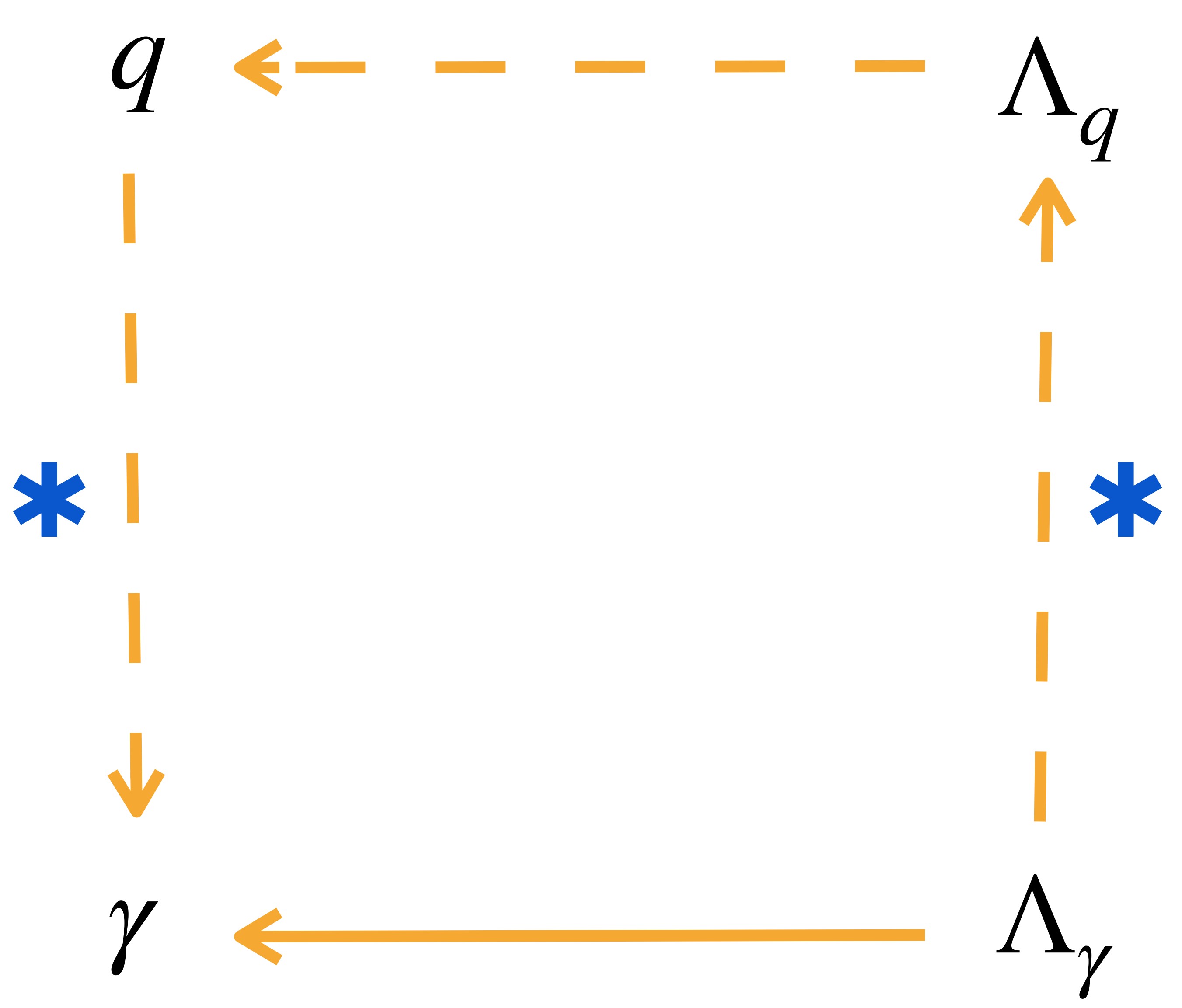
$$\big(-\Delta + q(x)\big)u = 0 \ \text{ in } \Omega$$
$$u = f \ \text{ on } \partial\Omega$$

