

Inverse scattering for the half line matrix Schrödinger operator

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Matrix Schrödinger equation on the half line

- $-\psi''(k, x) + V(x) \psi(k, x) = k^2 \psi(k, x), \quad x \in \mathbb{R}^+$
- $\mathbb{R}^+ := (0, +\infty)$, half line, $x > 0$; prime: x -derivative
- k^2 : spectral parameter
- potential $V(x)$: $n \times n$ matrix-valued, at times n -column vector
- bound-state wavefunction ψ : square-summable n -column vector

Relevant references for the characterization

- Z. S. Agranovich and V. A. Marchenko, *The inverse problem of scattering theory*, Gordon and Breach, New York, 1963.
- T. Aktosun and R. Weder, *Inverse scattering on the half line for the matrix Schrödinger equation*, J. Math. Phys. Anal. Geom. **14** (2018), 237–269.
- T. Aktosun and R. Weder, *Direct and inverse scattering for the matrix Schrödinger equation*, Springer Nature, May 2020.
- M. S. Harmer, *The matrix Schrödinger operator and Schrödinger operator on graphs*, PhD thesis, University of Auckland, New Zealand, 2004.

Applications

- scattering in quantum mechanics with internal structure (spin)
- quantum wires, quantum circuits
- scattering on quantum graphs
- boundary conditions at vertices of the graph

Selfadjoint boundary condition at $x = 0$

- $-B^\dagger \psi(0) + A^\dagger \psi'(0) = 0$

$$\begin{cases} A \text{ and } B \text{ constant } n \times n \text{ matrices} \\ A^\dagger A + B^\dagger B > 0 \quad \text{and} \quad B^\dagger A = A^\dagger B \end{cases}$$

- dagger \dagger : matrix adjoint (transpose and complex conjugate)
- Dirichlet: with $A = 0$ and $B = -I$, $\psi(0) = 0$

Selfadjoint boundary condition at $x = 0$

- $-B^\dagger \psi(0) + A^\dagger \psi'(0) = 0$
- boundary condition unaffected by invertible T in $(A, B) \mapsto (AT, BT)$
- $A^\dagger A + B^\dagger B > 0$ is the same as having the rank of $\begin{bmatrix} A \\ B \end{bmatrix}$ to be n
- analogy from the scalar ($n = 1$) case

$$(\cos \theta) \psi(0) + (\sin \theta) \psi'(0) = 0, \quad \theta \in (0, \pi]$$

Potential $V(x)$, $n \times n$ matrix-valued

- $V(x)^\dagger = V(x)$, selfadjoint potential
 - $V(x) \in L_1^1(\mathbb{R}^+) : \int_0^\infty dx (1+x) |V(x)| < +\infty$
 - $|V(x)|$ matrix operator norm
 - $\int_0^\infty dx |V(x)| < +\infty$ sufficient for results with $k \in \overline{\mathbb{C}^+} \setminus \{0\}$
 - physical solution $\Psi(k, x)$ satisfies Dirichlet/non-Dirichlet b.c.
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- Agranovich–Marchenko: $\int_0^\infty dx x |V(x)| < +\infty$
- physical solution $\Psi(k, x)$ satisfies only Dirichlet b.c., not non-Dirichlet b.c.

Faddeev class of input data sets \mathbf{D}

- \mathbf{D} : input data set; potential $V(x)$ and the boundary condition
- $-B^\dagger \psi(0) + A^\dagger \psi'(0) = 0$ with $B^\dagger A = A^\dagger B$ and $A^\dagger A + B^\dagger B > 0$
- $\mathbf{D} := \{V(x), A, B\}$ with uniqueness up to $(A, B) \mapsto (AT, BT)$
- $V(x)^\dagger = V(x)$ and $\int_0^\infty dx (1+x) |V(x)| < +\infty$

