

Time delay for dispersive quantum Hamiltonians

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- Scattering operator

$$S := W_+^* W_-$$

(unitarity)

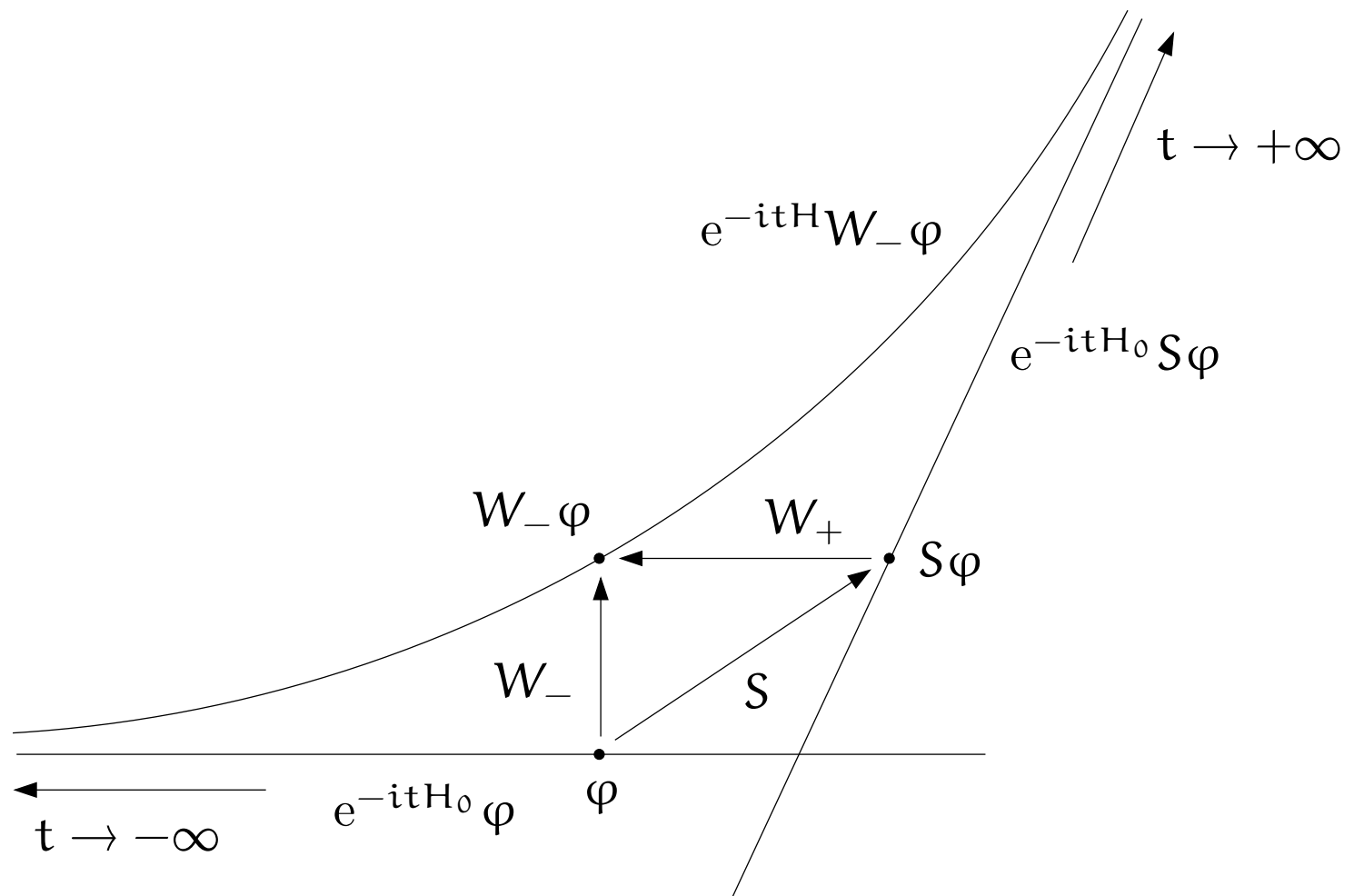


Figure 1: Wave operators W_{\pm} and scattering operator S

There exist Hilbert spaces \mathcal{H}_λ , $\lambda \in \sigma(H_0)$, and a unitary transformation

$$U : \mathcal{H} \rightarrow \int_{\sigma(H_0)}^{\oplus} d\lambda \mathcal{H}_\lambda$$

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S is decomposable in the spectral representation of H_0 , *i.e.* there exist unitary operators $S(\lambda)$ in \mathcal{H}_λ such that

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The collection $\{S(\lambda)\}$, $\lambda \in \sigma(H_0)$, is the scattering matrix.

