Inverse Schrödinger problem with internal measurements

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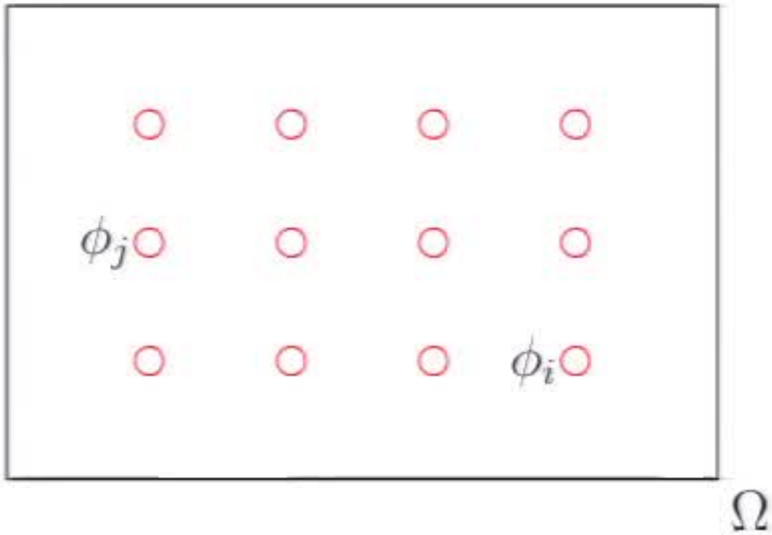
Schrödinger problem with internal measurements



$$\begin{cases} -\Delta u_j + q u_j = \phi_j \text{ in } \Omega \\ \qquad\qquad + \text{BC on } \partial\Omega \end{cases}$$

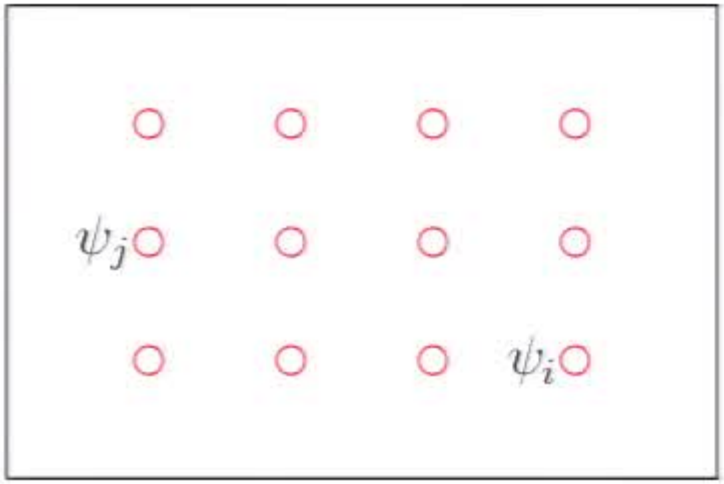
- $\phi_j(\mathbf{x})$ = source (or leak) term at j−th location
- $q(\mathbf{x})$ = (possibly complex) Schrödinger potential

Inverse Problem

Find q from measurements

$$M_{i,j}(t) = \int d\mathbf{x} \;\; \phi_i(\mathbf{x}) u_j(\mathbf{x}).$$

Application: Hydraulic Tomography



Ω

$$
\begin{cases}
S\dfrac{\partial v_j}{\partial t} = \nabla \cdot [\sigma \nabla v_j] + \psi_j \text{ in } \Omega \\
\qquad + \text{BC on } \partial\Omega \\
v_j(\mathbf{x}, 0) = \text{ Initial condition}
\end{cases}
$$

- $\psi_j(\mathbf{x}, t) =$ source (or leak) term at $j-$th well
- $v_j(\mathbf{x}, t) =$ head (hydraulic pressure) caused by $j-$th well
- $S(\mathbf{x}) =$ storage coefficient
- $\sigma(\mathbf{x}) =$ hydraulic conductivity

Inverse Problem

Find S and σ from measurements

$$M_{i,j}(t) = \int d\mathbf{x} \;\; \psi_i(\mathbf{x}, \cdot) \star_t v_j(\mathbf{x}, \cdot).$$

From Hydraulic Tomography to the Schrödinger problem

Fourier transform + Liouville identity $\rightsquigarrow v_j \equiv \sigma^{1/2}\widehat{u}_j$ satisfies

$$-\Delta v_j + \left(\sigma^{-1/2}\Delta\sigma^{1/2} + \imath\omega\sigma^{-1}S\right) v_j = \sigma^{-1/2}\widehat{\psi}_j \equiv \phi_j.$$

