Scattering Matrices and Weyl Functions

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Scattering system and wave operators

L, L_0 self-adjoint operators in a separable Hilbert space $\mathcal{H}$.
Describe $e^{-itL}\psi$ with $e^{-itL_0}\phi_\pm$ for $t \to \pm\infty$, i.e.

$$\|e^{-itL}\psi - e^{-itL_0}\phi_\pm\| = \|\psi - e^{itL}e^{-itL_0}\phi_\pm\| \to 0, \qquad t \to \pm\infty.$$

If $(L-\lambda)^{-1} - (L_0-\lambda)^{-1} \in \mathfrak{S}_1$ then the **wave operators**

$$W_\pm := s-\lim_{t\to\pm\infty} e^{itL}e^{-itL_0}P^{ac}(L_0) \text{ exist}, \quad \text{ran } W_\pm = \mathcal{H}^{ac}(L).$$

Define the **scattering operator** by

$$S : \mathcal{H}^{ac}(L_0) \to \mathcal{H}^{ac}(L_0), \qquad \phi_- \mapsto \phi_+ = W_+^* W_- \phi_-.$$

S is unitary in $\mathcal{H}^{ac}(L_0)$ and commutes with $L_0^{ac} = L_0|\mathcal{H}^{ac}(L_0)$.

Direct integrals and scattering matrix

There is a direct integral representation of $\mathcal{H}^{ac}(L_0)$,

$$\mathcal{H}^{ac}(L_0) \cong L^2(\sigma_{ac}(L_0), d\lambda, \mathcal{H}_\lambda) \text{ “ } = \text{ “} \int_{\sigma_{ac}(L_0)}^{\oplus} \mathcal{H}_\lambda \, d\lambda$$

such that

$$L_0^{ac} = L_0 | \mathcal{H}^{ac}(L_0) \cong \lambda.$$

Example: $L_0 = -\frac{d^2}{dx^2}$ in $L^2(\mathbb{R})$, $\sigma(L_0) = \sigma_{ac}(L_0) = [0, \infty)$.

$$-\frac{d^2}{dx^2} \text{ in } L^2(\mathbb{R}) \overset{\mathcal{F}}{\cong} \lambda^2 \text{ in } L^2(\mathbb{R}) \cong \lambda \text{ in } L^2([0,\infty), d\lambda, \mathbb{C}^2)$$

Scattering operator $S = W_+^* W_-$ of $\{L, L_0\}$ turns into multiplication

$$S \cong \{S(\lambda)\} \quad \text{in} \quad L^2(\sigma_{ac}(L_0), d\lambda, \mathcal{H}_\lambda);$$

$\{S(\lambda)\}$ **scattering matrix** of $\{L, L_0\}$.

Boundary triplets

$A \subset A^*$ closed symmetric operator in $\mathcal{H}$, $n_+(A) = n_-(A)$

Definition $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ boundary triplet for A^* if $\mathcal{G}$ Hilbert space, $\Gamma_0, \Gamma_1 :$ dom $A^* \to \mathcal{G}$ such that

$$\big(A^* f, g\big) - \big(f, A^* g\big) = \big(\Gamma_1 f, \Gamma_0 g\big) - \big(\Gamma_0 f, \Gamma_1 g\big), \quad f, g \in \text{dom}\, A^*,$$

$$\text{and} \quad \Gamma := \begin{pmatrix} \Gamma_0 \\ \Gamma_1 \end{pmatrix} : \text{dom}\, A^* \to \mathcal{G} \times \mathcal{G} \quad \text{is surjective.}$$

Gorbatchuk, Gorbatchuk and Derkach, Malamud

Example: (singular Sturm-Liouville operator)

$Af := -f'' + qf | \{f(0) = f'(0) = 0\}$ in $L^2(0, \infty)$, LP at ∞,

$A^* f = -f'' + qf$

Here $(A^* f, g) - (f, A^* g) = -f'\overline{g} + f\overline{g'}|_0^\infty = f'(0)\overline{g(0)} - f(0)\overline{g'(0)}$.