$$\Lambda_q : f \mapsto \partial_\nu u|_{\partial\Omega}$$

$$q = \frac{\Delta\gamma^{1/2}}{\gamma^{1/2}}, \quad u = \gamma^{1/2}v, \quad f = \gamma^{1/2}g$$

$$\nabla\cdot\big(\gamma(x)\nabla v\big) = 0 \ \text{ in } \Omega$$
$$v = g \ \text{ on } \partial\Omega$$

$$\Lambda_\gamma : g \mapsto \gamma\partial_\nu v|_{\partial\Omega}$$



We can solve similarly the uniqueness for the inverse problem with $\Lambda : \gamma \mapsto \Lambda_\gamma$ for $n \geq 3$ and $\gamma \in C^2(\bar{\Omega})$.

✱ Boundary reconstruction [Kohn, Vogelius 1984].

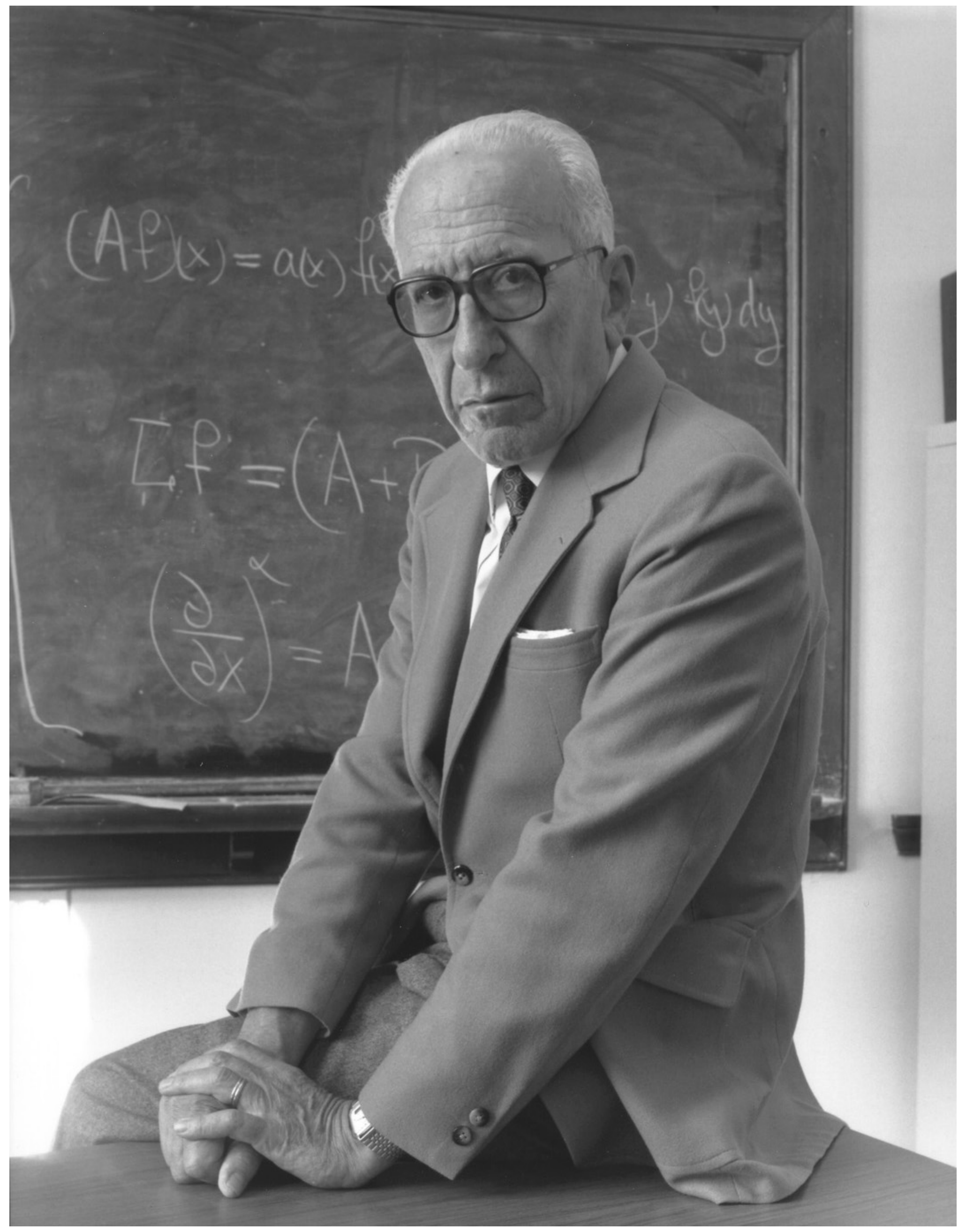
The inverse conductivity problem

Electrical conductivity of a medium ← Voltage and current on the boundary

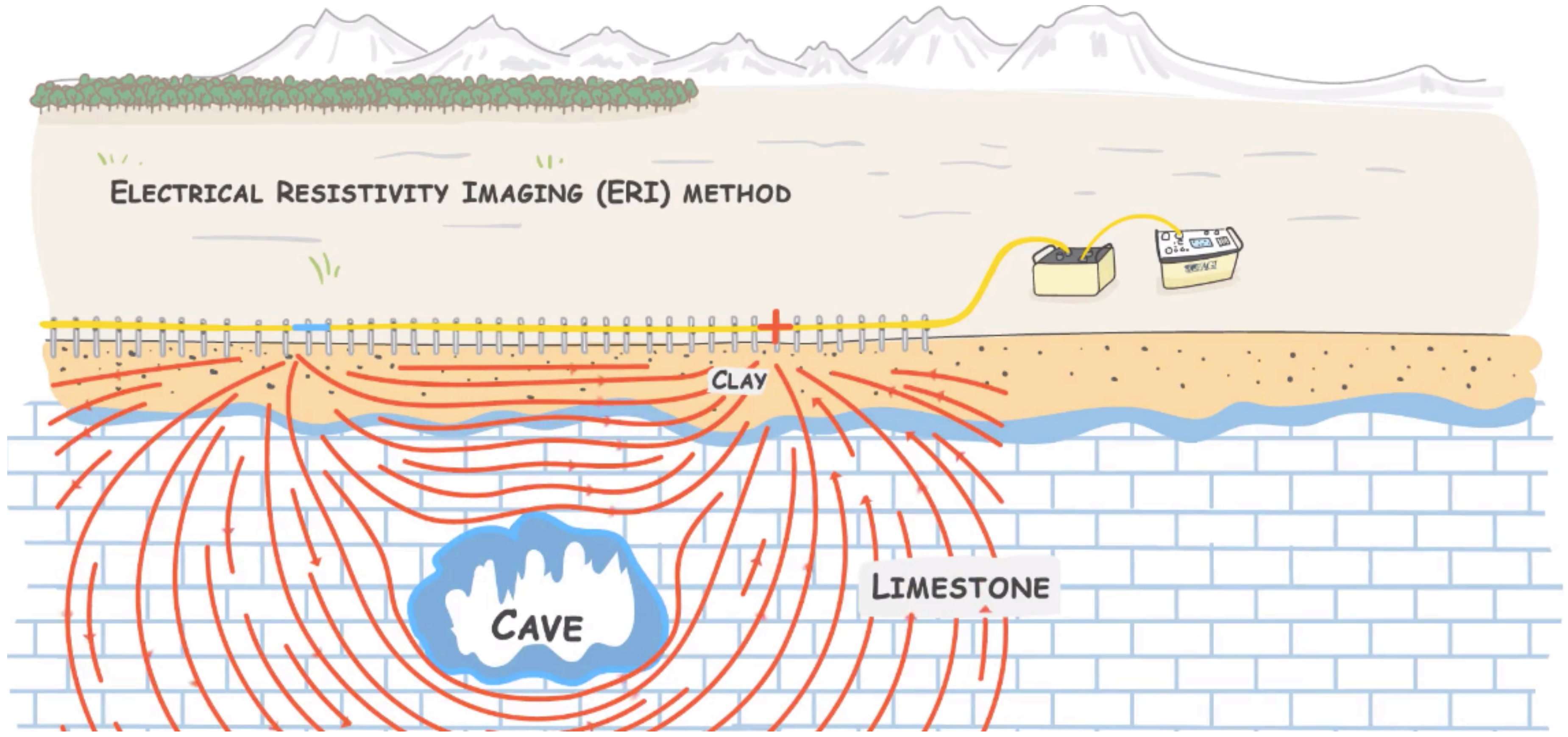
$\gamma : \Omega \to [c_1, c_2]$

$$\underbrace{\left\{ v|_{\partial\Omega}, \quad i \cdot v|_{\partial\Omega} = -\gamma \partial_\nu v|_{\partial\Omega} \right\}}_{\Lambda_\gamma}$$