If $\sigma|_{\operatorname{supp}\widehat{\phi}_i} = \text{known}$,

$$\widehat{M}_{i,j}(\omega) = \int d\mathbf{x}\ \widehat{\psi}_i(\mathbf{x},\omega)\widehat{u}_j(\mathbf{x},\omega) \quad \text{(HT meas. in frequency)}$$

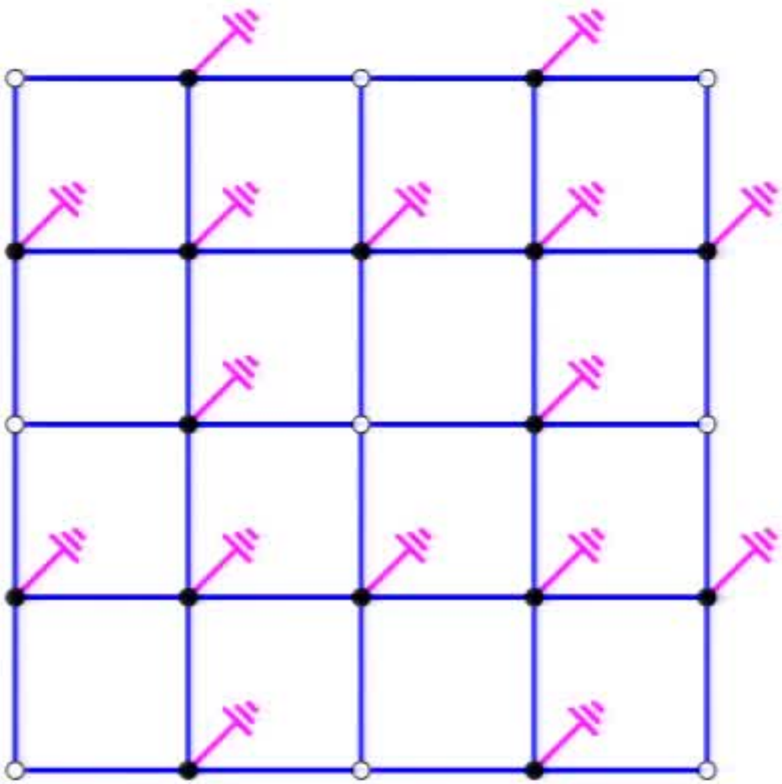
$$= \int d\mathbf{x}\ \underbrace{\frac{\widehat{\psi}_i(\mathbf{x},\omega)}{\sigma^{1/2}(\mathbf{x})}}_{\equiv\phi_i(\mathbf{x})} v_j(\mathbf{x}) \quad \text{(Schrödinger eq. meas.)}$$

Inverse problem

Find (complex) $q = \sigma^{-1/2}\Delta(\sigma^{1/2}) + \imath\omega S/\sigma$ from measurements

$$\widehat{M}_{i,j}(\omega) = \int d\mathbf{x}\ \widehat{\phi}_i(\mathbf{x},\omega)\widehat{u}_j(\mathbf{x},\omega)$$

Reduced order model based inversion



Main idea

1. Find reduced model parameters fitting data from continuum.
2. Use reduced model parameters to image continuum parameter.

Problem

Are reduced model parameters uniquely determined from data?

References: Borcea, Druskin (2001, 2002); Borcea, Druskin, GV (2008); Druskin, Moskow (2002); Borcea, Druskin, Mamonov (2010); Ding, Ren (2014); Druskin, Mamonov, Thaler, Zaslavsky (2016); Borcea, Mamonov, GV (2016); . . .