Marchenko class of scattering data sets \mathbf{S}

- scattering data set $\mathbf{S} := \{S(k), \{\kappa_j, M_j\}_{j=1}^N\}$
- scattering matrix $S(k)$ for $k \in \mathbb{R}$, $n \times n$ matrix-valued
- κ_j : distinct, positive numbers; N : nonnegative integer
- M_j : $n \times n$ constant matrix, nonnegative, hermitian, rank m_j
 M_j normalization matrix, Marchenko normalization matrix, norming matrix
- Marchenko class: \mathbf{S} satisfies properties **(1, 2, 3, 4)**

Marchenko class of scattering data sets \mathbf{S}

- scattering data set $\mathbf{S} := \{S(k), \{\kappa_j, M_j\}_{j=1}^N\}$
- $\{\kappa_j, M_j\}_{j=1}^N$: bound-state data; $-\kappa_j^2$ bound-state energy
- M_j has rank m_j , multiplicity of bound state with κ_j
- N number of bound states without counting multiplicities

$$\mathcal{N} := \sum_{j=1}^N m_j, \text{ number of bound states including multiplicities}$$

Faddeev class of input data sets \mathbf{D}

- \mathbf{D} : input data set; potential $V(x)$ and the boundary condition
- $-B^\dagger \psi(0) + A^\dagger \psi'(0) = 0$ with $B^\dagger A = A^\dagger B$ and $A^\dagger A + B^\dagger B > 0$
- $\mathbf{D} := \{V(x), A, B\}$ with uniqueness up to $(A, B) \mapsto (AT, BT)$
- $V(x)^\dagger = V(x)$ and $\int_0^\infty dx (1+x) |V(x)| < +\infty$

Direct and inverse scattering problems

- Direct problem: $\mathbf{D} \mapsto \mathbf{S}$, Inverse problem: $\mathbf{S} \mapsto \mathbf{D}$
- existence
- uniqueness
- construction, reconstruction
- characterization

Our main results

- 1-to-1 correspondence between Marchenko class and Faddeev class
- construction in $\mathbf{D} \mapsto \mathbf{S}$, construction in $\mathbf{S} \mapsto \mathbf{D}$, $\mathbf{S} \mapsto \mathbf{D} \mapsto \mathbf{S}$
- Dom(Inverse map): the “Marchenko class” of scattering data sets
- Dom(Direct map): the “Faddeev class” of input data sets
- Domain of the inverse map = Range of the direct map
- various equivalent descriptions of the Marchenko class

Trouble with the traditional formulation

- tradition: Dirichlet/non-Dirichlet b.c. is a part of scattering data set
- ours: Boundary condition should be a part of the input data set
- tradition: normalize $S(\pm\infty) = I$
- ours: do not normalize $S(\pm\infty) = I$
- tradition: define $S(k)$ differently with Dirichlet/non-Dirichlet b.c.
- ours: define $S(k)$ the same way with Dirichlet/non-Dirichlet b.c.

Traditional formulation, Ill-posedness of the inverse problem

- $\{S(k) \equiv I, \text{no bound states, Dirichlet b.c.}\} \mapsto \{V(x) \equiv 0\}$
- $\{S(k) \equiv I, \text{no bound states, Neumann b.c.}\} \mapsto \{V(x) \equiv 0\}$
- $\{S(k) \equiv I, \text{no bound states}\} \mapsto \begin{cases} \{V(x) \equiv 0, \text{Dirichlet b.c.}\} \\ \{V(x) \equiv 0, \text{Neumann b.c.}\} \end{cases}$
- Inverse problem is ill posed unless b.c. is part of scattering data
- Dirichlet/non-Dirichlet b.c. cannot be mixed

Our formulation, Well-posedness of the inverse problem

- scattering matrix $S(k)$ is properly defined
- b.c. is not a part of scattering data set \mathbf{S}
- b.c. is to be recovered from scattering data set \mathbf{S}
- Inverse problem is well posed
- Dirichlet/non-Dirichlet b.c. may be mixed

Direct problem: Construction for $\mathbf{D} \mapsto \mathbf{S}$

- $\mathbf{D} := \{V(x), A, B\}$ and $\mathbf{S} := \{S(k), \{\kappa_j, M_j\}_{j=1}^N\}$
- uniquely construct the Jost solution $f(k, x)$ by using $V(x)$ in

$$\begin{cases} -f''(k, x) + V(x) f(k, x) = k^2 f(k, x), \\ f(k, x) = e^{ikx} [I + o(1)], \quad x \rightarrow +\infty. \end{cases}$$

