Scattering matrices and Dirichlet-to-Neumann maps

Mark Malamud

Institute of Appl. Math. and Mech., Ukraine

Join talk with J. Behrndt and H. Neidhardt

St. Petersburg, June 24-30, 2016

Scattering matrix

Let A and B be self-adjoint op-s in $\mathfrak{H}$ and assume that they are resol. comparable, i.e. their resol. difference is a trace class op.,

$$(B-i)^{-1}-(A-i)^{-1}\in\mathfrak{S}_1(\mathfrak{H}). \tag{1}$$

Denote by $\mathfrak{H}^{ac}(A)$ the abs. continuous subspace of A and let $P^{ac}(A)$ be the orthog. proj-n in $\mathfrak{H}$ onto $\mathfrak{H}^{ac}(A)$. In accordance with the Birman-Krein th-m, under the assum. (1) the *wave op-s*

$$W_{\pm}(A,B):=s-\lim_{t\to\pm\infty}e^{itB}e^{-itA}P^{ac}(A)$$

exist and are complete, i.e. the ranges of $W_{\pm}(B,A)$ coincide with the absolutely continuous subspace $\mathfrak{H}^{ac}(B)$ of B. The *scattering op.* $S(A,B)$ of the *scattering system* is defined by

$$S(A,B)=W_{+}(A,B)^{*}W_{-}(A,B).$$

The op-r $S(A,B)$ commutes with A and is unitary in $\mathfrak{H}^{ac}(A)$, hence it is unitarily equivalent to a multiplication op-r induced by a family $\{S(A,B;\lambda)\}_{\lambda\in\mathbb{R}}$ of unitary oper-s in a spectral repres-n of the absol. continuous part A^{ac} of A,

$$A^{ac} := A \upharpoonright \mathrm{dom}(A) \cap \mathfrak{H}^{ac}(A).$$

The family $\{S(A,B;\lambda)\}_{\lambda\in\mathbb{R}}$ is called the *scattering matrix* of the scattering system $\{A,B\}$.

Boundary triples and their Weyl functions

Let S be a densely defined, closed, symmetric operator in a separable Hilbert space $\mathfrak{H}$.

Definition 1

A triple $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is called a *B-generalized bound. triple* for S^* if $\mathcal{H}$ is a Hilbert space and for some operator T in $\mathfrak{H}$ such that $\overline{T} = S^*$, the linear mappings $\Gamma_0, \Gamma_1 : \mathrm{dom}(T) \longrightarrow \mathcal{H}$ satisfy the abstract Green's identity

$$(Tf, g) - (f, Tg) = (\Gamma_1 f, \Gamma_0 g) - (\Gamma_0 f, \Gamma_1 g), \quad f, g \in \mathrm{dom}(T), \tag{2}$$

the op-r $A_0 := T \upharpoonright \ker(\Gamma_0)$ is self-adjoint in $\mathfrak{H}$, and $\mathrm{ran}(\Gamma_0) = \mathcal{H}$. If, in addition, the op-r $A_1 := T \upharpoonright \ker(\Gamma_1)$ is self-adjoint in $\mathfrak{H}$ and $\mathrm{ran}(\Gamma_1) = \mathcal{H}$, then the triple $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is called a *double B-generalized bound. triple* for S^*.

Definition 2

Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a B-gen-zed b-ry triple. The *Weyl func-n* $M(\cdot)$ and the *γ-field* $\gamma(\cdot)$ corresponding to Π are defined by

$$M(z)\Gamma_0 f_z := \Gamma_1 f_z, \quad f_z \in \mathfrak{N}_z = \ker(T - z),$$
$$\text{and} \quad \gamma(z) := \big(\Gamma_0 \upharpoonright \ker(T - z)\big)^{-1}, \quad z \in \rho(A_0).$$

Clearly, $M(z) = \Gamma_1 \gamma(z)$.

