Stationary scattering theory for unitary operators with an application to quantum walks

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Resolvents and smooth operators

- U, unitary operator in a Hilbert space $\mathcal{H}$ with spectral measure $E^U(\cdot)$, singular subspace $\mathcal{H}_{\mathrm{s}}(U)$, a.c. subspace $\mathcal{H}_{\mathrm{ac}}(U)$, projection on a.c. subspace $P_{\mathrm{ac}}(U)$, resolvent

$$R(z) := (1 - zU^*)^{-1}, \quad z \in \mathbb{C} \setminus \mathbb{S}^1,$$

and (Poisson) operator

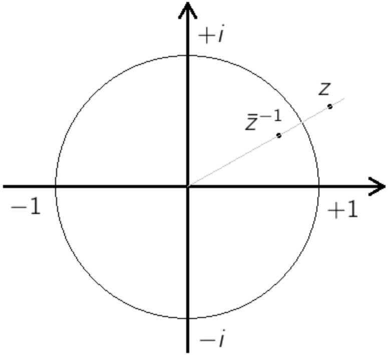
$$\delta(r,\theta) := \tfrac{1}{2\pi}(1 - r^2)\big|R(r\,\mathrm{e}^{i\theta})\big|^2, \quad r \in (0,\infty) \setminus \{1\},\ \theta \in [0, 2\pi).$$

- U_0, unitary operator in a Hilbert space $\mathcal{H}_0$ with ...
- $J \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$, identification operator from $\mathcal{H}_0$ to $\mathcal{H}$
- $V := JU_0 - UJ$, two-Hilbert spaces perturbation

The resolvent of U can be written as a geometric series

$$R(z) = \begin{cases} \sum_{n\geq 0}(zU^*)^n & \text{if } |z|<1 \\ -\sum_{n\geq 1}(z^{-1}U)^n & \text{if } |z|>1, \end{cases}$$

and one has the identity $R(\bar{z}^{-1})^* = -zU^*R(z)$ relating values inside/outside $\mathbb{S}^1$:



If $\mathcal{G}$ is a Hilbert space, then $T \in \mathscr{B}(\mathcal{H}, \mathcal{G})$ is locally U-smooth on a Borel set $\Theta \subset [0, 2\pi)$ if there is $c_\Theta \geq 0$ such that

$$\sum_{n \in \mathbb{Z}} \left\| T U^n E^U(\Theta)\varphi \right\|_{\mathcal{G}}^2 \leq c_\Theta \|\varphi\|_{\mathcal{H}}^2 \quad \text{for all } \varphi \in \mathcal{H}, \tag{A}$$

and T is U-smooth if (A) is satisfied with $\Theta = [0, 2\pi)$. Similarly, T is weakly locally U-smooth on Θ if the weak limit

$$\operatorname*{w-lim}_{\varepsilon \searrow 0} T\,\delta(1-\varepsilon, \theta) E^U(\Theta) T^* \text{ exists for a.e. } \theta \in [0, 2\pi), \tag{B}$$

and T is weakly U-smooth if (B) is satisfied with $\Theta = [0, 2\pi)$.

- T locally U-smooth on $\Theta \Rightarrow T$ weakly locally U-smooth on Θ.
- T locally U-smooth on $\Theta \Rightarrow \overline{E^U(\Theta) T^* \mathcal{G}^*} \subset \mathcal{H}_{\mathrm{ac}}(U)$.

Representation formulas for the wave operators

Set

$$g_{\pm}(\varepsilon) := \tfrac{1}{2\pi}\big(1-(1-\varepsilon)^{\pm 2}\big), \quad \varepsilon \in (0,1),$$

and define $w_{\pm}(U, U_0, J, \varepsilon) \in \mathscr{B}(\mathcal{H}_0, \mathcal{H})$ by the sesquilinear form

$$\begin{aligned}&\big\langle w_{\pm}(U, U_0, J, \varepsilon)\varphi_0, \varphi\big\rangle_{\mathcal{H}} \\ &:= \pm g_{\pm}(\varepsilon)\int_0^{2\pi} \mathrm{d}\theta \,\big\langle J R_0\big((1-\varepsilon)^{\pm 1}\,\mathrm{e}^{i\theta}\big)\varphi_0, R\big((1-\varepsilon)^{\pm 1}\,\mathrm{e}^{i\theta}\big)\varphi\big\rangle_{\mathcal{H}}\end{aligned}$$

for $\varphi_0 \in \mathcal{H}_0$ and $\varphi \in \mathcal{H}$.