- uniquely construct the Jost matrix $J(k)$ by using $A, B, f(k, x)$ via .06in
$$J(k) = f(-k^*, 0)^\dagger B - f'(-k^*, 0)^\dagger A, \quad k \in \overline{\mathbb{C}^+}.$$

- uniquely construct the scattering matrix $S(k)$ by using $J(k)$ via

$$S(k) = -J(-k) J(k)^{-1}, \quad k \in \mathbb{R}.$$

- uniquely construct the physical solution $\Psi(k, x)$ via

$$\Psi(k, x) = f(-k, x) + f(k, x) S(k), \quad k \in \mathbb{R}.$$

Direct problem: Construction for $\mathbf{D} \mapsto \mathbf{S}$

- $\mathbf{D} := \{V(x), A, B\}$ and $\mathbf{S} := \{S(k), \{\kappa_j, M_j\}_{j=1}^N\}$
- uniquely determine $\{\kappa_j\}_{j=1}^N$ as zeros $k = i\kappa_j$ of $\det[J(k)]$ in $k \in \mathbb{C}^+$.
- uniquely determine the orthogonal, hermitian $n \times n$ projection matrices $\{P_j\}_{j=1}^N$ projecting \mathbb{C}^n onto $\text{Ker}[J(i\kappa_j)^\dagger]$, $P_j = P_j$, $P_j^\dagger = P_j$.
- uniquely construct the $n \times n$ positive, hermitian matrices $\{B_j\}_{j=1}^N$ via $B_j := (I - P_j) + P_j \int_0^\infty dx f(i\kappa_j, x)^\dagger f(i\kappa_j, x) P_j$.
- uniquely construct the nonnegative, hermitian normalization matrices $\{M_j\}_{j=1}^N$ via $M_j = B_j^{-1/2} P_j$.

Inverse problem: Construction for $\mathbf{S} \mapsto \mathbf{D}$

- $\mathbf{S} := \{S(k), \{\kappa_j, M_j\}_{j=1}^N\}$ and $\mathbf{D} := \{V(x), A, B\}$
- uniquely construct the constant $n \times n$ matrices S_∞ and G_1 by using

$$S(k) = S_\infty + \frac{G_1}{ik} + o\left(\frac{1}{k}\right), \quad k \rightarrow \pm\infty.$$

- uniquely construct the $n \times n$ matrices $F_s(y)$ and $F(y)$ as

$$\begin{cases} F_s(y) := \frac{1}{2\pi} \int_{-\infty}^{\infty} dk [S(k) - S_\infty] e^{iky}, & y \in \mathbb{R}, \\ F(y) := F_s(y) + \sum_{j=1}^N M_j^2 e^{-\kappa_j y}, & y \in \mathbb{R}^+. \end{cases}$$

- for each fixed $x \geq 0$, determine $K(x, y)$ as the unique solution in $L^1(x < y < +\infty)$ to the Marchenko integral equation

$$K(x, y) + F(x+y) + \int_x^\infty dz K(x, z) F(z+y) = 0, \quad 0 \leq x < y.$$

Inverse problem: Construction for $\mathbf{S} \mapsto \mathbf{D}$

- $\mathbf{S} := \{S(k), \{\kappa_j, M_j\}_{j=1}^N\}$ and $\mathbf{D} := \{V(x), A, B\}$
- uniquely construct the potential $V(x)$ via $V(x) = -2 \frac{d K(x, x^+)}{dx}$.
- using $S_\infty, G_1, K(0, 0)$, obtain the boundary matrices A and B (unique up to a postmultiplication by an invertible matrix T) by solving
$$\begin{cases} (I - S_\infty) A = 0, \\ (I + S_\infty) B = [G_1 - S_\infty K(0, 0) - K(0, 0) S_\infty] A. \end{cases}$$
- uniquely construct the Jost solution as $f(k, x) = e^{ikx} + \int_x^\infty dy K(x, y) e^{iky}$.
- construct the physical solution as $\Psi(k, x) = f(-k, x) + f(k, x) S(k)$.
- construct the Jost matrix as $J(k) = f(-k^*, 0)^\dagger B - f'(-k^*, 0)^\dagger A$.