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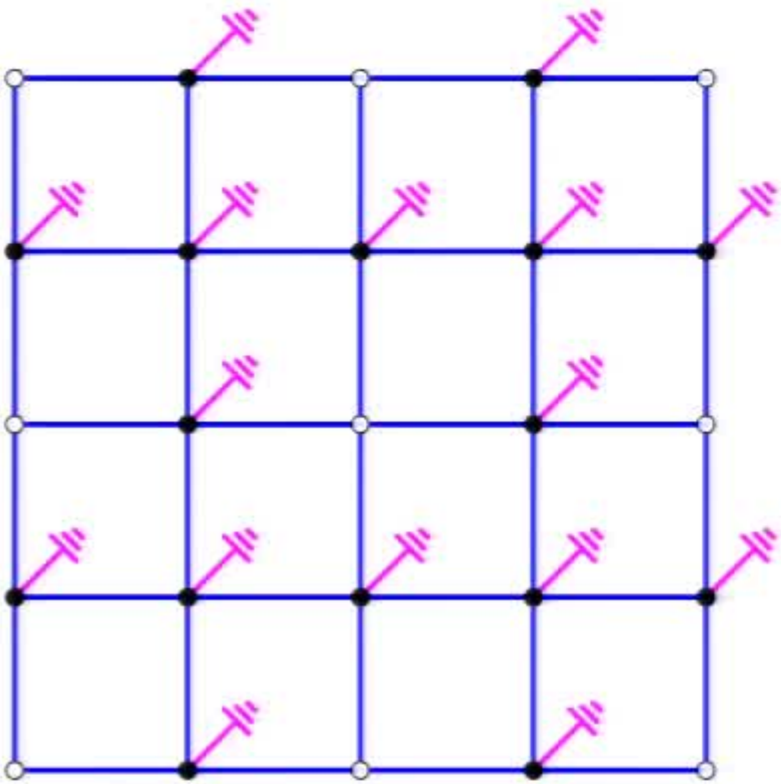

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Result preview

This work

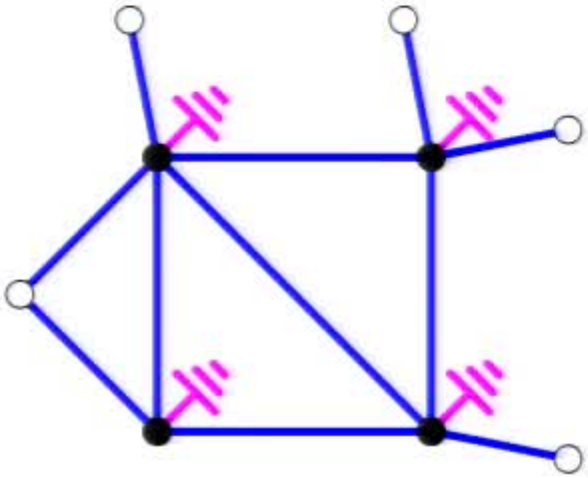
Jacobian injective at 1 pt $\Longrightarrow$ Non-linear problem uniqueness a.e.

Implicit function theorem would only give local uniqueness.
In general: Jacobian injective everywhere $\not\Rightarrow$ uniqueness.
(related to "Jacobian Conjecture" in algebraic geometry).

Flexible approach inspired by Complex Geometric Optics
(Calderón '80; Sylvester, Uhlmann '87):

1. Discrete inverse conductivity problem
2. Discrete inverse Schrödinger problem $\leftsquigarrow$ [today]
3. Matrix versions of 1 and 2.
4. Networks of springs, masses and dampers (part of 3):
    - Finding spring/damping constants given the masses.
    - Finding masses given the spring/damping constants

Inverse problems in a circuit



- γ = vector of admittances in blue
- q = vector of admittances in pink

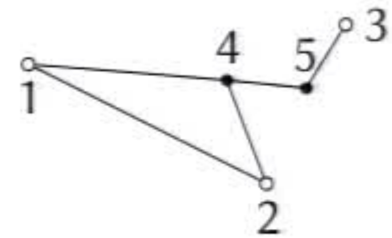
1. Discrete Conductivity Inverse Problem: Assuming no leaks ($q = 0$), find γ from electrical measurements at terminal nodes.
2. Discrete Schrödinger Inverse Problem: Assuming γ is known, find q from electrical measurements at terminal nodes.

Focus on uniqueness question:

Does the data determine the unknown (γ or q) uniquely?