Definition 3

A Nevanlinna function $M(\cdot) \in R[\mathcal{H}]$ is called $\mathfrak{S}_p$-regular for some $p \in (0, \infty]$ if it admits a representation

$$M(z) = C + K(z), \qquad K(\cdot) : \mathbb{C}_+ \longrightarrow \mathfrak{S}_p(\mathcal{H}), \quad z \in \mathbb{C}_+, \qquad (3)$$

where $C = C^* \in \mathcal{B}(\mathcal{H})$, $0 \in \rho(C)$, and $K(\cdot)$ is a strict Nevanlinna f-n with values in $\mathcal{B}(\mathcal{H})$, i.e. $K(\cdot) \in R^s[\mathcal{H}]$. The class of $\mathfrak{S}_p$-regular Nevanlinna functions is denoted by $R^{\mathrm{reg}}_{\mathfrak{S}_p}[\mathcal{H}]$.

Lemma 1

Let $M(\cdot)$ be an $\mathfrak{S}_1$-regular Nevanlinna function, $M(\cdot) \in R^{\mathrm{reg}}_{\mathfrak{S}_1}[\mathcal{H}]$. Then the following assertions hold.

(i) $M(\lambda + i0) = \lim_{\varepsilon \to +0} M(\lambda + i\varepsilon)$ exists for a.e. $\lambda \in \mathbb{R}$ in the norm of $\mathcal{B}(\mathcal{H})$;

(ii) $M(\lambda + i0)$ is boundedly invertible in $\mathcal{H}$ for a.e. $\lambda \in \mathbb{R}$;

(iii) $M(\lambda + i\varepsilon) - M(\lambda + i0) \in \mathfrak{S}_p(\mathcal{H})$ for $p \in (1, \infty]$, $\varepsilon > 0$ and a.e. $\lambda \in \mathbb{R}$, and

$$\lim_{\varepsilon \to +0} \|M(\lambda + i\varepsilon) - M(\lambda + i0)\|_{\mathfrak{S}_p(\mathcal{H})} = 0;$$

(iv) $\mathrm{Im}\, M(\lambda + i0) = \lim_{\varepsilon \to +0} \mathrm{Im}\, M(\lambda + i\varepsilon)$ exists for a.e. $\lambda \in \mathbb{R}$ in the $\mathfrak{S}_1$-norm.

Proposition 1

Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a B-generalized boundary triple for S^* such that the corresponding Weyl function $M(\cdot)$ is $\mathfrak{S}_p$-regular for some $p \in (0, \infty]$. Then the following assertions hold.

(i) Π is a double B-generalized boundary triple for S^*;

(ii) The Weyl function corresponding to the transposed B-generalized boundary triple $\Pi^\top$ is $\mathfrak{S}_p$-regular;

(iii) The operators A_0 and A_1 are $\mathfrak{S}_p$-resolvent comparable and the Krein type resolvent formula

$$(A_1 - z)^{-1} - (A_0 - z)^{-1} = -\gamma(z)M(z)^{-1}\gamma(\bar{z})^* \in \mathfrak{S}_p(\mathfrak{H}) \quad (4)$$

holds for all $z \in \rho(A_0) \cap \rho(A_1)$.

The following result is very important in applications.

Proposition 2

Let A and B be self-adjoint operators in $\mathfrak{H}$ such that

$$R_{B,A}(z) := (B - z)^{-1} - (A - z)^{-1} \in \mathfrak{S}_p(\mathfrak{H}) \tag{5}$$

holds for some $z \in \mathbb{C} \setminus \mathbb{R}$ and some $p \in (0, \infty]$, and assume that the closed symmetric operator $S = A \cap B$ is densely defined. Assume, in addition, that there exists $\lambda_0 \in \rho(A) \cap \rho(B) \cap \mathbb{R}$ such that

$$\pm R_{B,A}(\lambda_0) \geqslant 0. \tag{6}$$

If $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is a double B-generalized boundary triple for S^* such that $A = T \upharpoonright \ker(\Gamma_0)$ and $B = T \upharpoonright \ker(\Gamma_1)$ then the corresponding Weyl function $M(\cdot)$ is $\mathfrak{S}_p$-regular.