Choose $\mathcal{G} = \mathbb{C}$, $\Gamma_0 f := f(0)$, $\Gamma_1 f := f'(0)$.

Self-adjoint extensions and Weyl function

$A \subset A^*$, $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ boundary triplet for A^*. Then

$$\Theta \mapsto A_\Theta := A^* \restriction \ker(\Gamma_1 - \Theta\Gamma_0)$$

bijection between self-adjoint extensions and self-adjoint Θ in $\mathcal{G}$.

Example: $A_\Theta f = -f'' + qf | \{\Theta f(0) = f'(0)\}$, $\Theta \in \mathbb{R}$.

Let $f_\lambda \in \ker(A^* - \lambda)$, $\lambda \in \rho(A_0)$, $A_0 = A^* \restriction \ker \Gamma_0$. The function

$$M(\lambda) : \mathcal{G} \longrightarrow \mathcal{G}, \qquad \Gamma_0 f_\lambda \mapsto \Gamma_1 f_\lambda, \qquad \lambda \in \rho(A_0),$$

is called **Weyl function** of $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$.

* M is Titchmarsh Weyl function in singular Sturm-Liouville theory, if e.g. $q = 0$, then $M(\lambda) = i\sqrt{\lambda}$
* Spectral properties of A_Θ can be described with M
* $(A_\Theta - \lambda)^{-1} = (A_0 - \lambda)^{-1} + \gamma(\lambda)(\Theta - M(\lambda))^{-1}\gamma(\bar{\lambda})^*$

Scattering matrices and Weyl functions

Scattering system $\{L, L_0\}$ of self-adjoint operators such that

$$(L-\lambda)^{-1} - (L_0-\lambda)^{-1} \quad \text{finite rank}.$$

Then $A := L \cap L_0$ has finite defect, $\exists$ boundary triplet $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$, $\Theta = \Theta^*$ in $\mathcal{G}$ with $L_0 = A^* \upharpoonright \ker \Gamma_0$, $L = A^* \upharpoonright \ker (\Gamma_1 - \Theta\Gamma_0)$.

Theorem Let M be the Weyl function of $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$. Then

(i) $L_0^{ac} \cong \lambda$ in $L^2(\mathbb{R}, d\lambda, \mathcal{H}_\lambda)$, where $\mathcal{H}_\lambda = \text{ran}\,(\text{Im}\, M(\lambda + i0))$.

(ii) Scattering matrix $\{S(\lambda)\}$ of $\{L, L_0\}$ is

$$S(\lambda) = I_{\mathcal{H}_\lambda} + 2i\sqrt{\text{Im}\, M(\lambda+i0)}\big(\Theta - M(\lambda+i0)\big)^{-1}\sqrt{\text{Im}\, M(\lambda+i0)}$$

for a.e. $\lambda \in \mathbb{R}$.

see also [Adamyan, Pavlov 86], [Albeverio, Kurasov 99]

Singular Sturm-Liouville operators

Consider the scattering system $\{L, L_0\}$, where

$$L_0 = -\frac{d^2}{dx^2} + q|\{f(0) = 0\}, \quad L_\Theta = -f'' + q|\{\Theta f(0) = f'(0)\}$$

in $L^2(0,\infty)$, $-\frac{d^2}{dx^2} + q$ LP at ∞ and M Titchmarsh-Weyl function.

The scattering matrix is

$$S(\lambda) = \frac{\Theta - \overline{M(\lambda + i0)}}{\Theta - M(\lambda + i0)}, \qquad \text{for } q = 0: \ \frac{\Theta + i\sqrt{\lambda}}{\Theta - i\sqrt{\lambda}}.$$

If $q \in L^\infty \cap L^1$, $xq(x) \in L^1$ then the high energy asymptotic is

$$S(\lambda) \approx -1 \quad \text{as } \lambda \to +\infty.$$

Boundary condition Θ can NOT be recovered from $\lim_{\lambda \to +\infty} S(\lambda)$.

