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Time-Delay in Potential Scattering Theory

Some "Geometric" Results

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Abstract. Results on time-delay in potential scattering theory are given using properties of the generator of dilations ("geometric" method).

1. Introduction

The present paper is concerned with time-delay in potential scattering theory. Let $H_0 = -\Delta$ and $H = H_0 + V$ be the free and full Hamiltonian, respectively, in $\mathscr{H} = L^2(\mathbb{R}^n)$, with $V(x) = O(|x|^{-\beta})$, $\beta > 1$, as $|x| \to \infty$. Existence and completeness of the wave operators W_{\pm} is well known. To define the time-delay, consider first an orthogonal projection P in \mathscr{H} . The probability of finding the state $e^{-itH}f$ in $P\mathscr{H}$ at time t is given by $||Pe^{-itH}f||^2$.

The total time spent in $P\mathcal{H}$ is given by

$$\int_{-\infty}^{\infty} \|Pe^{-itH}f\|^2 dt.$$
(1.1)

It is not obvious that this integral is finite. Finiteness is in many cases obtained for some f by proving local H-smoothness of P.

Let us briefly state the main problems in time-delay. Let P_r denote multiplication by the characteristic function for the ball $\{|x| < r\}$. Let $f \in \mathscr{H}$. $e^{-itH_0}f$ and $e^{-itH}W_f$ are asymptotically equal as $t \to -\infty$. The difference of the times spent in $P_r\mathscr{H}$ by these two states is the time-delay for the ball $\{|x| < r\}$:

$$\Delta T_r(f) = \int_{-\infty}^{\infty} (\|P_r e^{-itH} W_- f\|^2 - \|P_r e^{-itH_0} f\|^2) dt.$$
(1.2)

As r tends to infinity, one expects a finite limit, at least for a dense set of $f \in \mathcal{H}$. The limit is the time-delay for f

$$\Delta T(f) = \lim_{r \to \infty} \Delta T_r(f).$$
(1.3)

From stationary considerations one expects $\Delta T(f)$ given as the expectation value of a selfadjoint operator T

$$\Delta T(f) = \langle f, Tf \rangle. \tag{1.4}$$

T is usually called the *Eisenbud-Wigner time-delay operator*. *T* is given explicitly in terms of the scattering operator $S = W_+^* W_-$. Let $S = \{S(\lambda)\}$ be the *S*-matrix decomposition in the spectral representation for H_0 . *T* is given by

$$T = \left\{ -iS(\lambda)^* \frac{d}{d\lambda} S(\lambda) \right\}.$$
 (1.5)

In order to define T by (1.5) one needs differentiability of the scattering matrix. We give two results. First assume $V(x) = O(|x|^{-1-\varepsilon-k})$ as $|x| \to \infty$ for some $\varepsilon > 0$ and some integer $k \ge 0$. Then $S(\lambda)$ is C^k as a function of λ with values in $B(L^2(S^{n-1}))$, S^{n-1} the unit sphere in \mathbb{R}^n . The result is obtained using the Kato-Kuroda representation for $S(\lambda)$. The second result is obtained for V satisfying

$$|(x \cdot \nabla)^{\ell} V(x)| \leq c(1+|x|)^{-1-\varepsilon}, \quad x \in \mathbb{R}^n,$$

for some c > 0, $\varepsilon > 0$, and $\ell = 0, 1, 2, ..., k$. For such potentials $S(\lambda)$ is C^k . This result is proved using a scaling argument.

The above problems (1.2)–(1.5) can be considered for any sequence P_r converging strongly to the identity. Geometric ideas related to the generator of dilations $D = \frac{1}{2i}(x \cdot \nabla + \nabla \cdot x)$ have played an important role in recent developments in scattering theory. See [8] for a review, and [21, 24] for important results, on which our results are based.

Let $P_{-}(P_{+})$ denote the spectral projection for *D* corresponding to $(-\infty, 0]$ ($[0, \infty)$). $P_{-} \mathscr{H}(P_{+} \mathscr{H})$ is the subspace of incoming (outgoing) states. In Sect. 5 we prove

$$\langle f, Tf \rangle = \int_{-\infty}^{\infty} (\|P_{-}e^{-itH_{0}}Sf\|^{2} - \|P_{-}e^{-itH_{0}}f\|^{2})dt$$
 (1.6)

for V satisfying one of the above conditions with k=1. It is part of our result that the integral in (1.6) is absolutely convergent for a dense set of f. Thus (1.6) shows that the difference of the times $e^{-itH_0}f$ and $e^{-itH_0}Sf$ spend in $P_-\mathscr{H}$ equals the time-delay. Replacing P_- by P_+ reverses the sign in (1.6), as expected.

