

Dissipative quantum systems: scattering theory and spectral singularities

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J.F. and **J. Fröhlich**, *Asymptotic completeness in dissipative scattering theory*, Adv. Math., 340, 300-362, (2018).

J.F. and **F. Nicoleau**, *Scattering matrices for dissipative quantum systems*, J. Funct. Anal., 9, 3062-3097, (2019).

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Introduction

The nuclear optical model

The nuclear optical model (I)

Quantum system

- Neutron targeted onto a complex nucleus
- Either the neutron is elastically scattered off the nucleus
- Or it is absorbed by the nucleus \implies Formation of a compound nucleus
- Concept of a compound nucleus was introduced by Bohr ('36)

Model

- Feshbach, Porter and Weisskopf ('54): nuclear optical model describing both elastic scattering and absorption
- "Pseudo-Hamiltonian" on $L^2(\mathbb{R}^3)$

$$H = -\Delta + V(x) - iW(x)$$

with V and W real-valued, compactly supported, $W \geq 0$

- Widely used in Nuclear Physics, refined versions include, e.g., spin-orbit interactions
- Empirical model

The nuclear optical model (II)

Interpretation

- $-iH$ generates a strongly continuous **semigroup of contractions** $\{e^{-itH}\}_{t \geq 0}$
- Dynamics described by the **Schrödinger equation**

$$\begin{cases} i\partial_t u_t = H u_t \\ u_0 \in \mathcal{D}(H) \end{cases}$$

If the neutron is initially in the normalized state u_0 , after a time $t \geq 0$, it is in the **unnormalized** state $e^{-itH} u_0$

- Probability that the neutron, initially in the normalized state u_0 (supposed to be orthogonal to bound states), eventually escapes from the nucleus:

$$p_{\text{scatt}}(u_0) = \lim_{t \rightarrow \infty} \|e^{-itH} u_0\|^2$$

- Probability of absorption:

$$p_{\text{abs}}(u_0) = 1 - \lim_{t \rightarrow \infty} \|e^{-itH} u_0\|^2$$

- If $p_{\text{scatt}}(u_0) > 0$ (and u_0 is orthogonal to bound states), one expects that there exists an (unnormalized) **scattering state** u_+ such that $\|u_+\|^2 = p_{\text{scatt}}(u_0)$ and

$$\lim_{t \rightarrow \infty} \|e^{-itH} u_0 - e^{it\Delta} u_+\| = 0$$

The nuclear optical model (III)

Aim

- Explicit expression of H rests on experimental scattering data
- Nuclear optical model generalizes to any quantum system S interacting with another system S' and susceptible of being absorbed by S'
- Need to develop the full **scattering theory** of a class of models

References: mathematical scattering theory for dissipative operators in Hilbert spaces

- Abstract framework: Lax-Phillips ['73], **Martin** ['75], **Davies** ['79, '80], Neidhardt ['85], Exner ['85], Petkov ['89], Kadowaki ['02, '03], Stepin ['04], ...
- Small perturbations: **Kato** ['66], Falconi-F-Fröhlich-Schubnel ['17], ...
- Schrödinger operators: Mochizuki ['68], **Simon** ['79], Wang-Zhu ['14], ...

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The abstract framework of dissipative scattering theory

Abstract model

The model

- \mathcal{H} complex Hilbert space
- Pseudo-Hamiltonian

$$H = H_0 + V - iC^*C = H_V - iC^*C,$$

with $H_0 \geq 0$, V symmetric, $C \in \mathcal{L}(\mathcal{H})$ and V, C relatively compact with respect to H_0

- H_V is self-adjoint, H is closed and maximal dissipative, with domains

$$\mathcal{D}(H) = \mathcal{D}(H_V) = \mathcal{D}(H_0)$$

- $-iH$ generates a strongly continuous semigroup of contractions $\{e^{-itH}\}_{t \geq 0}$. More precisely, $-iH$ generates a group $\{e^{-itH}\}_{t \in \mathbb{R}}$ s.t.

$$\|e^{-itH}\| \leq 1, \quad t \geq 0, \quad \|e^{-itH}\| \leq e^{\|C^*C\||t|}, \quad t \leq 0$$

- $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_0)$ and $\sigma(H) \setminus \sigma_{\text{ess}}(H)$ consists of an at most countable number of eigenvalues of finite algebraic multiplicities that can only accumulate at points of $\sigma_{\text{ess}}(H)$