Main abstract theorem

Theorem 1

Let A and B be self-adjoint operators in a Hilbert space $\mathfrak{H}$, assume that the closed symmetric operator $S = A \cap B$ is densely defined and simple, and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a B-generalized boundary triple for S^* such that $A = T \restriction \ker(\Gamma_0)$ and $B = T \restriction \ker(\Gamma_1)$. Assume, in addition, that the Weyl function $M(\cdot)$ corresponding to Π is $\mathfrak{S}_1$-regular.
Then $\{A, B\}$ is a complete scattering system and

$$L^2(\mathbb{R}, d\lambda, \mathcal{H}_\lambda), \qquad \mathcal{H}_\lambda := \overline{\operatorname{ran}(\operatorname{Im} M(\lambda + i0))},$$

forms a spectral representation of A^{ac} such that for a.e. $\lambda \in \mathbb{R}$ the scattering matrix $\{S(A, B; \lambda)\}_{\lambda \in \mathbb{R}}$ of the scattering system $\{A, B\}$ admits the representation

$$S(A, B; \lambda) = I_{\mathcal{H}_\lambda} - 2i\sqrt{\operatorname{Im} M(\lambda + i0)}\, M(\lambda + i0)^{-1} \sqrt{\operatorname{Im} M(\lambda + i0)}.$$

Birman-Krein formula

Corollary 1. Let A and B be resolvent comparable in $\mathfrak{H}$. Then:

(i) There exists a B-gen-zed b-ry triple $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ for S^* such that $A = T \upharpoonright \ker(\Gamma_0)$ and $B = T \upharpoonright \ker(\Gamma_1)$, and the corresponding Weyl function $M(\cdot)$ is $\mathfrak{S}_1$-regular.

(ii) The following limit exists for a.e. $\lambda \in \mathbb{R}$ and the function

$$\mathbb{R} \ni \lambda \mapsto \xi(\lambda) := \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \operatorname{tr} \operatorname{Im}\big(\log\big(M(\lambda + i\varepsilon)\big)\big) \qquad (7)$$

is a spectral shift function for the pair $\{B, A\}$

(iii) The scattering matrix $\{S(\lambda)\}_{\lambda \in \mathbb{R}}$ of the pair $\{A, B\}$ and the spectral shift function ξ in (7) are connected via

$$\det S(\lambda) = \exp\big(-2\pi i \xi(\lambda)\big) \qquad (8)$$

for a.e. $\lambda \in \mathbb{R}$ with $\operatorname{Im}(M(\lambda + i0)) \neq 0$.

Remark

Recall that if A and B are resolvent comparable, then there exists a real valued function $\xi(\cdot) \in L^1_{loc}(\mathbb{R})$ such that

$$\operatorname{tr}\left((A-z)^{-1} - (B-z)^{-1}\right) = \int_{\mathbb{R}} \frac{1}{(t-z)^2}\,\xi(t)\,dt, \quad z \in \mathbb{C}_+ \cup \mathbb{C}_-, \tag{9}$$

and $\int_{\mathbb{R}} \frac{1}{1+t^2}\,\xi(t)\,dt < \infty$. Such a function $\xi(\cdot)$ is called a *spectral shift function* (SSF) of the pair $\{B, A\}$. We emphasize that $\xi(\cdot)$ is defined uniquely up to an additive constant, i.e. $\xi_1(\cdot)$ is a SSF alongside with $\xi(\cdot)$ if and only if $\xi_1(\cdot) = \xi(\cdot) + c,\ c \in \mathbb{R}$.

Formula (8) is the famous Birman-Krein formula connecting the determinant of the scattering matrix with the Krein spectral shift function. It is an immediate consequence of Theorem 1.

Formula (7) for (one of) the SSF was obtained in terms of the Weyl func-n corresponding to an ordinary b-ry triplet in [1].

Schrödinger operators. Let $\Omega \subset \mathbb{R}^n$ be an exterior domain, let

$$\mathcal{L} = -\Delta + V, \qquad V \in L^\infty(\Omega). \tag{10}$$

be a Schrödinger diff. expr-n with a potential $V = \bar{V} \in L^\infty(\Omega)$. With expression (10) one naturally associates the min. oper-r

$$S_{min} f = \mathcal{L} f, \qquad \mathrm{dom}(S_{min}) = \big\{ f \in H^2(\Omega) : \gamma_D f = \gamma_N f = 0 \big\}. \tag{11}$$

and realizations

$$\begin{aligned} A_D f &= \mathcal{L} f, \qquad \mathrm{dom}(A_D) = \big\{ f \in H^2(\Omega) : \gamma_D f = 0 \big\}, \\ A_N f &= \mathcal{L} f, \qquad \mathrm{dom}(A_N) = \big\{ f \in H^2(\Omega) : \gamma_N f = 0 \big\}, \end{aligned} \tag{12}$$

where γ_D and γ_N are the Dirichlet and Neumann traces, and

$$A_\alpha f = \mathcal{L} f, \qquad \mathrm{dom}(A_\alpha) = \big\{ f \in H^{3/2}_\Delta(\Omega) : \alpha \gamma_D f = \gamma_N f \big\}. \tag{13}$$