Lemma

Let $\mathscr{D}_0 \subset \mathcal{H}_0$ and $\mathscr{D} \subset \mathcal{H}$ be dense sets, and assume that for each $\varphi_0 \in \mathscr{D}_0$ and $\varphi \in \mathscr{D}$ the limits

$$a_\pm(\varphi_0, \varphi, \theta) := \pm \lim_{\varepsilon \searrow 0} g_\pm(\varepsilon) \left\langle JR_0\big((1-\varepsilon)^{\pm 1} \mathrm{e}^{i\theta}\big)\varphi_0, R\big((1-\varepsilon)^{\pm 1} \mathrm{e}^{i\theta}\big)\varphi \right\rangle_{\mathcal{H}}$$

exist for a.e. $\theta \in [0, 2\pi)$. Then, the following weak limits exist

$$w_\pm(U, U_0, J) := \operatorname*{w-lim}_{\varepsilon \searrow 0} w_\pm(U, U_0, J, \varepsilon) P_{\mathrm{ac}}(U_0).$$

Idea of the proof.

Apply a generalisation of Lebesgue's dominated convergence theorem (Vitali's theorem) to exchange limit and integral. □

The weak limits $w_{\pm}(U, U_0, J)$ are the stationary wave operators for the triple (U, U_0, J). When they exist, they posses the usual properties of wave operators

$$\mathcal{H}_{\mathrm{s}}(U_0) \subset \ker w_{\pm}(U, U_0, J) \quad \text{and} \quad \operatorname{Ran} w_{\pm}(U, U_0, J) \subset \mathcal{H}_{\mathrm{ac}}(U)$$

and the intertwinning relation [1]

$$w_{\pm}(U, U_0, J) E^{U_0}(\Theta) = E^{U}(\Theta) w_{\pm}(U, U_0, J), \quad \Theta \subset [0, 2\pi) \text{ Borel set.}$$

[1] Similar to the self-adjoint case [Yafaev 1992].

Assume there exist a Hilbert space $\mathcal{G}$ and operators $G_0 \in \mathscr{B}(\mathcal{H}_0, \mathcal{G})$, $G \in \mathscr{B}(\mathcal{H}, \mathcal{G})$ such that $V = G^* G_0$.

Theorem (Stationary wave operators)

Assume that for each φ_0 in a dense set $\mathscr{D}_0 \subset \mathcal{H}_0$

$$\operatorname*{s-lim}_{\varepsilon \searrow 0} G_0 U_0^* R_0\big((1-\varepsilon)^{\pm 1} \mathrm{e}^{i\theta}\big)\varphi_0 \text{ exist for a.e. } \theta \in [0, 2\pi),$$

and suppose that G is weakly U-smooth. Then, the stationary wave operators $w_\pm(U, U_0, J)$ exist and satisfy the representation formulas

$$\big\langle w_\pm(U, U_0, J)\varphi_0, \varphi\big\rangle_{\mathcal{H}} = \int_0^{2\pi} \mathrm{d}\theta \, a_\pm(\varphi_0, \varphi, \theta), \quad \varphi_0 \in \mathscr{D}_0, \ \varphi \in \mathcal{H}.$$

Idea of the proof.

Use the assumptions on G_0 and G to show that $a_\pm(\varphi_0, \varphi, \theta)$ exist for a.e. $\theta \in [0, 2\pi)$, and apply the previous lemma. □

Theorem (Strong wave operators)

Assume that for each φ_0 in a dense set $\mathscr{D}_0 \subset \mathcal{H}_0$

$$\operatorname*{s-lim}_{\varepsilon \searrow 0} G_0 U_0^* R_0\big((1-\varepsilon)^{\pm 1} \mathrm{e}^{i\theta}\big)\varphi_0 \text{ exist for a.e. } \theta \in [0, 2\pi),$$

and that $B_\pm(\theta) := \text{w-lim}_{\varepsilon \searrow 0} GR\big((1-\varepsilon)^{\pm 1} \mathrm{e}^{i\theta}\big)G^*$ exist for a.e. $\theta \in [0, 2\pi)$. Then, the strong wave operators

$$W_\pm(U, U_0, J) := \operatorname*{s-lim}_{n \to \pm\infty} U^n J U_0^{-n} P_{\mathrm{ac}}(U_0)$$

exist and coincide with the stationary wave operators $w_\pm(U, U_0, J)$.