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Heuristically, the time delay of an outgoing radial wave packet with respect to the associated free incoming wave packet (peaked around the kinetic energy λ) is given by derivative of the phase shift:

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(Eisenbud-Wigner time delay, 60's)

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Take a function $f \in L^\infty(\mathbb{R}^d)$ decaying to 0 at infinity such that $f = 1$ on a bounded neighbourhood Σ of 0. Let $Q \equiv (Q_1, \dots, Q_d)$ be the vector position operator in \mathcal{H} .

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Example: $f(Q/r)$ is the (exact) localization operator in $\mathcal{B}_r := \{\mathbf{x} \in \mathbb{R}^d \mid |\mathbf{x}| < r\}$ if $f = \chi_{\mathcal{B}_1}$.

Let $\varphi \in \mathcal{H}$ be an appropriate normalised scattering state.

- Sojourn time of the freely evolving state $e^{-itH_0} \varphi$ in Σ_r :

$$T_r^0(\varphi) := \int_{\mathbb{R}} dt \langle e^{-itH_0} \varphi, f(Q/r) e^{-itH_0} \varphi \rangle$$

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(definition introduced by Jauch, Misra, and Sinha in the 70's, when $f = \chi_{\mathcal{B}_1}$ and $H_0 = -\Delta$)

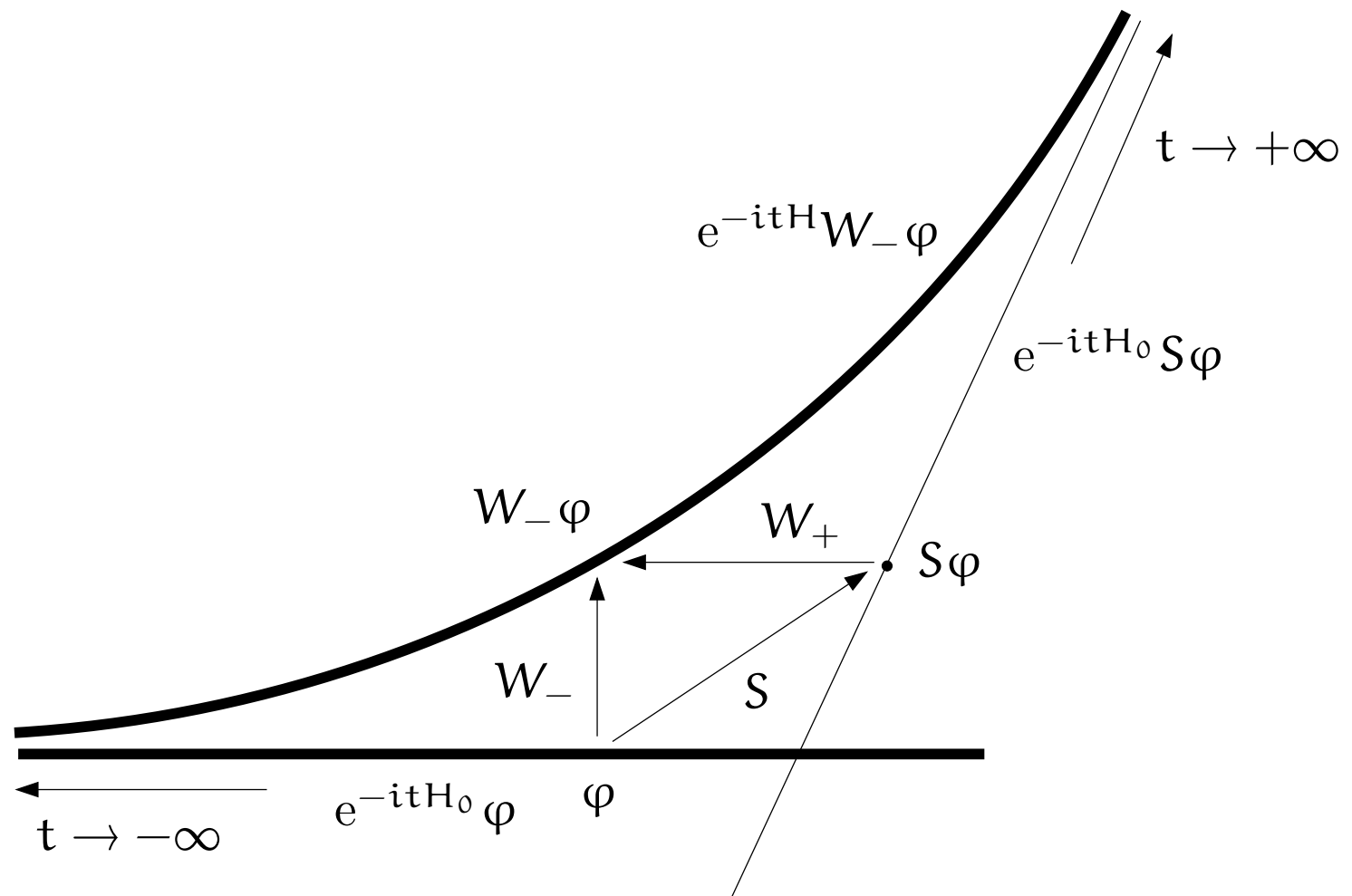


Figure 2: Interpretation of $\tau_r^{\text{in}}(\varphi)$

If $f = \chi_{\mathcal{B}_1}$, $H_0 = -\Delta$, and H is appropriate, $\tau_r^{\text{in}}(\varphi)$ exists for each $r > 0$, and

$$\begin{aligned} \lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi) &= \int_0^\infty d\lambda \left\langle (\mathcal{U}\varphi)(\lambda), -i\mathcal{S}(\lambda)^* \left(\frac{d\mathcal{S}(\lambda)}{d\lambda} \right) (\mathcal{U}\varphi)(\lambda) \right\rangle_{L^2(\mathbb{S}^{d-1})} \\ &\equiv \langle \varphi, \tau_{\text{E-W}} \varphi \rangle. \end{aligned}$$

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(Amrein, Cibils, Jensen, Martin, 80's and 90's)

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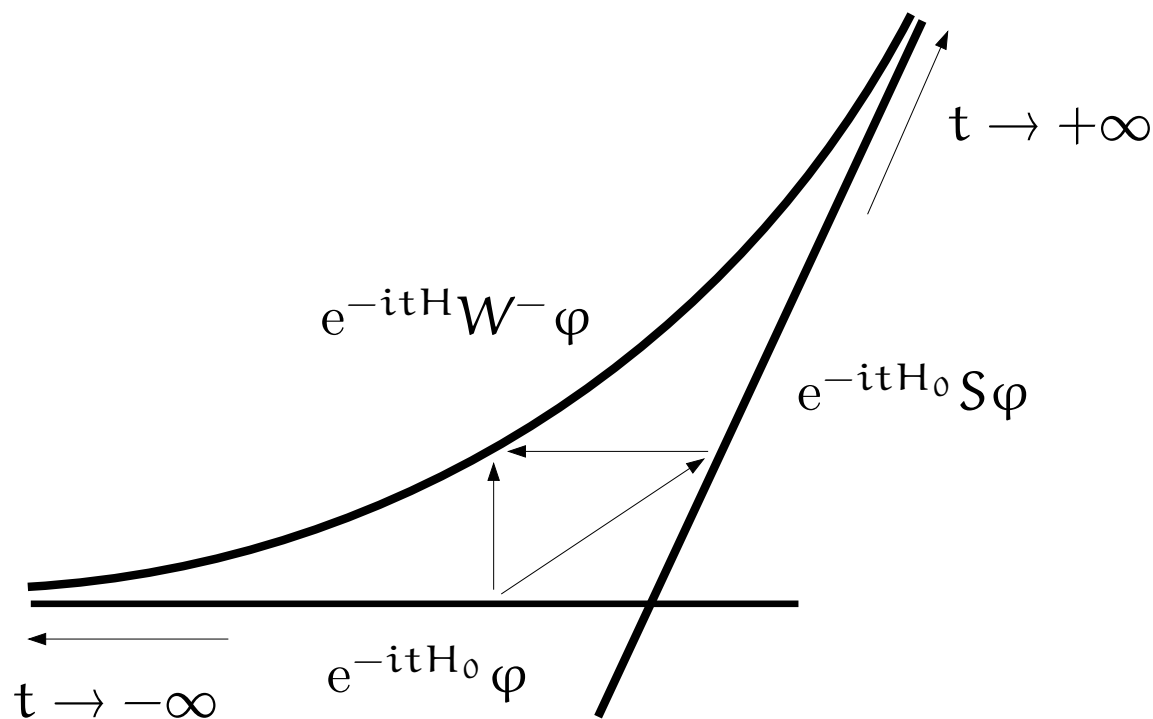


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- scattering in quantum waveguides (TdA 06),
- scattering for one-dimensionnal anisotropic potentials (Amrein-Jacquet 07).