Dirichlet-to-Neumann map

Mote that for any $\psi \in H^{1/2}(\partial\Omega)$ and $z \in \rho(A_D)$ there exists a unique solution $f_z \in H^1_\Delta(\Omega)$ of the boundary value problem

$$-\Delta f_z + V f_z = z f_z, \qquad \gamma_D f_z = \psi \in H^{1/2}(\partial\Omega). \tag{17}$$

The solution operator is given by

$$P_D(z) : H^{1/2}(\partial\Omega) \longrightarrow H^1_\Delta(\Omega) \subset L^2(\Omega), \qquad \psi \mapsto f_z. \tag{18}$$

For $z \in \rho(A_D)$ the *Dirichlet-to-Neumann map* $\Lambda_{1/2}(z)$ is defined by

$$\Lambda_{1/2}(z) : H^{1/2}(\partial\Omega) \longrightarrow H^{-1/2}(\partial\Omega), \qquad \psi \mapsto \gamma_N P_D(z)\psi, \tag{19}$$

Theorem 2

Let $\Omega \subset \mathbb{R}^2$ be an exterior domain with a C^∞-smooth boundary, let $V \in L^\infty(\Omega)$ and $\alpha \in L^\infty(\partial\Omega)$ be real valued functions, and let A_D and A_α be the self-adjoint Dirichlet and Robin realizations of $\mathcal{L} = -\Delta + V$ in $L^2(\Omega)$ in (12) and (13), respectively. Let $\Lambda_{1/2}(\cdot)$ be the Dirichlet-to-Neumann map defined in (19), and let

$$M_\alpha^D(z) := \widetilde{\jmath^{-1}}(\alpha - \Lambda_{1/2}(z))\jmath^{-1}, \quad z \in \rho(A_D), \tag{20}$$

where $\jmath : H^{1/2}(\partial\Omega) \longrightarrow L^2(\partial\Omega)$ denotes a positive definite self-adj. op. in $L^2(\partial\Omega)$ with $\mathrm{dom}(\jmath) = H^{1/2}(\partial\Omega)$ as in (14)–(15). Then $\{A_D, A_\alpha\}$ is a complete scattering system and

$$L^2(\mathbb{R}, d\lambda, \mathcal{H}_\lambda), \qquad \mathcal{H}_\lambda := \overline{\mathrm{ran}(\mathrm{Im}\, M_\alpha^D(\lambda + i0))},$$

forms a spectral representation of A_D^{ac} such that for a.e. $\lambda \in \mathbb{R}$

the scattering matrix $\{S(A_D, A_\alpha; \lambda)\}_{\lambda\in\mathbb{R}}$ of the scattering system $\{A_D, A_\alpha\}$ admits the representation

$$S(A_D, A_\alpha; \lambda) = I_{\mathcal{H}_\lambda} - 2i\sqrt{\mathrm{Im}\, M_\alpha^D(\lambda + i0)}\, M_\alpha^D(\lambda + i0)^{-1}\sqrt{\mathrm{Im}\, M_\alpha^D(\lambda + i0)}.$$

Remark. In connection with this result we mention the papers [2], [3], [4].

[1] M. Malamud, H. Neidhardt, Trace formulas for additive and non-additive perturbations $\backslash\backslash$ Advances in Math., v. 274 (2015), p. 736-832.

[2] Bagraev, N.T., Mikhailova, A.B., Pavlov, B.S., Prokhorov, L.V., Yafyasov, A.M.: Parameter regime of a resonance quantum switch. Phys. Rev. B **71**, 165308 (2005)

[3] Pavlov, B.S., Antoniou, I.: Jump-start in the analytic perturbation procedure for the Friedrichs model. J. Phys. A **38** 4811–4823 (2005)

[4] Mikhailova, A.B., Pavlov, B.S., Prokhorov, L.V.: Intermediate Hamiltonian via Glazman's splitting and analytic perturbation for meromorphic matrix-functions. Math. Nachr. **280**, 1376–1416 (2007)

Thank you!