Idea of the proof.

The assumptions on G_0 and G guarantee the existence of the operators $W_\pm(U, U_0, J)$ and $w_\pm(U, U_0, J)$.

To show that they coincide, one has to use power series for the resolvents in $w_\pm(U, U_0, J)$ to obtain an infinite series involving powers U^n and U_0^{-n}, and then use a Tauberian theorem to prove that this series converges to

$$\operatorname*{s-lim}_{n \to \pm\infty} U^n J U_0^{-n} P_{\mathrm{ac}}(U_0) = W_\pm(U, U_0, J).$$

□

Example (Trace class perturbation)

The assumptions of the theorem are satisfied for the set $\mathscr{D}_0 = \mathcal{H}_0$ *when* V *is trace class, or equivalently when the operators* G_0 *and* G *are Hilbert-Schmidt.*

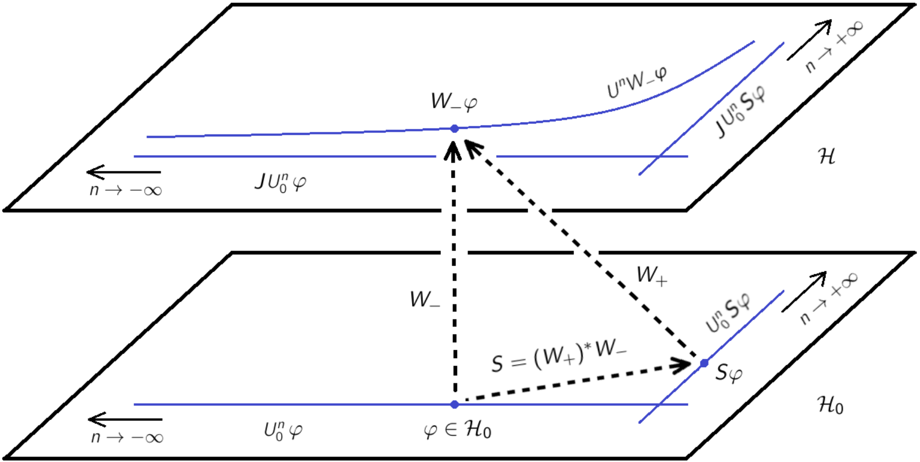
Representation formulas for the scattering matrix

If the strong wave operators $W_\pm(U, U_0, J)$ exist, then the scattering operator is defined as

$$S(U, U_0, J) := W_+(U, U_0, J)^* \, W_-(U, U_0, J).$$

Basic properties:

- $S(U, U_0, J) \restriction \mathcal{H}_{\mathrm{s}}(U_0) = 0$,
- $\mathrm{Ran}\, S(U, U_0, J) \subset \mathcal{H}_{\mathrm{ac}}(U_0)$,
- If $W_\pm(U, U_0, J) \restriction \mathcal{H}_{\mathrm{ac}}(U_0)$ are isometric, then $S(U, U_0, J) \restriction \mathcal{H}_{\mathrm{ac}}(U_0)$ is unitary if and only if $\mathrm{Ran}\, W_-(U, U_0, J) = \mathrm{Ran}\, W_+(U, U_0, J)$.


$W_- \varphi$
$U^n W_- \varphi$
$J U_0^n S \varphi$
$n \to +\infty$
$\mathcal{H}$
$n \to -\infty$
$J U_0^n \varphi$
W_+
W_-
$U_0^n S \varphi$
$n \to +\infty$
$S = (W_+)^* W_-$
$S\varphi$
$\mathcal{H}_0$
$n \to -\infty$
$U_0^n \varphi$
$\varphi \in \mathcal{H}_0$