The discrete Dirichlet problem

Let $\mathcal{G} = (V, E)$ be an undirected graph with no self edges.
$V = B \cup I \equiv$ vertex set (Boundary + Interior)
$E \subset V \times V \equiv$ edge set



- Discrete gradient: $\nabla : \mathbb{C}^V \to \mathbb{C}^E$. If $i \sim j$, $(\nabla u)(\{i, j\}) = u(i) - u(j)$.
- Discrete Laplacian: $L_\gamma : \mathbb{C}^V \to \mathbb{C}^V$, with $L_\gamma \equiv \nabla^* \mathrm{diag}\,(\gamma)\nabla$, $\gamma \in \mathbb{C}^E$.
- Physical interpretation:

$$(L_\gamma u)(i) = \text{net current at node } i \text{ for node voltages } u \in \mathbb{C}^V.$$

The $\gamma, q-$Dirichlet problem

Let $\gamma \in \mathbb{C}^E$, $q \in \mathbb{C}^I$. Given $f \in \mathbb{C}^B$ find $u \in \mathbb{C}^V$ s.t.

$$\begin{cases} (L_\gamma u)_I + q \odot u_I = 0, \\ \qquad u_B = f. \quad \text{(boundary condition)} \end{cases}$$

Dirichlet problem well-posedness

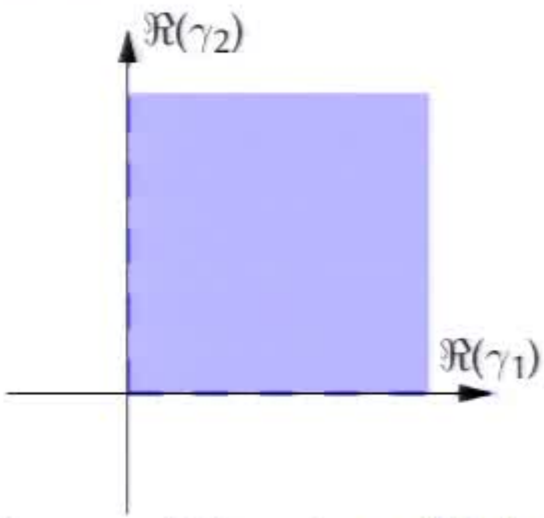
We say the $\gamma, q-$Dirichlet problem is well-posed if it admits a unique solution for all boundary data.

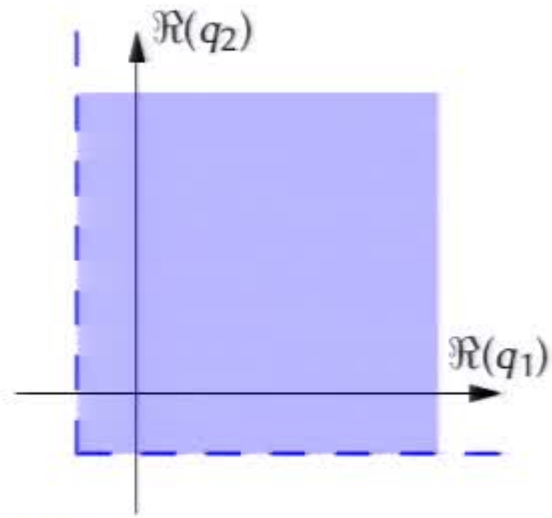
Proposition

When $\gamma \in \mathbb{C}^E$ and $q \in \mathbb{C}^I$ are such that:

i. $\Re(\gamma) > 0$ and
ii. $\Re(q) > -\lambda_{\min}((L_{\Re\gamma})_{II})$

then the $\gamma, q-$Dirichlet problem is well-posed.





Note: This condition is sufficient but not necessary.

Dirichlet to Neumann map

Recall:

$$(L_\gamma u)(i) = \text{net current at node } i \text{ for node voltages } u \in \mathbb{C}^V.$$

Dirichlet to Neumann or voltage to current map

$$\Lambda_{\gamma,q} : \mathbb{C}^B \to \mathbb{C}^B$$
$$f \to (L_\gamma u)_B = \text{currents flowing out of } B \text{ nodes.}$$

Here u is the solution to the γ, $q-$Dirichlet problem with BC f:

$$\begin{cases} (L_\gamma u)_I + q \odot u_I = 0, \\ u_B = f. \end{cases}$$

(assumes γ, $q-$Dirichlet problem is well posed)

Uniqueness results on finite graphs

Discrete conductivity inverse problem

- All terminals ($I = \emptyset$): Kirchhoff 1845.
- Rectangular graphs: Curtis, Morrow '90.
- Circular planar graphs: Curtis, Mooers, Morrow '94; Colin de Verdière '94; Curtis, Ingerman, Morrow '98.
- Any graph + monotonicity: Chung, Berenstein '05; Chung '10. If $\gamma_1 \geq \gamma_2$ then same boundary data $\Rightarrow$ same conductivity
- Cylindrical graphs: Lam, Pylyavskyy '12 (no uniqueness).