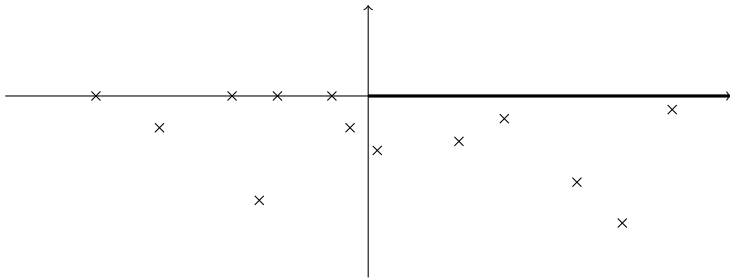


FIGURE: Form of the spectrum of H .

Example

Example to keep in mind:

$$\mathcal{H} = L^2(\mathbb{R}^3), \quad H_0 = -\Delta, \quad H_V = -\Delta + V(x) = H_V^*, \quad C = W(x)^{\frac{1}{2}}$$

Spectral subspaces

Space of bound states

$$\mathcal{H}_b(H) = \text{Span}\{u \in \mathcal{D}(H), \exists \lambda \in \mathbb{R}, Hu = \lambda u\}$$

Generalized eigenstates corresponding to non-real eigenvalues

- For $\lambda \in \sigma(H) \setminus \sigma_{\text{ess}}(H)$, **Riesz projection** defined by

$$\Pi_\lambda = \frac{1}{2i\pi} \int_\gamma (z\text{Id} - H)^{-1} dz,$$

where γ is a circle centered at λ , of sufficiently small radius

- $\text{Ran}(\Pi_\lambda)$ spanned by generalized eigenvectors of H associated to λ , $u \in \mathcal{D}(H^k)$ s.t. $(H - \lambda)^k u = 0$
- Space of **generalized eigenstates corresponding to non-real eigenvalues**:

$$\mathcal{H}_p(H) = \text{Span}\{u \in \text{Ran}(\Pi_\lambda), \lambda \in \sigma(H), \text{Im } \lambda < 0\}$$

“Dissipative space”

$$\mathcal{H}_d(H) = \{u \in \mathcal{H}, \lim_{t \rightarrow \infty} \|e^{-itH}u\| = 0\} \supset \mathcal{H}_p(H)$$

The adjoint operator H^*

Properties of H^*

- $H^* = H_0 + V + iC^*C$
- $\lambda \in \sigma(H^*)$ if and only if $\bar{\lambda} \in \sigma(H)$
- iH^* generates the strongly continuous contraction semigroup $\{e^{itH^*}\}_{t \geq 0}$
- Spectral subspaces

$$\mathcal{H}_b(H^*) = \text{Span}\{u \in \mathcal{D}(H), \exists \lambda \in \mathbb{R}, H^*u = \lambda u\},$$

$$\mathcal{H}_p(H^*) = \text{Span}\{u \in \text{Ran}(\Pi_\lambda^*), \lambda \in \sigma(H^*), \text{Im } \lambda > 0\},$$

$$\mathcal{H}_d(H^*) = \{u \in \mathcal{H}, \lim_{t \rightarrow \infty} \|e^{itH^*}u\| = 0\}$$

The wave operators

The wave operator $W_-(H, H_0)$

- Defined by

$$W_-(H, H_0) = \text{s-lim}_{t \rightarrow \infty} e^{-itH} e^{itH_0}$$

- If it exists, $W_-(H, H_0)$ is a **contraction**
- $W_-(H, H_0)H_0 = HW_-(H, H_0)$

The wave operator $W_+(H_0, H)$

- Defined by

$$W_+(H_0, H) = \text{s-lim}_{t \rightarrow \infty} e^{itH_0} e^{-itH} \Pi_b(H)^\perp$$

where $\Pi_b(H)^\perp$ denotes the orthogonal projection onto $\mathcal{H}_b(H)^\perp$

- If it exists, $W_+(H_0, H)$ is a **contraction**
- $H_0 W_+(H_0, H) = W_+(H_0, H)H$
- Under some conditions, $W_+(H_0, H) = W_+(H^*, H_0)^*$
- For $u \in \mathcal{H}_b(H)^\perp$,

$$u_+ = W_+(H_0, H)u \iff \lim_{t \rightarrow \infty} \|e^{-itH}u - e^{-itH_0}u_+\| = 0$$