Let $\widehat{\sigma}_0$ be a core of the spectrum of U_0. Then, there exist for a.e. $\theta \in \widehat{\sigma}_0$ Hilbert spaces $\mathfrak{h}_0(\theta)$ and an operator

$$F_0 : \mathcal{H}_0 \to \int_{\widehat{\sigma}_0}^{\oplus} \mathrm{d}\theta \, \mathfrak{h}_0(\theta) \quad \text{(spectral transformation)},$$

which is unitary from $\mathcal{H}_{\mathsf{ac}}(U_0)$ to $\int_{\widehat{\sigma}_0}^{\oplus} \mathrm{d}\theta \, \mathfrak{h}_0(\theta)$, vanishes on $\mathcal{H}_{\mathsf{s}}(U_0)$, and diagonalises $U_0 \upharpoonright \mathcal{H}_{\mathsf{ac}}(U_0)$. Namely, if

$$U_0^{(\mathsf{ac})} := U_0 \upharpoonright \mathcal{H}_{\mathsf{ac}}(U_0) \quad \text{and} \quad F_0^{(\mathsf{ac})} := F_0 \upharpoonright \mathcal{H}_{\mathsf{ac}}(U_0),$$

then we have the direct integral decomposition

$$F_0^{(\mathsf{ac})} U_0^{(\mathsf{ac})} \big(F_0^{(\mathsf{ac})}\big)^* = \int_{\widehat{\sigma}_0}^{\oplus} \mathrm{d}\theta \; \mathrm{e}^{i\theta} \, .$$

$\mathcal{H}_{\mathrm{ac}}(U_0)$ is a reducing subspace for $S(U, U_0, J)$ and the restriction

$$S^{(\mathrm{ac})}(U, U_0, J) := S(U, U_0, J) \upharpoonright \mathcal{H}_{\mathrm{ac}}(U_0)$$

commutes with $U_0^{(\mathrm{ac})}$. Thus $S^{(\mathrm{ac})}(U, U_0, J)$ decomposes in $\int_{\widehat{\sigma}_0}^{\oplus} \mathrm{d}\theta\, \mathfrak{h}_0(\theta)$, that is, there exist for a.e. $\theta \in \widehat{\sigma}_0$ operators $S(\theta) \in \mathscr{B}\big(\mathfrak{h}_0(\theta)\big)$ such that

$$F_0^{(\mathrm{ac})} S^{(\mathrm{ac})}(U, U_0, J) \big(F_0^{(\mathrm{ac})}\big)^* = \int_{\widehat{\sigma}_0}^{\oplus} \mathrm{d}\theta\, S(\theta).$$

The family $\{S(\theta)\}_{\theta \in \widehat{\sigma}_0}$ is called the scattering matrix for the triple (U, U_0, J).

Similarly, if the stationary wave operators $w_\pm(U_0, U_0, J^*J)$ exist, then $\mathcal{H}_{\rm ac}(U_0)$ is a reducing subspace for $w_\pm(U_0, U_0, J^*J)$, and

$$w_\pm^{(\rm ac)}(U_0, U_0, J^*J) := w_\pm(U_0, U_0, J^*J) \restriction \mathcal{H}_{\rm ac}(U_0)$$

commutes with $U_0^{(\rm ac)}$. Thus, there exist for a.e. $\theta \in \widehat{\sigma}_0$ operators $u_\pm(\theta) \in \mathscr{B}\big(\mathfrak{h}_0(\theta)\big)$ such that

$$F_0^{(\rm ac)} w_\pm^{(\rm ac)}(U_0, U_0, J^*J)\big(F_0^{(\rm ac)}\big)^* = \int_{\widehat{\sigma}_0}^{\oplus} \mathrm{d}\theta\, u_\pm(\theta).$$

Example (One-Hilbert space case)

If $\mathcal{H}_0 = \mathcal{H}$ *and* $J = 1_{\mathcal{H}_0}$, *then one has*

$$w_\pm(U_0, U_0, J^*J) = w_\pm(U_0, U_0, 1_{\mathcal{H}_0}) = 1_{\mathcal{H}_0},$$

and $u_\pm(\theta) = 1_{\mathfrak{h}_0(\theta)}$ *for a.e.* $\theta \in \widehat{\sigma}_0$.

Theorem (Scattering matrix)

Assume that for each φ_0 in a dense set $\mathscr{D}_0 \subset \mathcal{H}_0$

$$\operatorname*{s-lim}_{\varepsilon \searrow 0} G_0 U_0^* R_0\big((1-\varepsilon)^{\pm 1}\,\mathrm{e}^{i\theta}\big)\varphi_0 \text{ exist for a.e. } \theta \in [0, 2\pi),$$

that $B_\pm(\theta) = \text{w-lim}_{\varepsilon \searrow 0} GR\big((1-\varepsilon)^{\pm 1}\,\mathrm{e}^{i\theta}\big)G^*$ exist for a.e. $\theta \in [0, 2\pi)$, and that G_0 is weakly U_0-smooth. Then, we have for a.e. $\theta \in \widehat{\sigma}_0$ the representation formulas for the scattering matrix:

$$S(\theta) = u_+(\theta) + 2\pi\big(Z_0(\theta, GJU_0)Z_0(\theta, G_0)^* - Z_0(\theta, G_0)B_+(\theta)Z_0(\theta, G_0)^*\big),$$
$$S(\theta) = u_-(\theta) - 2\pi\big(Z_0(\theta, G_0)Z_0(\theta, GJU_0)^* - Z_0(\theta, G_0)B_-(\theta)Z_0(\theta, G_0)^*\big),$$

with

$$Z_0(\theta, T_0)\zeta = \big(F_0 T_0^* \zeta\big)(\theta), \quad T_0 \in \mathscr{B}(\mathcal{H}_0, \mathcal{G}),\ \zeta \in \mathcal{G},\ \text{a.e. } \theta \in \widehat{\sigma}_0.$$

Idea of the proof.

Apply the results that precede + some integrals calculations.

□

Application to anisotropic quantum walks

In the Hilbert space

$$\mathcal{H} := \ell^2(\mathbb{Z}, \mathbb{C}^2) = \left\{ \Psi : \mathbb{Z} \to \mathbb{C}^2 \mid \sum_{x \in \mathbb{Z}} \|\Psi(x)\|^2_{\mathbb{C}^2} < \infty \right\},$$

the evolution operator of the quantum walk is $U := SC$ with

$$(S\Psi)(x) := \begin{pmatrix} \Psi^{(0)}(x+1) \\ \Psi^{(1)}(x-1) \end{pmatrix}, \quad \Psi = \begin{pmatrix} \Psi^{(0)} \\ \Psi^{(1)} \end{pmatrix} \in \mathcal{H},\ x \in \mathbb{Z}, \quad \text{(shift)}$$

$$(C\Psi)(x) := C(x)\Psi(x), \quad \Psi \in \mathcal{H},\ x \in \mathbb{Z},\ C(x) \in \mathrm{U}(2). \quad \text{(coin)}$$

The operator U is unitary because S and C are unitary.

C is short-range and anisotropic at infinity:

Assumption (Anisotropic coin)

There exist $C_\ell, C_\mathsf{r} \in \mathrm{U}(2)$, $\kappa_\ell, \kappa_\mathsf{r} > 0$, *and* $\varepsilon_\ell, \varepsilon_\mathsf{r} > 0$ *such that*

$$\left\| C(x) - C_\ell \right\|_{\mathscr{B}(\mathbb{C}^2)} \leq \kappa_\ell \left| x \right|^{-1-\varepsilon_\ell} \quad \text{if } x < 0$$
$$\left\| C(x) - C_\mathsf{r} \right\|_{\mathscr{B}(\mathbb{C}^2)} \leq \kappa_\mathsf{r} \left| x \right|^{-1-\varepsilon_\mathsf{r}} \quad \text{if } x > 0,$$

with indexes ℓ *for "left" and* r *for "right".*

Quantum walks satisfying this are called quantum walks with an anisotropic coin.

The assumption provides operators $U_\star := SC_\star$ ($\star = \ell, \mathrm{r}$) describing the asymptotic behaviour of U on the left and on the right.

It also suggests to define the free evolution operator as

$$U_0 := U_\ell \oplus U_\mathrm{r} \quad \text{in} \quad \mathcal{H}_0 := \mathcal{H} \oplus \mathcal{H},$$

and to define the identification operator $J : \mathcal{H}_0 \to \mathcal{H}$ as

$$J(\Psi_0) := j_\ell \, \Psi_{0,\ell} + j_\mathrm{r} \, \Psi_{0,\mathrm{r}}, \quad \Psi_0 = (\Psi_{0,\ell}, \Psi_{0,\mathrm{r}}) \in \mathcal{H}_0,$$

with

$$j_\mathrm{r}(x) := \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x \leq -1 \end{cases} \quad \text{and} \quad j_\ell := 1 - j_\mathrm{r}.$$

If the matrices $C_\star$ are not anti-diagonal, then U_0 has purely a.c. spectrum and the strong wave operators $W_\pm(U, U_0, J)$ exist and are complete [Richard-Suzuki-T. 2018-2019].

Furthermore, the assumption implies that V is trace class. Thus one can verify the validity of the representation formulas for the stationary wave operators and the scattering matrix.

Thank you

References

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