Dirac operators and inverse problem

Let $a > 0$ and A be the Dirac operator on $\mathbb{R}$:

$$Af = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right) f' + \left(\begin{smallmatrix} a & 0 \\ 0 & -a \end{smallmatrix}\right) f, \qquad \text{dom } A = W_2^1(\mathbb{R}, \mathbb{C}^2) | \{f(0) = 0\}.$$

Then $n_\pm(A) = 2$, dom $A^* = W_2^1(\mathbb{R}_-, \mathbb{C}^2) \oplus W_2^1(\mathbb{R}_+, \mathbb{C}^2)$ and

$$\Gamma_0 f = \begin{pmatrix} f_2(0-) \\ f_1(0+) \end{pmatrix}, \quad \Gamma_1 f = \begin{pmatrix} f_1(0-) \\ f_2(0+) \end{pmatrix}, \quad f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \in \text{dom } A^*,$$

$\{L, L_0\}$ self-adj. extensions, $L = A^* \upharpoonright \ker(\Gamma_1 - \Theta\Gamma_0)$, $L_0 = A^* \upharpoonright \ker \Gamma_0$, then scattering matrix $\{S(\lambda)\}$ can be calculated.

High energy asymptotics: If $\Theta = \Theta^*$ 2×2-matrix, then

$$\lim_{|\lambda| \to +\infty} S(\lambda) = 1 + 2i(\Theta - i)^{-1}.$$

Boundary condition $\Theta = i(S(\infty) + 1)(S(\infty) - 1)^{-1}$ can be recovered.

Schrödinger operators with point interactions

Consider the symmetric operator

$$H = -\Delta, \qquad \text{dom}\, H := \{ f \in W_2^2(\mathbb{R}^3) : f(0) = 0 \},$$

then $n_\pm(H) = 1$ and $H^* = -\Delta$,

$$\text{dom}\, H^* = \left\{ f = \xi_0 \frac{e^{-r}}{r} + \xi_1 e^{-r} + f_H, \xi_0, \xi_1 \in \mathbb{C},\ f_H \in \text{dom}\, H \right\}$$

and $\{\mathbb{C}, \Gamma_0, \Gamma_1\}$

$$\Gamma_j f := 2\sqrt{\pi}\, \xi_j, \quad f = \xi_0 \frac{e^{-r}}{r} + \xi_1 e^{-r} + f_H \in \text{dom}\, H^*,\ j = 0, 1,$$

is a boundary triplet with Weyl function $M(\lambda) = i\sqrt{\lambda} + 1$, here $H^* \upharpoonright \ker \Gamma_0 = -\Delta \upharpoonright H^2(\mathbb{R}^3)$.

Scattering matrix for $\{H_\Theta, -\Delta\}$ is

$$S(\lambda) = 1 + 2i\sqrt{\lambda}\big(\Theta - (i\sqrt{\lambda} + 1)\big)^{-1}.$$

Spectral shift function

Scattering system $\{L, L_0\}$ of self-adjoint operators such that

$$(L-\lambda)^{-1} - (L_0-\lambda)^{-1} \quad \text{finite rank}.$$

Then $A := L \cap L_0$ has finite defect, $\exists$ boundary triplet $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$, $\Theta = \Theta^*$ in $\mathcal{G}$ with $L_0 = A^* \upharpoonright \ker \Gamma_0$, $L = A^* \upharpoonright \ker (\Gamma_1 - \Theta\Gamma_0)$.

Theorem Let M be the Weyl function of $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$. Then

$$\xi(\lambda) = \frac{1}{\pi} \mathrm{Im} \left(\mathrm{tr}(\log (M(\lambda + i0) - \Theta)) \right)$$

is a spectral shift function for $\{L, L_0\}$ with $0 \leq \xi(\lambda) \leq n$, i.e.

$$\mathrm{tr} \left((L-\lambda)^{-1} - (L_0-\lambda)^{-1} \right) = -\int_{\mathbb{R}} \frac{\xi(t)}{(t-\lambda)^2}\, dt, \qquad \int_{\mathbb{R}} \frac{\xi(t)}{1+t^2}\, dt < \infty.$$

If $(L-\lambda)^{-1} - (L_0-\lambda)^{-1}$ rank 1, [Langer Snoo Yavrian 01].