Verification in $\mathbf{S} \mapsto \mathbf{D}$

- $\mathbf{S} := \{S(k), \{\kappa_j, M_j\}_{j=1}^N\}$ and $\mathbf{D} := \{V(x), A, B\}$
- constructed $V(x)$ is hermitian: $V(x)^\dagger = V(x)$.
- constructed $V(x) \in L_1^1(\mathbb{R}^+) : \int_0^\infty dx (1+x) |V(x)| < +\infty$.
- constructed A and B satisfy $A^\dagger A + B^\dagger B > 0$ and $B^\dagger A = A^\dagger B$.
- constructed physical sol $\Psi(k, x)$ satisfies $-B^\dagger \Psi(k, 0) + A^\dagger \Psi'(k, 0) = 0$.
- constructed bound states $\{\Psi_j(x)\}_{j=1}^N$ satisfy $-B^\dagger \Psi_j(0) + A^\dagger \Psi'_j(0) = 0$.

Marchenko class of scattering data sets $\mathbf{S} := \{S(k), \{\kappa_j, M_j\}_{j=1}^N\}$

- Marchenko class: \mathbf{S} satisfies properties **(1, 2, 3, 4)**

$$(1) : \begin{cases} S(-k) = S(k)^\dagger = S(k)^{-1}, & k \in \mathbb{R}, \\ S(k) = S_\infty + \frac{G_1}{ik} + o\left(\frac{1}{k}\right), & k \rightarrow \pm\infty, \\ F_s(y) \in L^1(\mathbb{R}^+) \cap L^\infty(\mathbb{R}), \quad F_s(y) := \frac{1}{2\pi} \int_{-\infty}^{\infty} dk [S(k) - S_\infty] e^{iky}. \end{cases}$$

$$(2) : F'_s(y) \in L^1_1(\mathbb{R}^+) : \quad \int_0^\infty dy (1+y) |F'_s(y)| < +\infty.$$

(3) : The physical sol $\Psi(k, x)$ satisfies $-B^\dagger \Psi(k, 0) + A^\dagger \Psi'(k, 0) = 0$.

(4) : Let $F(y) := F_s(y) + \sum_{j=1}^N M_j^2 e^{-\kappa_j y}$. Then, $X(y) \equiv 0$ is the only solution in $L^1(\mathbb{R}^+)$ to

$$X(y) + \int_0^\infty dz X(z) F(z+y) = 0, \quad y \in \mathbb{R}^+.$$

Characterization of the scattering data in $\mathbf{S} \mapsto \mathbf{D}$

- $\mathbf{S} := \{S(k), \{\kappa_j, M_j\}_{j=1}^N\}$ and $\mathbf{D} := \{V(x), A, B\}$
- 1-to-1 correspondence between Marchenko class and Faddeev class
- \mathbf{S} in Marchenko class, \mathbf{D} in Faddeev class, $\mathbf{S} \mapsto \mathbf{D} \mapsto \mathbf{S}$
- Marchenko class: \mathbf{S} satisfies properties **(1, 2, 3, 4)**
- Faddeev class: potential with $V(x)^\dagger = V(x)$ and $\int_0^\infty dx (1+x) |V(x)| < +\infty$
and b.c. with boundary matrices with $B^\dagger A = A^\dagger B$ and $A^\dagger A + B^\dagger B > 0$
- equivalent characterization formulations: \mathbf{S} satisfies **(1*, 2*, 3*, 4*)**