In Sect. 6 results pertaining to (1.3) and (1.4) are given. The main results are Theorems 6.2 and 6.4, which establish results on time-delay under *general* assumptions on P_r and S. The main application is to $P_r = \chi_r(D)$, the spectral projection for D corresponding to [-r, r]. (1.2)–(1.5) are proved for this sequence under the assumption $V(x) = O(|x|^{-4-\varepsilon})$ as $|x| \to \infty$. No spherical symmetry is assumed. This choice of P_r corresponds roughly to the localization $|x \cdot p| \leq r$ in phase space. In the original formulation one had $|x| \leq r$ in configuration space. For states with finite energy support away from zero these localizations are almost equivalent.

Let us now briefly mention some previous results on time-delay. The problem was first studied by Eisenbud [7] and Wigner [29] in a stationary formulation.

(1.5) was introduced by Smith [27]. The time-dependent formulation (1.2) and (1.3) was introduced by Jauch and Marchand [10]. Results on convergence of the trace of certain operators related to (1.2) was proved in [11] and thus established the connection between time-delay and the derivative of the total phase shift (Krein's spectral shift function). (1.3) is not proved in [11].

Rigorous proofs of (1.2)–(1.5) have been given by Martin [20] for a class of simple scattering systems [i.e. $S(\lambda)$ scalar]. It is essential in his proof to have $S(\lambda)$ scalar. By considering fixed angular momentum he applies the results to potential scattering for V radial, $V(|x|) = O(|x|^{-4-\varepsilon})$ as $|x| \to \infty$. These results are here obtained as a special case of the theorems in Sect. 6. A presentation of Martin's results is given [1], together with some further discussion of time-delay, and the condition on the potential is improved in [9].

Lavine [18] has found a different expression for the limit (1.3). Narnhofer has proposed a different definition of time-delay, [23]. We have omitted discussion of these subjects to keep the paper reasonably short. For more recent results in the physics literature, see [5]. In classical scattering theory time-delay has been discussed by Lax-Phillips [19]. See also Amrein and Wollenberg [2] for an approach closer to the problems (1.2)–(1.5).

Note that [23] contains geometrical considerations showing that a spherically symmetric choice for P_r is natural.

2. Notation and Preliminary Results

This section contains the notation used and some preliminary results on various spaces and operators. Our basic Hilbert space is $\mathscr{H} = L^2(\mathbb{R}^n)$. The norm and inner product are denoted $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$, respectively. The weighted L^2 -space is given by

$$L_s^2(\mathbb{R}^n) = \{ f \in L_{\text{loc}}^2(\mathbb{R}^n) | \| f \|_s = \| (1+x^2)^{s/2} f \|_{L^2} < \infty \}.$$

Let $\mathscr{G}(\mathbb{R}^n)$ denote the Schwartz space of rapidly decreasing functions, and $\mathscr{G}'(\mathbb{R}^n)$ the tempered distributions. For any $m, s \in \mathbb{R}$ the weighted Sobolev space is given by

$$H^{m,s}(\mathbb{R}^n) = \{ f \in \mathscr{S}'(\mathbb{R}^n) | \| f \|_{m,s} = \| (1+x^2)^{s/2} (1-\Delta)^{m/2} f \|_{L^2} < \infty \}.$$

An equivalent norm is given by

$$||f||'_{m,s} = ||(1-\Delta)^{m/2}(1+x^2)^{s/2}f||_{L^2}.$$

Note that $H^{0,s}(\mathbb{R}^n) = L^2_s(\mathbb{R}^n)$ and $H^{0,0}(\mathbb{R}^n) = L^2(\mathbb{R}^n)$. The inner product on $L^2(\mathbb{R}^n)$ induces a natural duality between $H^{m,s}(\mathbb{R}^n)$ and $H^{-m,-s}(\mathbb{R}^n)$ for any $m, s \in \mathbb{R}$. It is denoted $\langle \cdot, \cdot \rangle$.

The Fourier transform \mathcal{F} is given by

$$(\mathscr{F}f)(\xi) = (2\pi)^{-n/2} \int f(x) e^{-ix \cdot \xi} dx.$$

$$(2.1)$$

 \mathscr{F} is bounded from $H^{m,s}(\mathbb{R}^n)$ to $H^{s,m}(\mathbb{R}^n)$ for any $s, m \in \mathbb{R}$.