The scattering operator and matrices

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The scattering operator $S(H, H_0)$

- Defined by

$$S(H, H_0) = W_+(H^*, H_0)^* W_-(H, H_0) = W_+(H_0, H) W_-(H, H_0)$$

- If it exists, $S(H, H_0)$ is a **contraction**
- $S(H, H_0)$ **commutes with H_0**

The scattering matrices $S(\lambda)$

- Defined by the fiber decomposition

$$S(H, H_0) = \int_{\Lambda}^{\oplus} S(\lambda) d\lambda \quad \text{in} \quad \mathcal{H} = \int_{\Lambda}^{\oplus} \mathcal{H}(\lambda) d\lambda, \quad \Lambda = \sigma(H_0)$$

- If H_0 has a **purely absolutely continuous** spectrum of **constant multiplicity**, then

$$\mathcal{H}(\lambda) = \mathcal{M}$$

and $S(H, H_0)$ acts in $\mathcal{H} = L^2(\Lambda; \mathcal{M})$ as

$$[S(H, H_0)u](\lambda) = S(\lambda)u(\lambda)$$

Basic assumptions

(H1) Spectrum of H_0

The spectrum of H_0 is **purely absolutely continuous** and has a **constant multiplicity** (which may be infinite)

(H2) Spectrum of H_V

H_V has **finitely many eigenvalues** counting multiplicity, **no embedded eigenvalues**, and $\sigma_{\text{sc}}(H_V) = \emptyset$

(H3) Wave operators for H_V and H_0

The **wave operators**

$$W_{\pm}(H_V, H_0) = \text{s-lim}_{t \rightarrow \pm\infty} e^{itH_V} e^{-itH_0}, \quad W_{\pm}(H_0, H_V) = \text{s-lim}_{t \rightarrow \pm\infty} e^{itH_0} e^{-itH_V} \Pi_{\text{ac}}(H_V)$$

exist and are asymptotically complete, i.e.,

$$\text{Ran}(W_{\pm}(H_V, H_0)) = \mathcal{H}_{\text{ac}}(H_V) = \mathcal{H}_{\text{pp}}(H_V)^{\perp},$$

$$\text{Ran}(W_{\pm}(H_0, H_V)) = \mathcal{H}$$

Regularity of C w.r.t. H_V

(H4) Relative smoothness of C with respect to H_V

There exists a constant $c_V > 0$, such that

$$\int_{\mathbb{R}} \|C e^{-itH_V} \Pi_{\text{ac}}(H_V) u\|^2 dt \leq c_V^2 \|\Pi_{\text{ac}}(H_V) u\|^2,$$

for all $u \in \mathcal{H}$

Remarks

- Estimates of this form considered in [Kato '66]
- The following estimate is *always* satisfied

$$\int_0^\infty \|C e^{-itH} u\|^2 dt \leq \frac{1}{2} \|u\|^2$$

Basic results

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Existence and properties of the wave operators

Suppose (H1)–(H4). Then

- * $W_-(H, H_0)$ and $W_+(H_0, H)$ exist
- * $W_-(H, H_0)$ is an **injective** contraction and

$$\overline{\text{Ran}(W_-(H, H_0))} = (\mathcal{H}_b(H^*) \oplus \mathcal{H}_d(H^*))^\perp$$

- * $W_+(H_0, H)$ is a contraction with **dense range** and

$$\text{Ker}(W_+(H_0, H)) = \mathcal{H}_b(H) \oplus \mathcal{H}_d(H)$$

- * $S(H, H_0)$ exists and is a contraction

Definition of asymptotic completeness and consequences

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Definition

- $W_-(H, H_0)$ is said to be **asymptotically complete** if

$$\text{Ran}(W_-(H, H_0)) = (\mathcal{H}_b(H^*) \oplus \mathcal{H}_p(H^*))^\perp$$

- Main issues: prove that $\mathcal{H}_d(H^*) = \mathcal{H}_p(H^*)$ and that $\text{Ran}(W_-(H, H_0))$ is **closed**