Discrete Schrödinger problem

- Circular Planar Graphs: Araúz, Carmona, Encinas '14-'15.

This work

- Linearized problem uniqueness $\Rightarrow$ non-linear problem uniqueness a.e.
- Simple uniqueness test: no explicit topological restrictions
- γ and q can be **complex** and/or **matrix valued**

The Continuum Schrödinger inverse problem

Find q from Dirichlet to Neumann map $\Lambda_q : f \to \boldsymbol{n} \cdot \nabla u|_{\partial\Omega}$, where u solves

$$\begin{cases} -\Delta u + qu = 0 \text{ in } \Omega, \\ u = f \text{ on } \partial\Omega. \end{cases}$$

Here $\Omega \subset \mathbb{R}^d$ is a domain with smooth boundary $\partial\Omega$.

Uniqueness question

Does Λ_q determine q uniquely?

$\rightsquigarrow$ YES in $d \geq 3$ (Sylvester, Uhlmann '87). Method is called Complex Geometric Optics (CGO) and has been used in other uniqueness problems:

- Maxwell equations: Ola, Somersalo '96
- Linear isotropic elasticity: Nakamura, Uhlmann '94; Eskin, Ralston '02.
- Schrödinger equation with magnetic potential: Nakamura, Sun, Uhlmann '95.
- ...

The Complex Geometric Optics method for Schrödinger

1. Interior Identity: If $-\Delta u^{(i)} + q_i u^{(i)} = 0$, $i = 1, 2$:

$$\int_{\partial\Omega} \left[(\Lambda_{q_1} - \Lambda_{q_2})(u^{(1)}|_{\partial\Omega})\right] u^{(2)}|_{\partial\Omega}\, dS = \int_{\Omega} (q_1 - q_2) u^{(1)} u^{(2)}\, dx$$

2. Products of solutions to $\Delta u = 0$ are dense in $L^2(\Omega)$: (Calderón '80)

   With $y, \xi \in \mathbb{R}^d$, $y \cdot y = \xi \cdot \xi$ and $y \cdot \xi = 0$

   $\Rightarrow u_\pm(x) = \exp[x \cdot (\pm y + i\xi)] \equiv$ harmonic.

   $\Rightarrow$ products $u_+ u_- = \exp[2ix \cdot \xi] \equiv$ Fourier basis for $L^2(\Omega)$.

3. Show 2 $\Rightarrow$ products of solutions $u^{(1)} u^{(2)}$ are dense in $L^2(\Omega)$ via high frequency asymptotics (Sylvester, Uhlmann '87).

4. Uniqueness follows:

$$\Lambda_{q_1} = \Lambda_{q_2} \Rightarrow \overline{q_1} - \overline{q_2} \text{ is } \perp \text{ to dense set in } L^2(\Omega)$$
$$\Rightarrow q_1 = q_2.$$

A discrete version of the CGO method?

1. Interior Identity: If $u^{(i)}$ solves γ, q_i−Dirichlet problem, $i = 1, 2$:

$$\int_B u_B^{(2)} \odot [(\Lambda_{\gamma,q_1} - \Lambda_{\gamma,q_2}) u_B^{(1)}] = \int_I (q_1 - q_2) \odot u_I^{(1)} \odot u_I^{(2)}.$$

2. Products of solutions to $\gamma, 0$−Dir. problem are dense in (span) $\mathbb{C}^I$
   This property is assumed for e.g. $q = 0$!
3. Show **2** $\Rightarrow$ products of solutions $u_I^{(1)} \odot u_I^{(2)}$ span $\mathbb{C}^I$
   $\rightsquigarrow$ holds for almost all q_1, q_2 in appropriate set. (more details soon. . .)
4. "Uniqueness almost everywhere" follows:

$$\Lambda_{\gamma,q_1} = \Lambda_{\gamma,q_2} \Rightarrow \overline{q_1} - \overline{q_2} \text{ is } \perp \text{ to } \mathbb{C}^I$$
$$\Rightarrow q_1 = q_2, \text{ for a.a. } q_1, q_2.$$