Let $H_0 = -\Delta$. H_0 is an unbounded selfadjoint operator in $L^2(\mathbb{R}^n)$ with domain $\mathscr{D}(H_0) = H^{2,0}(\mathbb{R}^n)$, but we will also consider H_0 as a bounded operator from $H^{m,s}(\mathbb{R}^n)$ to $H^{m-2,s}(\mathbb{R}^n)$.

In the present paper the dilation group, $U(\theta)$, and its generator, D, play important roles. Let $f \in \mathcal{H} = L^2(\mathbb{R}^n)$ and $\theta \in \mathbb{R}$. Then

$$(U(\theta)f)(x) = e^{\frac{\theta}{2}n} f(e^{\theta}x), \qquad (2.2)$$

and $U(\theta) = e^{i\theta D}$, where

$$D = \frac{1}{2i} (x \cdot \nabla + \nabla \cdot x).$$
(2.3)

D is essentially selfadjoint on $\mathscr{S}(\mathbb{R}^n)$. *D* is considered both as an unbounded selfadjoint operator on \mathscr{H} , and as a bounded operator from $H^{m,s}(\mathbb{R}^n)$ to $H^{m-1,s-1}(\mathbb{R}^n)$. Note also that the condition

$$\|(D^2+1)^{3/2}f\| < \infty$$

is equivalent to the conditions

$$||D^{j}f|| < \infty$$
 for $j = 0, 1, 2, 3$.

Let $\phi \in C_0^{\infty}((0, \infty))$ and define $\phi(H_0)$ using the functional calculus. Using the Fourier transform it is easy to see that $\phi(H_0)$ is bounded from $H^{m,s}(\mathbb{R}^n)$ to $H^{m,s}(\mathbb{R}^n)$ for any $m, s \in \mathbb{R}$.

The quantum mechanical operators can be considered in various representations. We use configuration space, momentum space, and the spectral representation spaces for H_0 and D. These spaces are related by unitary operators. To simplify notation, let $\mathcal{P} = L^2(S^{n-1})$, S^{n-1} the unit sphere in \mathbb{R}^n . The spaces are defined as follows.

 $\mathscr{H}_{c} = L^{2}(\mathbb{R}^{n})$, configuration space.

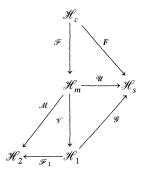
 $\mathcal{H}_m = L^2(\mathbb{R}^n)$, momentum space.

 $\mathscr{H}_s = L^2(0, \infty; \mathscr{P})$, spectral representation space for H_0 .

 $\mathscr{H}_1 = L^2(\mathbb{R}; \mathscr{P})$, auxiliary space.

 $\mathscr{H}_2 = L^2(\mathbb{R}; \mathscr{P})$, spectral representation space for *D*.

The unitary maps between these spaces are given in the following diagram.



The operators are defined below. It is straightforward to check that the operators are unitary, and that the diagram commutes. We omit the details.

$$\begin{aligned} \mathcal{F}: & \mathscr{H}_c \to \mathscr{H}_m \text{ is the Fourier transform as defined in (2.1).} \\ \mathscr{U}: & \mathscr{H}_m \to \mathscr{H}_s \text{ is given by } (\mathscr{U}f)(\lambda, \omega) = 2^{-1/2} \lambda^{(n-2)/4} f(\lambda^{1/2} \omega) \\ & \text{with} \end{aligned}$$

$$(\mathscr{U}^{-1}g)(\xi) = (\mathscr{U}^{-1}g)(|\xi|\omega) = 2^{1/2}|\xi|^{-\frac{n-2}{2}}g(|\xi|^2,\omega)$$

- $F = \mathcal{UF} : \mathscr{H}_c \to \mathscr{H}_s$ gives the spectral representation for H_0 , viz. FH_0F^{-1} is multiplication by λ in \mathscr{H}
- \mathcal{M} : $\mathscr{H}_m \to \mathscr{H}_2$ is the Mellin transform. It is conveniently described by $\mathcal{M} = \mathcal{F}, \mathcal{N}$

$$\mathcal{V}: \qquad \mathcal{H}_m \to \mathcal{\hat{H}}_1 \text{ is given by } (\mathcal{V}f)(\tau, \omega) = e^{\overline{2}^{\tau}} f(e^{\tau} \omega)$$
with

$$(\mathscr{V}^{-1}h)(\xi) = (\mathscr{V}^{-1}h)(|\xi|\omega) = |\xi|^{-\frac{n}{2}}h(\ln|\xi|,\omega).$$