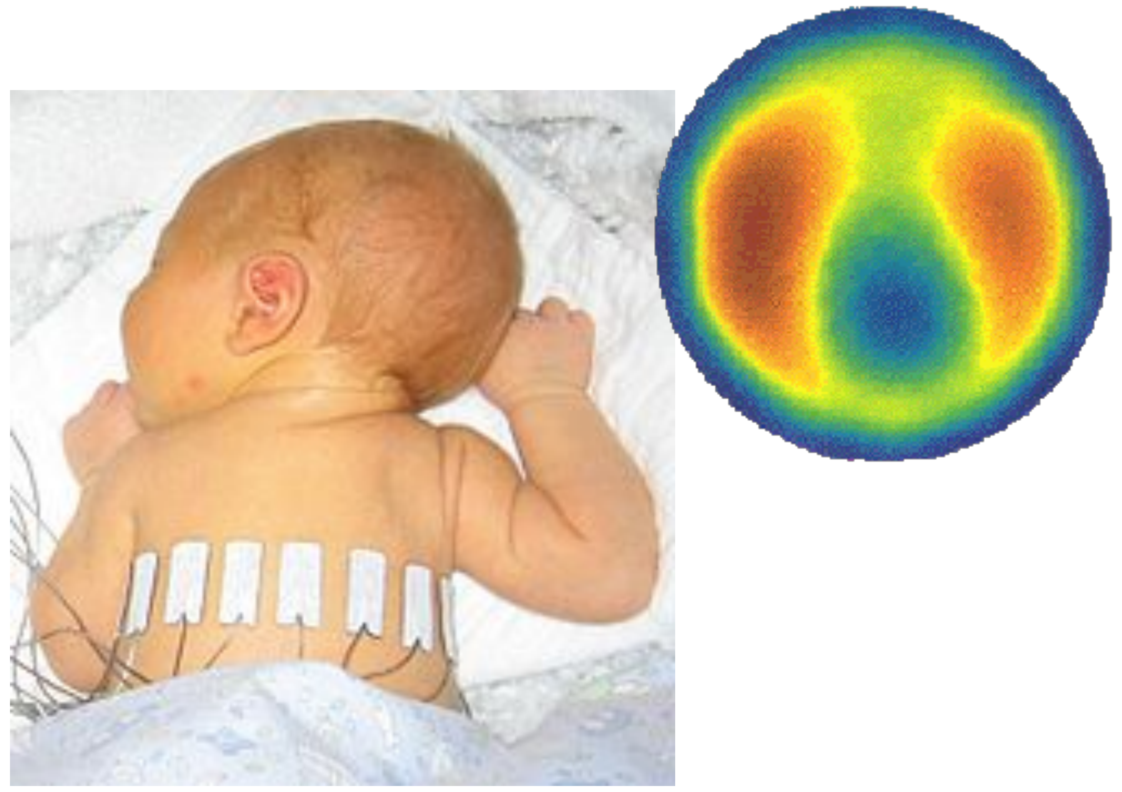
Calderón problem



Alberto Calderón
Argentina 1920 - USA 1998



Electrical
Resistivity
Tomography



Electrical
Impedance
Tomography

Electrical conductivity of a medium ← Voltage and current on the boundary

$\gamma : \Omega \to [c_1, c_2]$

$$\underbrace{\{\, v|_{\partial\Omega},\quad i\cdot\nu|_{\partial\Omega} = -\gamma\partial_\nu v|_{\partial\Omega} \,\}}_{\Lambda_\gamma}$$

- In one dimension, the Calderón problem has no solution.
- If $n = 2$, uniqueness by Astala, Päivarinta for $L^\infty(\Omega)$ conductivities (2006).
- If $n \geq 3$, uniqueness, stability and reconstruction by Uhlmann, Sylvester, Alessandrini, Nachman, Novikov, among others, for $C^2(\bar{\Omega})$ conductivities (1980's); and for less regular conductivities by Brown, Haberman, Tataru, Caro, Rogers, García, Zhang, GF and others, up to Lipschitz conductivities (in the Hölder class) (1990's-2020's).

❖ Stability does not hold unless a priori information is assumed. Stability results look like $\|q_1 - q_2\|_{L^2(\Omega)} \lesssim \left(-\log(\|\Lambda_{q_1} - \Lambda_{q_2}\|_*)\right)^{-\alpha}$ (assuming $\|q_j\|_{L^\infty(\Omega)} \leq M$). This is optimal [Mandache 2001], but under extra assumptions, it might become better.

An inverse problem for data-driven prediction in QM