Consequences of asymptotic completeness

- * Direct sum decomposition

$$\mathcal{H} = \mathcal{H}_b(H) \oplus \mathcal{H}_p(H) \oplus (\mathcal{H}_b(H^*) \oplus \mathcal{H}_p(H^*))^\perp$$

and the restriction of H to $(\mathcal{H}_b(H^*) \oplus \mathcal{H}_p(H^*))^\perp$ is similar to H_0

- * $W_+(H_0, H) : \mathcal{H} \rightarrow \mathcal{H}$ is **surjective** and

$$\text{Ker}(W_+(H_0, H)) = \mathcal{H}_b(H) \oplus \mathcal{H}_p(H)$$

- * $S(H, H_0) : \mathcal{H} \rightarrow \mathcal{H}$ is **bijective**

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Regular spectral point and spectral singularity

Notation

Recall that

$$\Lambda = \sigma(H_0) = \sigma_{\text{ess}}(H)$$

and set

$$R(z) = (H - z)^{-1}, \quad R_V(z) = (H_V - z)^{-1}, \quad R_0(z) = (H_0 - z)^{-1}$$

Definition

$\lambda \in \dot{\Lambda}$ is a **regular spectral point** of H if there exists a compact interval $K_\lambda \subset \mathbb{R}$ whose interior contains λ and such that the limit

$$CR(\mu - i0^+)C^* = \lim_{\varepsilon \downarrow 0} CR(\mu - i\varepsilon)C^*$$

exists uniformly in $\mu \in K_\lambda$ in the norm topology of $\mathcal{L}(\mathcal{H})$. If λ is not a regular spectral point of H , we say that λ is a **“spectral singularity”** of H

Equivalent possible definitions of a regular spectral point

Theorem [F., Nicoleau]

Suppose

- (H1)–(H4)
- V is **strongly smooth** w.r.t. H_0 and C is **strongly smooth** w.r.t. H_V

Let $\lambda \in \mathring{\Lambda}$. The following conditions are equivalent:

- * λ is a **regular spectral point** of H
- * λ is not an accumulation point of eigenvalues of H located in $\lambda - i(0, \infty)$ and the limit

$$CR(\lambda - i0)C^* := \lim_{\varepsilon \downarrow 0} CR(\lambda - i\varepsilon)C^*$$

exists in the norm topology of $\mathcal{L}(\mathcal{H})$

- * $I - iCR_V(\lambda - i0)C^*$ is invertible in $\mathcal{L}(\mathcal{H})$
- * $S(\lambda)$ is invertible in $\mathcal{L}(\mathcal{M})$

Proposition [F., Nicoleau]

$\{\text{Spectral singularities of } H\} = \text{closed set of Lebesgue measure } 0$

Properties of the scattering matrices

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Theorem [F., Nicoleau]

Under the previous assumptions, for all $\lambda \in \mathring{\Lambda}$,

- * $S(\lambda)$ is a **contraction**
- * $S(\lambda) - I$ is **compact**
- * If in addition $\dim \mathcal{M} = +\infty$, then $\|S(\lambda)\| = 1$

Consequences: Properties of the scattering operator

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Theorem [F., Nicoleau]

Under the previous assumptions, if $\dim \mathcal{M} = +\infty$,

$$\|S(H, H_0)\| = 1$$

Suppose in addition that

- $\Lambda \setminus \dot{\Lambda}$ is finite
- All $\lambda \in \Lambda \setminus \dot{\Lambda}$ are regular in a suitable sense (if Λ is right-unbounded, we assume in addition that $+\infty$ is regular).

Then

- * $S(H, H_0)$ is invertible in $\mathcal{L}(\mathcal{H}) \iff H$ has no spectral singularities in $\dot{\Lambda}$
- * If the previous equivalent conditions hold, then

$$\text{Ran}(W_-(H, H_0)) = (\mathcal{H}_b(H^*) \oplus \mathcal{H}_d(H^*))^\perp$$

- * In particular,

H has a spectral singularity $\implies W_-(H, H_0)$ is not asymptotically complete

Spectral singularity of finite order

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Definition

We say that $\lambda \in \mathring{\Lambda}$ is a spectral singularity of H of **finite order** if λ is a spectral singularity of H and there exists $\nu \in \mathbb{N}^*$ and a compact interval K_λ , whose interior contains λ , such that the limit

$$\lim_{\varepsilon \downarrow 0} (\mu - \lambda)^\nu CR(\mu - i\varepsilon)C^*$$

exists uniformly in $\mu \in K_\lambda$ in the norm topology of $\mathcal{L}(\mathcal{H})$