Many other formulations of characterization the scattering data

- **S** in Marchenko class, **D** in Faddeev class
- Marchenko class: **S** satisfies properties **(1, 2, 3, 4)**
- Marchenko class: **S** satisfies properties **(1, 2, III + V, 4)**
- Marchenko class: **S** satisfies properties **(1, 2, L, 4 + 5)**
- Marchenko class: **S** satisfies properties **(I + VI, 2, A, 4)**
- several equivalent formulations for each of **(3), (4), (III), (V)**
(3_a), (3_b); (4_a), (4_b), (4_c), (4_d), (4_e); (III_a), (III_b), (III_c)
(V_a), (V_b), (V_c), (V_d), (V_e), (V_f), (V_g), (V_h)

Properties (III) and (V)

(III) : $F'_s \in L^1(\mathbb{R}^-) \oplus L^2(\mathbb{R}^-)$, and $X(y) \equiv 0$ is the only solution in $L^2(\mathbb{R}^-)$ to

$$-X(y) + \int_{-\infty}^0 dz X(z) F_s(z+y) = 0, \quad y \in \mathbb{R}^-.$$

(V) : There are precisely $\sum_{j=1}^N \text{rank}[M_j]$ linearly independent solutions in $L^1(\mathbb{R}^+)$ to

$$X(y) + \int_0^\infty dz X(z) F_s(z+y) = 0, \quad y \in \mathbb{R}^+.$$

Properties (L), (4), (5)

$$(L) : \left\{ \begin{array}{l} S(k) \text{ is continuous in } k \in \mathbb{R}, \\ \arg[\det S(0^+)] - \arg[\det S(+\infty)] = \pi [2\mathcal{N} + \mu - n + n_D], \\ \mu = \text{multiplicity of eigenvalue } +1 \text{ of } S(0), \\ n_D = \text{multiplicity of eigenvalue } -1 \text{ of } S_\infty, \\ \mathcal{N} = \sum_{j=1}^N \text{rank}[M_j]. \end{array} \right.$$

(4) : Let $\overset{\circ}{F}(y) := F_s(y) + \sum_{j=1}^N M_j^2 e^{-\kappa_j y}$. Then, $X(y) \equiv 0$ is the only solution in $L^2(\mathbb{R}^+)$ to

$$X(y) + \int_0^\infty dz X(z) F(z+y) = 0, \quad y \in \mathbb{R}^+.$$

(5) : $F'_s \in L^1(\mathbb{R}^-) \oplus L^2(\mathbb{R}^-)$.

Properties (I), (VI), (A)

$$(I) : \begin{cases} S(-k) = S(k)^\dagger = S(k)^{-1}, & k \in \mathbb{R}, \\ S(k) = S_\infty + O\left(\frac{1}{k}\right), & k \rightarrow \pm\infty, \\ F_s(y) \in L^1(\mathbb{R}^+) \cap L^\infty(\mathbb{R}), \quad F_s(y) := \frac{1}{2\pi} \int_{-\infty}^{\infty} dk [S(k) - S_\infty] e^{iky}. \end{cases}$$

(VI) : $S(k)$ is continuous in $k \in \mathbb{R}$.

$$(A) : \begin{cases} \text{There exists at least one solution } h(k) \in \mathbf{H}^2(\mathbb{C}^+) \text{ to} \\ h(-k) + S(k) h(k) = g(k), \quad k \in \mathbb{R}, \\ \text{for every } g(k) \text{ in a dense subspace of } L^2(\mathbb{R}) \text{ satisfying} \\ g(-k) = S(k) g(k), \quad k \in \mathbb{R}. \end{cases}$$

Example 1: The scattering data in the Marchenko class

$$n = 1, \quad S(k) = -\frac{k+i}{k-i}, \quad \text{no bound states.}$$

This scattering data set belongs to the Marchenko class.

$$S(0) = 1, \quad S_\infty = -1, \quad G_1 = 2, \quad \mu = 1, \quad n_D = 1, \quad \mathcal{N} = 0,$$

$$F_s(y) = \begin{cases} 2e^{-y}, & y \in \mathbb{R}^+, \\ 0, & y \in \mathbb{R}^-, \end{cases}$$

$$K(0, 0) = -1, \quad f(k, x) = e^{ikx} \left[1 - \frac{i}{k+i} \frac{e^{-x}}{\cosh x} \right],$$

$$V(x) = -2 \operatorname{sech}^2 x, \quad \Psi(k, x) = -\frac{2ik}{k-i} \sin kx - \frac{1}{k-i} (\cos kx)(\tanh x),$$

$$A = 0, \quad J(k) = \frac{k}{k+i} B, \quad \Psi(k, 0) = 0, \quad \Psi'(k, 0) = -2i(k+i), \quad \text{where } B \text{ is an arbitrary nonzero constant.}$$