 $\mathscr{H}_1 \rightarrow \mathscr{H}_2$ is the one-dimensional Fourier transform of vector-valued \mathcal{F}_1 : functions:

$$(\mathscr{F}_1 f)(\sigma) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\tau) e^{-i\sigma\tau} d\tau.$$

[As in (2.1) the integral is convergent in the mean for $f \in \mathcal{H}_1$.] $\mathscr{H}_1 \to \mathscr{H}_s$ is given by $\mathscr{G} = \mathscr{U} \mathscr{V}^{-1}$. Explicitly we have

$$(\mathscr{G}g)(\lambda,\omega) = 2^{-1/2}\lambda^{-1/2}g(\frac{1}{2}\ln\lambda,\omega)$$
$$(\mathscr{G}^{-1}f)(\tau,\omega) = 2^{1/2}e^{\tau}g(e^{2\tau},\omega).$$

 \mathcal{G} :

As usual, the same letter is used to denote a quantum mechanical observable in various representations. Hence $H_0 = -\Delta$ in $\hat{\mathscr{H}_c}, H_0 =$ multiplication by ξ^2 in \mathscr{H}_m , and H_0 = multiplication by λ in \mathcal{H}_s .

Note also that in
$$\mathscr{H}_c D = \frac{1}{2i}(x \cdot \nabla + \nabla \cdot x)$$
, in $\mathscr{H}_m D = -\frac{1}{2i}(\xi \cdot \nabla + \nabla \cdot \xi)$, in \mathscr{H}_2

D = multiplication by $-\sigma$, and in $\mathscr{H}_s D = -\frac{1}{i} \left(\lambda \frac{d}{d\lambda} + \frac{d}{d\lambda} \lambda \right)$. We have chosen the above signs to obtain consistency with [24].

Let $P_+(P_-)$ be the spectral projection for *D* corresponding to $[0, \infty)((-\infty, 0])$. We have $P_+ + P_- = 1$. Due to the choice of signs P_+ is given by multiplication by the characteristic function for $(-\infty, 0]$ in \mathscr{H}_2 .

Using the operators summarized in the diagram above we can find P_{-} as an explicit convolution operator in \mathscr{H}_s . We state the result, but omit the computation. Let vp denote the Cauchy principal value. Then $P_{-} - \frac{1}{2}I$ is represented in \mathscr{H}_{s} by

$$-\frac{1}{2\pi i} \frac{1}{\lambda^{1/2} \mu^{1/2}} v p\left(\frac{1}{\ln \lambda - \ln \mu}\right).$$
(2.4)

Boundedness of this operator can be seen directly using results on the Hilbert transform, see e.g. [28].

Let $\chi_r(D)$ denote the spectral projection for D corresponding to [-r, r]. In $\mathscr{H}_s \chi_r(D)$ is given by the kernel

$$\kappa_{r}(\lambda,\mu) = \frac{1}{4\pi} \frac{1}{\lambda^{1/2} \mu^{1/2}} \frac{\sin\left(\frac{r}{2}(\ln\lambda - \ln\mu)\right)}{\ln\lambda - \ln\mu}.$$
(2.5)

For two Hilbert spaces \mathscr{H} and \mathscr{H} we let $B(\mathscr{H}, \mathscr{H})$ denote the bounded operators from \mathscr{H} to \mathscr{H} . As usual we write $B(\mathscr{H}) = B(\mathscr{H}, \mathscr{H})$.

In many cases we write L^2 instead of $L^2(\mathbb{R}^n)$, $H^{m,s}$ instead of $H^{m,s}(\mathbb{R}^n)$, etc. $C^k(\mathbb{R}^n)$ denotes continuously differentiable functions on \mathbb{R}^n , etc.

3. The Eisenbud-Wigner Time-Delay Operator

Let $H_0 = -\Delta$ and $H = H_0 + V$ in $\mathscr{H}_c = L^2(\mathbb{R}^n)$, where V is a short range potential. The wave operators

$$W_{\pm} = \underset{t \to \pm \infty}{s-\lim} e^{itH} e^{-itH_0}$$

exist and are complete. Hence we have a unitary scattering operator $S = W_+^* W_-$. In $\mathscr{H}_s S$ has a decomposition $S = \{S(\lambda)\}$; $S(\lambda)$ is the scattering matrix. The Eisenbud-Wigner time-delay operator is formally given by

$$T = \left\{ -iS(\lambda)^* \frac{d}{d\lambda} S(\lambda) \right\}.$$
(3.1)

In this section we give conditions on V that ensure the differentiability of $\lambda \mapsto S(\lambda)$ in operator norm on $B(\mathscr{P})$. These results imply for a large class of potentials the existence of T as a selfadjoint operator commuting with H_0 . For two classes of potentials the differentiability of $S(\lambda)$ is well known. If V is short range and dilation-analytic, $S(\lambda)$ is analytic, see [4]. If V is exponentially decaying, $S(\lambda)$ is analytic, see for instance [3].