Consequences

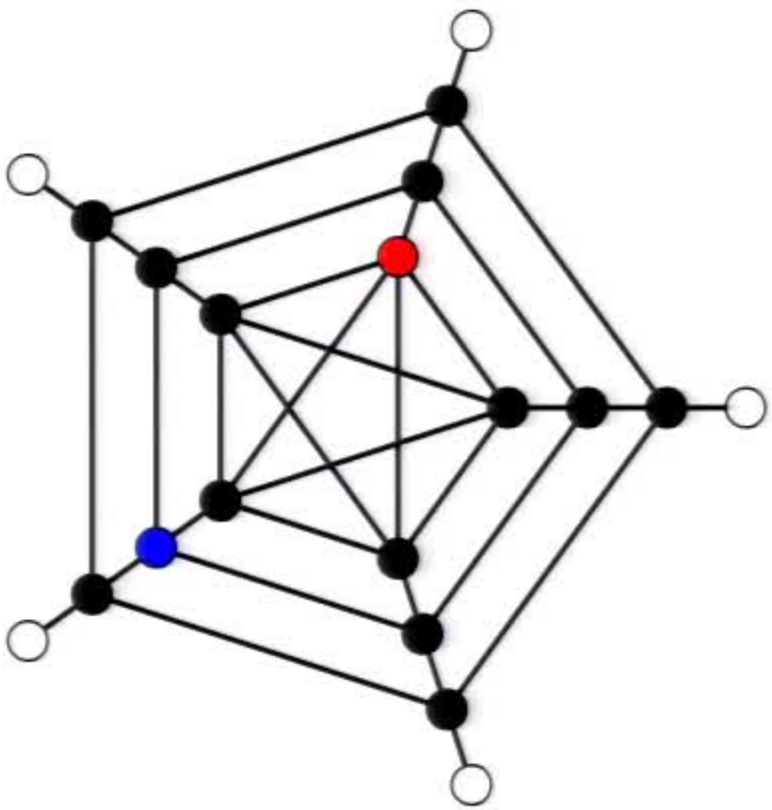
Fact: $W(q,q)^T = D_q\Lambda_{\gamma,q}$ = Jacobian of $\Lambda_{\gamma,q}$ at q.

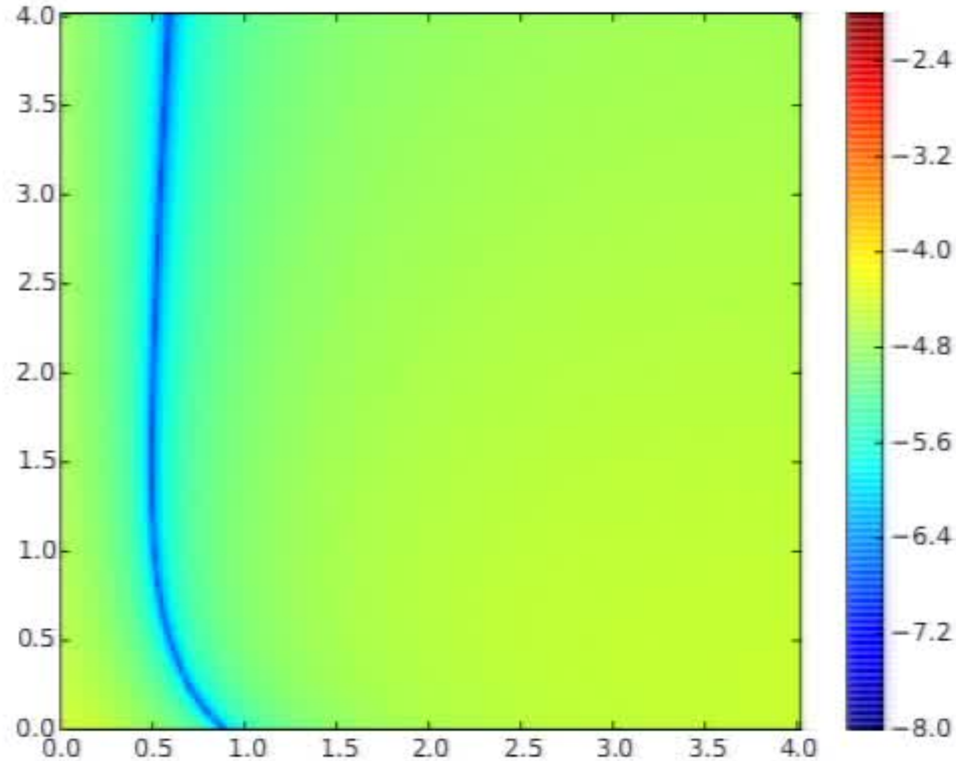
If Jacobian is injective at some p with $\Re(p) > \zeta \equiv -\lambda_{\min}((L_{\Re\gamma})_{II})$ we get:

1. Uniqueness for a.a. $(q_1, q_2) \in \{z \in \mathbb{C}^I \mid \Re(z) > \zeta\}^2$.
2. Injective Jacobian for a.a. $q \in \{z \in \mathbb{C}^I \mid \Re(z) > \zeta\}$.
3. Equivalence classes for equivalence relation $q_1 \sim q_2 \Leftrightarrow \Lambda_{\gamma,q_1} = \Lambda_{\gamma,q_2}$ must be of zero measure in $\{z \in \mathbb{C}^I \mid \Re(z) > \zeta\}$.

- Note #1: Instead of identifying the (q_1, q_2) that have the same boundary data, we show they belong to the zero set of an analytic function.
- Note #2: Can use real analytic functions instead of complex analytic to obtain similar results if $\gamma \in \mathbb{R}^E$ and $q \in \mathbb{R}^I$.

A zero set example for Schrödinger

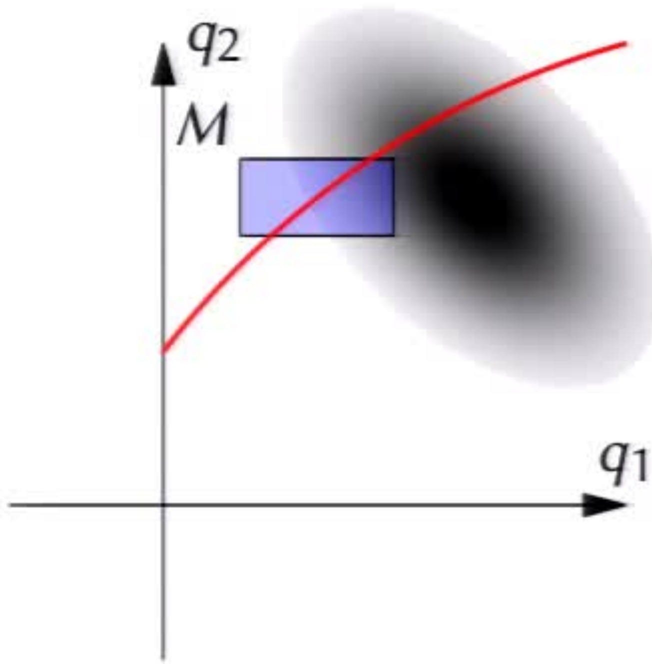




Smallest singular value of $W(xp, yq)$ for $(x, y) \in [0, 4]^2$.

Probabilistic interpretation of uniqueness a.e.

If uniqueness a.e. holds, $(Q_1, Q_2) \equiv$ absolutely continuous random variable and M is a non-zero probability event:



- $W(Q_1, Q_2)$ is full rank knowing that $(Q_1, Q_2) \in M$ almost surely.
- $\mathbb{E}\left[\|\Lambda_{\gamma,Q_1} - \Lambda_{\gamma,Q_2}\| \mid (Q_1, Q_2) \in M\right] > 0.$

What about Newton's method?