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Further conditions

(H5) Pure point spectrum of H

H has **at most finitely many eigenvalues**

(H6) Spectral singularities of H

- H has **at most finitely many spectral singularities** in $\mathring{\Lambda}$
- Each spectral singularity is of **finite order**
- If Λ is right-unbounded, **$+\infty$ is regular**

Dissipative space

Theorem [F., Fröhlich]

Suppose (H1)–(H6). Then

$$\mathcal{H}_d(H) = \mathcal{H}_p(H)$$

Remarks

- Finding conditions implying this result quoted as open in [Davies '80]
- For small perturbations, the theorem follows from similarity of H and H_0 [Kato '66], implying that $\mathcal{H}_d(H) = \mathcal{H}_p(H) = \{0\}$
- Interpretation for the nuclear optical model: unless the initial state is a linear combination of generalized eigenstates corresponding to non-real eigenvalues of H , the **probability that the neutron eventually escapes from the nucleus is always strictly positive**

Idea

Generalization of spectral projections for non self-adjoint operators **with spectral singularities**

Consequence: Asymptotic completeness

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Theorem [F., Fröhlich]

Suppose (H1)–(H6). Then

* H has no spectral singularities in $\Lambda \implies W_-(H, H_0)$ is asymptotically complete
i.e.,

$$\text{Ran}(W_-(H, H_0)) = (\mathcal{H}_b(H^*) \oplus \mathcal{H}_p(H^*))^\perp$$

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Application: the nuclear optical model (I)

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Setting

On $\mathcal{H} = L^2(\mathbb{R}^3)$,

$$H_0 = -\Delta, \quad H_V = H_0 + V(x), \quad H = H_V - iW(x)$$

References

- Spectral and scattering theories for (H_V, H_0) : Kato ['66], Reed-Simon ['78], Isozaki-Kitada ['85], Koch-Tataru ['06], Yafaev ['10]
- Relative smoothness/Analysis at threshold: Kato ['66], Jensen-Kato ['79], Constantin-Saut ['89], Ben Artzi-Klainerman ['92], Jensen-Nenciu ['01], Fournais-Skibsted ['04], Schlag ['07]
- Mourre's theory: Mourre ['81], Boutet de Monvel-Georgescu ['96]
- Resonances theory: Sjöstrand ['02], Dyatlov-Zworski ['18]
- Dissipative framework: Simon ['79], Wang ['11,'12]

Application: the nuclear optical model (II)

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Theorem

Let $V, W \in L^\infty(\mathbb{R}^3; \mathbb{R})$. Assume that

- $V \in C^2(\mathbb{R}^3)$ s.t. for $|\alpha| \leq 2$, $\partial_x^\alpha V(x) = \mathcal{O}(\langle x \rangle^{-\rho-|\alpha|})$ with $\rho > 3$,
- $W(x) \geq 0$, $W(x) > 0$ on a non-trivial open set, $W(x) = \mathcal{O}(\langle x \rangle^{-\delta})$ with $\delta > 2$,
- 0 is neither an eigenvalue nor a resonance of H_V

Then,

- * $S(\lambda) \in \mathcal{L}(L^2(S^2))$ is invertible $\iff \lambda$ is not a spectral singularity of H
- * $S(H, H_0)$ is invertible in $\mathcal{L}(L^2(\mathbb{R}^3))$ $\iff H$ has no spectral singularities in Λ
- * If the previous equivalent conditions hold, then

$$\text{Ran}(W_-(H, H_0)) = \mathcal{H}_d(H^*)^\perp$$

Application: the nuclear optical model (III)

Theorem

Let $V, W \in L^\infty(\mathbb{R}^3; \mathbb{R})$. Assume that

- V and W are **compactly supported**,
- $W(x) \geq 0$, $W(x) > 0$ on a **non-trivial open set**,
- 0 is **neither an eigenvalue nor a resonance** of H_V