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Let us consider again the wave function $\Psi(t,x)$ describing the quantum state of some moving particles under the influence of a potential $V(t,x)$. Its evolution is described by the Schrödinger equation

$$i\hbar\partial_t\Psi = \left(-\frac{\hbar}{2m}\Delta + V\right)\Psi \longrightarrow i\partial_t u = (-\Delta + V)u$$

If $V \in L^1\big((0,T), L^\infty(\mathbb{R}^N)\big)$, given any initial state $f \in L^2(\mathbb{R}^n)$, there exists a unique $u \in C\big([0,T], L^2(\mathbb{R}^n)\big)$ solving

$$\begin{cases} i\partial_t u = (-\Delta + V)u \text{ in } [0,T]\times\mathbb{R}^n, \\ u(0,\cdot) = f \text{ in } \mathbb{R}^n. \end{cases} \quad (⚛)$$

"physical solutions"

Define the initial-to-final map as $\mathscr{U}_T^V : f \mapsto u(T,\cdot)$, with u solving (⚛).

$\Lambda : V \to \mathscr{U}_T^V$ — The forward problem is well posed (as a map from $L^1\big((0,T), L^\infty(\mathbb{R}^N)\big)$ to $\mathscr{B}\big(L^2(\mathrm{R}^n), L^2(\mathrm{R}^n)\big)$).

IP: Can we find V (and therefore the evolution of the quantum state) from the knowledge of $\mathscr{U}_T^V$?

Uniqueness: [Caro, Ruiz 2024] (under some decaying conditions on V_j)

1. $\mathscr{U}_T^{V_1} = \mathscr{U}_T^{V_2} \Rightarrow \int_{(0,T)\times\mathbb{R}^n} (V_1 - V_2)u_{V_1}\overline{u}_{\overline{V}_2}\,dt\,dx = 0$ for "physical solutions".
2. Density of products does not hold with "physical solutions".

Thank you very much
for your attention

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