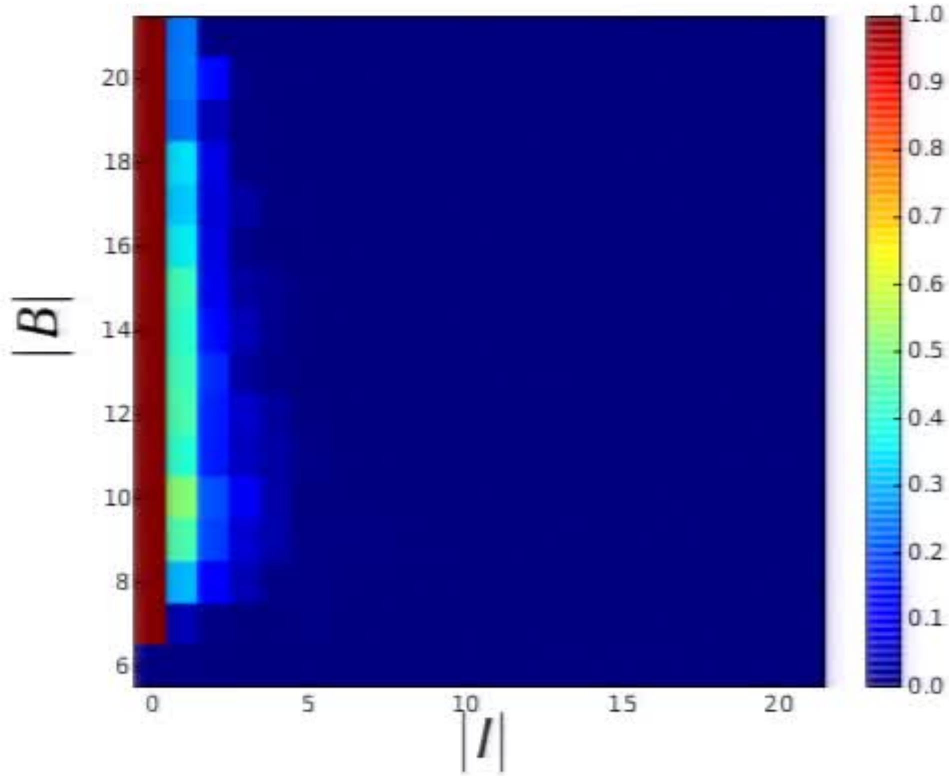
Newton's Method

$q^{(0)} = \text{given}$
for $k = 0, 1, 2, \ldots$
    Find step $\delta q^{(k)}$ s.t. $D_q \Lambda_{\gamma, q^{(k)}} \delta q^{(k)} = \Lambda_{\gamma, q^{(k)}} - \Lambda_{\gamma, q}$
    Choose step length $t_k > 0$
    Update $q^{(k+1)} = q^{(k)} + t_k \delta q^{(k)}$

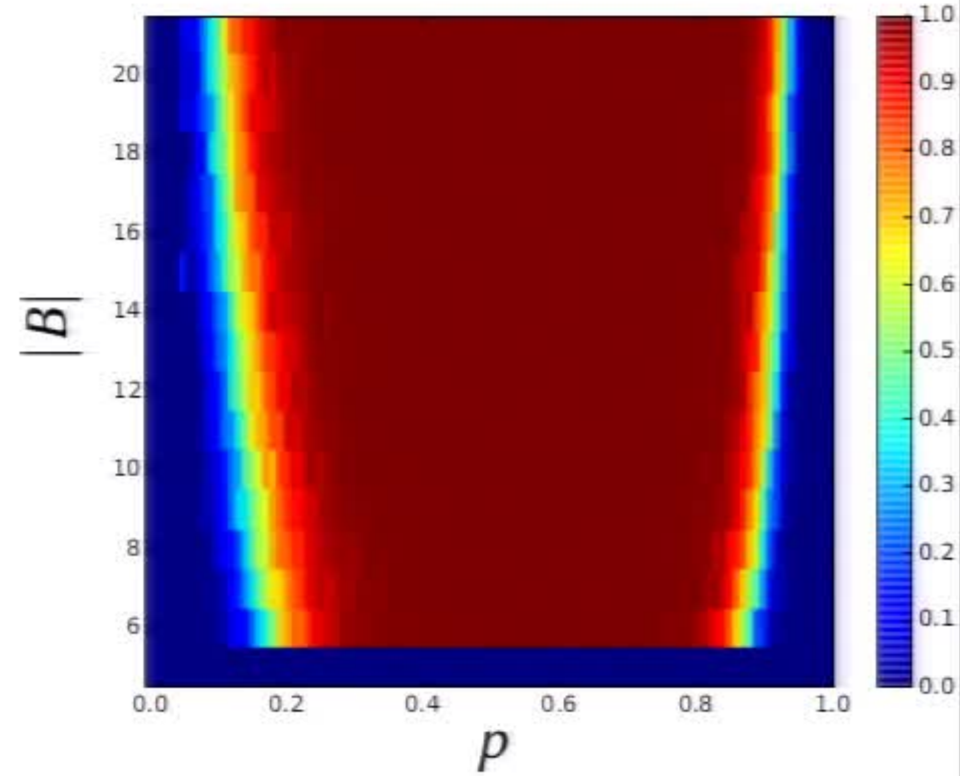
Theorem

If Jacobian $D_q \Lambda_{\gamma, q^{(k)}}$ is injective, then all feasible choices of the next iterate $q^{(k+1)}$ are such that the Jacobian is injective, up to finitely many exceptions.

Numerical comparison: conductivity vs Schrödinger



(a) Conductivity with $|E| = 21$



(b) Schrödinger with $|I| = 21$