Then

- * $\mathcal{H}_d(H) = \mathcal{H}_p(H)$
- * $W_-(H, H_0)$ is **asymptotically complete** $\iff \text{Ran}(W_-(H, H_0)) = \mathcal{H}_p(H^*)^\perp$
 $\iff H$ has no **spectral singularities**
- * If the previous equivalent conditions hold, then
 - * $S(H, H_0)$ is **invertible** in $\mathcal{L}(L^2(\mathbb{R}^3))$,
 - * The restriction of H to $\mathcal{H}_p(H^*)^\perp$ is **similar to H_0**
 - * There exist $m_1 > 0$ and $m_2 > 0$ such that, for all $u \in \mathcal{H}_p(H^*)^\perp$,

$$m_1 \|u\| \leq \|e^{-itH} u\| \leq m_2 \|u\|, \quad t \in \mathbb{R}$$

Application: the nuclear optical model (IV)

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Remarks

- Spectral singularity = real resonance
- H has no real eigenvalues
- [Wang '11]: 0 cannot be a resonance of H
- [Wang '12]: For any $\lambda > 0$, one can construct smooth compactly supported potentials V and W such that λ is a spectral singularity of H
- Work in progress: prove that “generically”, there is no spectral singularity

Application: scattering for Lindblad master equations (I)

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References

- Davies ['80]
- Different approach: Alicki ['81], Alicki-Frigerio ['83]
- Falconi-F.-Fröhlich-Schubnel ['16]

Application: scattering for Lindblad master equations (II)

Lindbladian and quantum dynamical semigroup

- If one considers a quantum particle interacting with a dynamical target, takes the trace over the degrees of freedom of the target and studies the reduced effective evolution of the particle, then, in the kinetic limit, the dynamics of the particle is given by a **quantum dynamical semigroup** $\{e^{-it\mathcal{L}}\}_{t \geq 0}$ generated by a **Lindbladian** \mathcal{L}

- On $\mathcal{J}_1(\mathcal{H})$ (space of trace-class operators), \mathcal{L} is given by

$$\mathcal{L}(\rho) = H\rho - \rho H^* + i \sum_{j \in \mathbb{N}} W_j \rho W_j^*, \quad H = H_V - \frac{i}{2} \sum_{j \in \mathbb{N}} W_j^* W_j,$$

where, for all $j \in \mathbb{N}$, $W_j \in \mathcal{L}(\mathcal{H})$, and $\sum_{j \in \mathbb{N}} W_j^* W_j \in \mathcal{L}(\mathcal{H})$

- H is a **dissipative operator** on \mathcal{H}
- On a suitable domain, \mathcal{L} is the generator of a **quantum dynamical semigroup** $\{e^{-it\mathcal{L}}\}_{t \geq 0}$ (strongly continuous semigroup on $\mathcal{J}_1(\mathcal{H})$) such that, for all $t \geq 0$, $e^{-it\mathcal{L}}$ preserves the trace and is a completely positive operator)
- **Free dynamics**: group of isometries $\{e^{-it\mathcal{L}_0}\}_{t \in \mathbb{R}}$,

$$\mathcal{L}_0(\rho) = H_0\rho - \rho H_0$$

Application: scattering for Lindblad master equations (III)

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Modified wave operator ([Davies '80], [Alicki '81])

- $\Pi_{\text{pp}}^\perp : \mathcal{H} \rightarrow \mathcal{H} : \text{orthogonal projection onto } (\mathcal{H}_b(H) \oplus \mathcal{H}_p(H))^\perp$
- Modified wave operator:

$$\tilde{\Omega}_+(\mathcal{L}_0, \mathcal{L}) := s\text{-}\lim_{t \rightarrow +\infty} e^{it\mathcal{L}_0} (\Pi_{\text{pp}}^\perp e^{-it\mathcal{L}} (\cdot) \Pi_{\text{pp}}^\perp)$$

Theorem

Suppose that Hypotheses (H1)–(H6) hold and that H has **no spectral singularities** in Λ . Then $\tilde{\Omega}_+(\mathcal{L}_0, \mathcal{L})$ **exists on $\mathcal{J}_1(\mathcal{H})$**

Interpretation

For all $\rho \in \mathcal{J}_1(\mathcal{H})$ with $\rho \geq 0$ and $\text{tr}(\rho) = 1$, the number $\text{tr}(\tilde{\Omega}_+(\mathcal{L}_0, \mathcal{L})\rho) \in [0, 1]$ is interpreted as the **probability that the particle**, initially in the state ρ , **eventually escapes from the target**