Example 2: The scattering data not in the Marchenko class

$$n = 1, \quad S(k) = \frac{k}{k+i}, \quad \text{no bound states.}$$

This scattering data set does not belong to the Marchenko class even though (2, III + V, 4) hold. Only (1) does not hold: $S(k)^\dagger \neq S(k)^{-1}$.

(L) does not hold because $\mathcal{N} = -1/2$, not a nonnegative integer.

$$\mathbf{S} \mapsto \mathbf{D} \not\mapsto \mathbf{S}, \quad \mathbf{D} \text{ yields } S(k) = \frac{k - i/2}{k + i/2}.$$

Example 3: The scattering data not in the Marchenko class

$$n = 1, \quad S(k) = i \frac{k - i}{k + i}, \quad \text{no bound states.}$$

This scattering data set does not belong to the Marchenko class even though **(2, III + V, 4)** hold. Only **(1)** does not hold: $S(-k) \neq S(k)^\dagger$.

$A = B = 0$, not satisfying $A^\dagger A + B^\dagger B > 0$.

Example 4: The scattering data not in the Marchenko class

$$n = 1, \quad S(k) = \frac{k+i}{k-i}, \quad \text{no bound states.}$$

This scattering data set does not belong to the Marchenko class even though (1, 2, III) hold.
Only (4, V) do not hold.

$$V(x) = \frac{8e^{2x}}{(e^{2x} - 1)^2}, \quad V \notin L^1(\mathbb{R}^+),$$

$$V(x) = \frac{2}{x^2} - \frac{2}{3} + \frac{2x^2}{15} + O(x^4), \quad x \rightarrow 0,$$

$K(0, 0) = -\infty$, and hence no A and B satisfying $A^\dagger A + B^\dagger B > 0$.

Example 5: The scattering data not in the Marchenko class

$$n = 1, \quad S(k) = \left(\frac{k-i}{k+i} \right)^2, \quad \text{no bound states.}$$

This scattering data set does not belong to the Marchenko class even though (1, 2, 4, V) hold.
Only (III) does not hold.

$K(0, 0) = 0, \quad V(x) \equiv 0, \quad B = 2A$, with A as any nonzero constant.

(3) fails: $-B^\dagger \Psi(k, 0) + A^\dagger \Psi'(k, 0) \neq 0$,

$$\Psi(k, 0) = \frac{2k^2 - 2}{(k+i)^2}, \quad \Psi'(k, 0) = \frac{4k^2}{(k+i)^2}.$$

(L) fails because $\mathcal{N} = -1$, not a nonnegative integer.

Example 6: The scattering data in the Marchenko class

$$n=2, \quad S(k) = \frac{1}{(k-i)\left(k-\frac{i}{3}\right)} \begin{bmatrix} k(k+i) & \frac{i}{3}(k+i) \\ \frac{i}{3}(k+i) & k(k+i) \end{bmatrix}, \text{ one bound state at } k=i$$

of multiplicity two with $M_1 = \begin{bmatrix} 1 + \frac{1}{\sqrt{2}} & 1 - \frac{1}{\sqrt{2}} \\ 1 - \frac{1}{\sqrt{2}} & 1 + \frac{1}{\sqrt{2}} \end{bmatrix}$.

This scattering data set belongs to the Marchenko class

$$V(x) = -\frac{8e^{2x/3}}{9(2+e^{2x/3})^2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad B = \frac{1}{18} \begin{bmatrix} -17 & 1 \\ 1 & -17 \end{bmatrix} A, \text{ with } A \text{ being any invertible } 2 \times 2 \text{ matrix.}$$