Gérard-TdA 06: If $f = \chi_\Sigma$ with $\Sigma = -\Sigma$, $H_0 = -\Delta$, and H is appropriate, then $\tau_r(\varphi)$ exists for each $r > 0$, and

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If $f = \chi_{\mathcal{B}_1}$, the second contribution vanishes, and all the time delays coincide:

$$\lim_{r \rightarrow \infty} \tau_r(\varphi) = \lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi) = \langle \varphi, \tau_{E-W} \varphi \rangle.$$

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Could we extend the theory in order to get a unified picture of the problem?

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Notation: Given a function $h \in C^1(\mathbb{R}^d; \mathbb{R})$, we denote by $\kappa(h)$ the set of critical values of h , *i.e.*

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- $\kappa(h)$ has measure zero if $h \in C^d(\mathbb{R}^d; \mathbb{R})$.
- $\kappa(h)$ is finite if h is a polynomial.
- $\kappa(h)$ is closed if $|h(\mathbf{x})| \rightarrow \infty$ as $|\mathbf{x}| \rightarrow \infty$.

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Assumption (hypoelliptic-type): The function $h : \mathbb{R}^d \rightarrow \mathbb{R}$ is of class C^m for some $m \geq 3$, and satisfies the following conditions:

- (i) $|h(\mathbf{x})| \rightarrow \infty$ as $|\mathbf{x}| \rightarrow \infty$.
- (ii) $\sum_{|\alpha| \leq m} |(\partial^\alpha h)(\mathbf{x})| \leq \text{Const.} (1 + |h(\mathbf{x})|)$.
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H_0 has purely absolutely continuous spectrum in $\mathbb{R} \setminus \kappa(h)$.

Example: h can be an elliptic symbol of degree $s > 0$, *i.e.* $h \in C^\infty(\mathbb{R}^d; \mathbb{R})$, $|(\partial^\alpha h)(\mathbf{x})| \leq C_\alpha \langle \mathbf{x} \rangle^{s-|\alpha|}$ for each multi-index α , and $|h(\mathbf{x})| \geq C |\mathbf{x}|^s$, for some $C > 0$, outside a compact set.

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is well-defined.

Example: If f is radial, *i.e.* $f(\mathbf{x}) = f_0(|\mathbf{x}|)$ for a.e. $\mathbf{x} \in \mathbb{R}^d$, then

$$R_f(\mathbf{x}) = R_{f_0}(1) - \ln |\mathbf{x}|,$$

and

$$(\nabla R_f)(\mathbf{x}) = -\mathbf{x}^{-2}\mathbf{x}.$$

Theorem: Suppose that $f \in \mathcal{S}(\mathbb{R}^d)$ is even and satisfies $f = 1$ on a bounded neighbourhood of $\mathbf{0}$. Let \mathbf{h} be as above. Then there exists a dense set of vectors φ such that

$$\begin{aligned} & \lim_{r \rightarrow \infty} \int_0^\infty dt \langle \varphi, [e^{i\mathbf{t}\mathbf{h}(\mathbf{P})} f(\mathbf{Q}/r) e^{-i\mathbf{t}\mathbf{h}(\mathbf{P})} - e^{-i\mathbf{t}\mathbf{h}(\mathbf{P})} f(\mathbf{Q}/r) e^{i\mathbf{t}\mathbf{h}(\mathbf{P})}] \varphi \rangle \\ & = \langle \varphi, \mathbf{A}_f \varphi \rangle, \end{aligned}$$

where

$$\mathbf{A}_f := \mathbf{Q} \cdot (\nabla \mathbf{R}_f)[(\nabla \mathbf{h})(\mathbf{P})] + (\nabla \mathbf{R}_f)[(\nabla \mathbf{h})(\mathbf{P})] \cdot \mathbf{Q}.$$

Remark: If f is radial, A_f reduces to the operator

$$A := -\left(Q \cdot \frac{(\nabla \mathbf{h})(\mathbf{P})}{(\nabla \mathbf{h})(\mathbf{P})^2} + \frac{(\nabla \mathbf{h})(\mathbf{P})}{(\nabla \mathbf{h})(\mathbf{P})^2} \cdot Q\right).$$