We consider the following classes of potentials. For simplicity we consider only multiplicative V. Theorem 3.5 can easily be extended to a class of nonlocal V.

Assumption 3.1. a) *V* is multiplication by a realvalued function such that V defines a compact operator from $H^{1,0}(\mathbb{R}^n)$ to $H^{-1,\beta}(\mathbb{R}^n)$ for some $\beta > 1$.

b) V is multiplication by a realvalued function such that V defines a compact operator from $H^{2,0}(\mathbb{R}^n)$ to $H^{0,\beta}(\mathbb{R}^n)$ for some $\beta > 1$.

Obviously b) implies a). In case a) $V: H^{1,s}(\mathbb{R}^n) \to H^{-1,\beta+s}(\mathbb{R}^n)$ is compact, and in case b) $V: H^{2,s}(\mathbb{R}^n) \to H^{0,\beta+s}(\mathbb{R}^n)$ is compact, for any $s \in \mathbb{R}$, because V commutes with multiplication by $(1+x^2)^{s/2}$. In case a) $H = H_0 + V$ is the quadratic form sum, and in case b) $H = H_0 + V$ is the operator sum.

Assumption 3.2. Let V be a realvalued function. Assume that for some $s > \frac{1}{2}$ and integer $k \ge 0$ the map

$$\theta \mapsto U(\theta) V U(-\theta), \mathbb{R} \to B(L^2_{-s}, L^2_s)$$

is k times continuously differentiable. Here $U(\theta)$ is the dilation-group, see (2.2).

The following condition is sufficient for V to satisfy Assumption 3.2. Let $V \in C^k(\mathbb{R}^n)$ and assume there exist $\delta > 0$, c > 0 such that

$$|(x \cdot \nabla)^{\ell} V(x)| \le c(1+|x|)^{-1-\delta}$$
(3.2)

for all $x \in \mathbb{R}^n$ and ℓ , $0 \le \ell \le k$. If V satisfies (3.2) it is well known that H has no positive eigenvalues, see [26].

The following results are derived using the explicit representation for the scattering matrix given in [16]. Let us briefly describe it. Let $\gamma(\mu)$ be the trace operator defined for $f \in C_0^{\infty}(\mathbb{R}^n)$ by $(\gamma(\mu)f)(\omega) = f(\mu\omega), \mu > 0, \omega \in S^{n-1}$. $\gamma(\mu)$ extends to a bounded operator $\gamma(\mu) \in B(H^{s,m}(\mathbb{R}^n), L^2(S^{n-1}))$ for any $s > \frac{1}{2}, m \in \mathbb{R}$.

Lemma 3.3. Let $m \in \mathbb{R}$, $s > k + \frac{1}{2}$, $k \ge 0$ an integer. Then $\mu \mapsto \gamma(\mu)$ is k times continuously differentiable in norm on $B(H^{s,m}(\mathbb{R}^n), L^2(S^{n-1}))$.

Proof. Consider first k = 1 and m = 0. Let $T: \mu \mapsto \gamma(\mu), T: (0, \infty) \rightarrow B(H^{s,m}, L^2(S^{n-1}))$. The obvious guess for the derivative is $DT(\mu) = \gamma(\mu) \frac{\partial}{\partial r}, \frac{\partial}{\partial r} = \frac{1}{|x|} x \cdot \nabla$. Let $f \in C_0^{\infty}(\mathbb{R}^n)$.