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Hence, if f is radial and H_0 has purely absolutely continuous spectrum, the theorem gives

$$\begin{aligned} & \lim_{r \rightarrow \infty} \int_0^\infty dt \langle \varphi, [e^{ith(P)} f(Q/r) e^{-ith(P)} - e^{-ith(P)} f(Q/r) e^{ith(P)}] \varphi \rangle \\ &= \int_{\sigma(H_0)} d\lambda \left\langle (\mathcal{U}\varphi)(\lambda), -2i \frac{d(\mathcal{U}\varphi)}{d\lambda}(\lambda) \right\rangle_{\mathcal{H}_\lambda}, \end{aligned}$$

where $\mathcal{U} : \mathcal{H} \rightarrow \int_{\sigma(H_0)} d\lambda \mathcal{H}_\lambda$ is a spectral transformation for $H_0 = h(P)$.

7 Existence of symmetrised time delay

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Let H be any selfadjoint perturbation of $H_0 = \mathfrak{h}(P)$ satisfying the following condition.

Assumption W_{\pm} : The wave operators W_{\pm} exist and are complete, and any operator $T \in \mathcal{B}(\mathcal{D}(\langle Q \rangle^{-\rho}), \mathcal{H})$, with $\rho > \frac{1}{2}$, is locally H -smooth on $\mathbb{R} \setminus \{\kappa(\mathfrak{h}) \cup \sigma_{\text{pp}}(H)\}$.

Theorem: Let $f \geq 0$ be an even function in $\mathcal{S}(\mathbb{R}^d)$ such that $f = 1$ on a bounded neighbourhood of 0 . Let \mathfrak{h} be as above. Suppose that Assumption W_{\pm} holds. Then, if φ satisfies some technical conditions, one has

$$\lim_{r \rightarrow \infty} \tau_r(\varphi) = \frac{1}{2} \langle \varphi, \mathcal{S}^*[\mathcal{A}_f, \mathcal{S}]\varphi \rangle.$$

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Remark 1: If f is radial and H_0 has purely absolutely continuous spectrum, we get the identity of symmetrised time delay and Eisenbud-Wigner time delay for dispersive Hamiltonians $H_0 = \mathfrak{h}(P)$:

$$\lim_{r \rightarrow \infty} \tau_r(\varphi) = \int_{\sigma(H_0)} d\lambda \langle (\mathcal{U}\varphi)(\lambda), -i\mathcal{S}(\lambda)^* \frac{d\mathcal{S}(\lambda)}{d\lambda} (\mathcal{U}\varphi)(\lambda) \rangle_{\mathcal{H}_\lambda}.$$

Remark 2: One can always write the symmetrised time delay as the sum of the contribution of the radial component of the localization function f (Eisenbud-Wigner) and the contribution of the non-radial component of f :

$$\lim_{r \rightarrow \infty} \tau_r(\varphi) = \frac{1}{2} \langle \varphi, S^*[A, S]\varphi \rangle + \frac{1}{2} \langle \varphi, S^*[\widetilde{A}_f, S]\varphi \rangle,$$

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Remark 3: Appart technical conditions, we only need to suppose that the localization function f is even to get the existence of symetrised time delay.

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If $\mathbf{p} \in \mathbb{R}^d$ and f is real, the number $F_f(\mathbf{p}) \equiv \int_{\mathbb{R}} dt f(t\mathbf{p})$ can be seen as the sojourn time in the region defined by the localization function f of a free classical particle moving along the trajectory $\mathbb{R} \ni t \mapsto \mathbf{x}(t) := t\mathbf{p}$.

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Let $F_f : \mathbb{R}^d \setminus \{0\} \rightarrow \mathbb{C}$ be defined by

$$F_f(\mathbf{x}) := \int_{\mathbb{R}} d\mu f(\mu\mathbf{x}).$$

If $\mathbf{p} \in \mathbb{R}^d$ and f is real, the number $F_f(\mathbf{p}) \equiv \int_{\mathbb{R}} dt f(t\mathbf{p})$ can be seen as the sojourn time in the region defined by the localization function f of a free classical particle moving along the trajectory $\mathbb{R} \ni t \mapsto \mathbf{x}(t) := t\mathbf{p}$.

$F_f[(\nabla\mathbf{h})(P)]$ is a “quantum analog” of $F_f(\mathbf{p})$, since $(\nabla\mathbf{h})(P)$ is the quantum velocity operator.

Theorem: Let $f \in \mathcal{S}(\mathbb{R}^d)$ be even. Let \mathbf{h} be as above. Suppose that Assumption W_{\pm} holds. Assume that

$$[F_f[(\nabla \mathbf{h})(\mathbf{P})], \mathcal{S}] = 0. \quad (1)$$

Then, if φ satisfies some technical conditions, one has

$$\lim_{r \rightarrow \infty} [\mathsf{T}_r^0(\mathcal{S}\varphi) - \mathsf{T}_r^0(\varphi)] = 0.$$

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Then, if φ satisfies some technical conditions, one has

$$\lim_{r \rightarrow \infty} [\mathsf{T}_r^0(S\varphi) - \mathsf{T}_r^0(\varphi)] = 0.$$

In particular, time delay and symmetrized time delay satisfy

$$\lim_{r \rightarrow \infty} [\tau_r^{\text{in}}(\varphi) - \tau_r(\varphi)] = 0.$$

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Using the change of variables $\mu := t/r$, $\nu := 1/r$, and the parity of f , one gets

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&= \lim_{\nu \searrow 0} \int_{\mathbb{R}} d\mu \langle \varphi, \mathsf{S}^* \left[\frac{1}{\nu} \{ f[\nu Q + \mu(\nabla h)(\mathsf{P})] - f[\mu(\nabla h)(\mathsf{P})] \}, \mathsf{S} \right] \varphi \rangle
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&= \lim_{\nu \searrow 0} \int_{\mathbb{R}} d\mu \langle \varphi, \mathsf{S}^*[\frac{1}{\nu} \{ f[\nu Q + \mu(\nabla h)(\mathsf{P})] - f[\mu(\nabla h)(\mathsf{P})] \}, \mathsf{S}] \varphi \rangle \\
&= \int_{\mathbb{R}} d\mu \langle \varphi, \mathsf{S}^*[Q \cdot (\nabla f)[\mu(\nabla h)(\mathsf{P})], \mathsf{S}] \varphi \rangle \\
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- Let h be a polynomial of degree 1, *i.e.* $h(\mathbf{x}) = v_0 + \mathbf{v} \cdot \mathbf{x}$ for some $v_0 \in \mathbb{R}$, $\mathbf{v} \in \mathbb{R}^d \setminus \{\mathbf{0}\}$. Then $F_f[(\nabla h)(\mathbf{P})]$ reduces to the scalar $F_f(\mathbf{v})$, and thus it commutes with S .

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(This covers the case of the Friedrichs Hamiltonian.)

- Suppose that f and h are radial, *i.e.* $f(\mathbf{x}) = f_0(|\mathbf{x}|)$ and $h(\mathbf{x}) = h_0(|\mathbf{x}|)$ with, say, $h'_0 \geq 0$ on \mathbb{R}_+ . Then $F_f[(\nabla h)(\mathbf{P})] = F_f(h'_0(|\mathbf{P}|))$ is diagonalizable in the spectral representation of $H_0 \equiv h(\mathbf{P})$. So it commutes with S .

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- Let \mathbf{h} be a polynomial of degree 1, *i.e.* $\mathbf{h}(\mathbf{x}) = \mathbf{v}_0 + \mathbf{v} \cdot \mathbf{x}$ for some $\mathbf{v}_0 \in \mathbb{R}$, $\mathbf{v} \in \mathbb{R}^d \setminus \{\mathbf{0}\}$. Then $F_f[(\nabla \mathbf{h})(\mathbf{P})]$ reduces to the scalar $F_f(\mathbf{v})$, and thus it commutes with \mathbf{S} .

(This covers the case of the Friedrichs Hamiltonian.)

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(This covers the Schrödinger case $\mathbf{h}_0(\rho) = \rho^2$, the square-root Klein-Gordon case $\mathbf{h}_0(\rho) = \sqrt{1 + \rho^2}$, and many others.)

9 Existence of usual time delay

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Theorem: Let $f \geq 0$ be an even function in $\mathcal{S}(\mathbb{R}^d)$ such that $f = 1$ on a bounded neighbourhood of 0 . Let h be as above. Suppose that Assumption W_{\pm} holds. Assume that

$$[F_f[(\nabla h)(P)], S] = 0.$$

Then, if φ satisfies some technical conditions, one has

$$\lim_{r \rightarrow \infty} \tau_r^{\text{in}}(\varphi) = \lim_{r \rightarrow \infty} \tau_r(\varphi) = \frac{1}{2} \langle \varphi, S^*[A_f, S]\varphi \rangle.$$

10 Some references

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