We then have

$$\left(\left(\frac{1}{h}(T(\mu+h)-T(\mu))-DT(\mu)\right)f\right)(\omega)=\frac{1}{h}\int_{0}^{h}\left(\frac{\partial f}{\partial r}((\mu+\xi)\omega)-\frac{\partial f}{\partial r}(\mu\omega)\right)d\xi.$$

Hence

$$\begin{split} \left\| \left(\frac{1}{h} (T(\mu+h) - T(\mu)) - DT(\mu) \right) f \right\|_{L^{2}(S^{n-1})} \\ & \leq \frac{1}{h} \int_{0}^{h} \left\| \frac{\partial f}{\partial r} ((\mu+\xi) \cdot) - \frac{\partial f}{\partial r} (\mu \cdot) \right\|_{L^{2}(S^{n-1})} d\xi \\ & \leq \left\| \frac{\partial f}{\partial r} \right\|_{H^{s-1}(\mathbb{R}^{n})} \cdot \frac{1}{h} \int_{0}^{h} \left\| \gamma(\mu+\xi) - \gamma(\mu) \right\|_{B(H^{s-1}(\mathbb{R}^{n}), L^{2}(S^{n-1}))} d\xi \\ & \leq c \left\| f \right\|_{H^{s}(\mathbb{R}^{n})} \cdot \frac{1}{h} \int_{0}^{h} |\xi|^{\delta} d\xi \leq c \left\| f \right\|_{H^{s}(\mathbb{R}^{n})} |h|^{\delta}. \end{split}$$

In the last step we used the Hölder continuity of $\gamma(\mu)$, see [16]. Since $DT(\mu) = \gamma(\mu) \frac{\partial}{\partial r}$ is continuous in operator norm, the result is proved for k = 1, m = 0. Using the expression for $DT(\mu)$ the result for any k follows easily. For $m \neq 0$ we note that boundedness of $\gamma(\mu): H^{s,m} \to L^2(S^{n-1})$ is equivalent to boundedness of

$$\gamma(\mu)(1+x^2)^{-m/2}: H^{s,0} \to L^2(S^{n-1}).$$

Obviously $\gamma(\mu)(1+x^2)^{-m/2} = (1+\mu^2)^{-m/2}\gamma(\mu)$, and the result for $m \neq 0$ follows from this result.

Let $R(\zeta) = (H - \zeta)^{-1}$ be the resolvent. The boundary values

$$R(\lambda \pm i0) = \lim_{\varepsilon \perp 0} R(\lambda \pm i\varepsilon), \ \lambda > 0, \ \lambda \notin \sigma_p(H)$$

exist in $B(H^{-1,s}, H^{1,-s'})$ for $s, s' > \frac{1}{2}$. Here $\sigma_p(H)$ denotes the point spectrum of H.

The scattering matrix is given by

$$S(\lambda) = 1 - \pi i \lambda^{n/2 - 1} \gamma(\lambda^{1/2}) \mathscr{F}(V - VR(\lambda + i0) V) \mathscr{F}^* \gamma(\lambda^{1/2})^*$$
(3.3)

for $\lambda \in (0, \infty) \setminus \sigma_p(H)$, see [16].

Lemma 3.4. Let $k \ge 0$ be an integer. Let V satisfy Assumption 3.1 a) with $\beta > k+1$. Let $s, s' > k + \frac{1}{2}$. Then $\lambda \mapsto R(\lambda + i0)$ is k times continuously differentiable as a map from $(0, \infty) \setminus \sigma_p(H)$ to $B(H^{-1,s}, H^{1,-s'})$.

Proof. The result is proved using the technique in [13]. Since we do not require decay estimates in λ , we can allow local singularities in *V*. Details are omitted. See also [22] for similar results. \Box

Theorem 3.5. Let V satisfy Assumption 3.1 a) with $\beta > k+1$, $k \ge 0$ an integer. Then $S(\lambda)$ is k times continuously differentiable in λ , $\lambda \in (0, \infty) \setminus \sigma_p(H)$, with values in $B(\mathscr{P})$.

Proof. Using (3.3) and Lemmas 3.3, 3.4 we see that all operators in the expression for $S(\lambda)$ are k times continuously differentiable, provided we can verify the conditions on s, s' in Lemmas 3.3 and 3.4. Omitting constants and the factor $\lambda^{n/2-1}$ we have typical terms

$$\left(\left(\frac{d}{d\lambda}\right)^{\ell_1}(\gamma(\lambda^{1/2})\mathscr{F})\right)V\left(\frac{d}{d\lambda}\right)^{\ell_3}(\mathscr{F}^*\gamma(\lambda^{1/2})^*)$$

and

$$\left(\left(\frac{d}{d\lambda}\right)^{\ell_1}(\gamma(\lambda^{1/2})\mathscr{F})\right)V\left(\left(\frac{d}{d\lambda}\right)^{\ell_2}R(\lambda+i0)\right)V\left(\frac{d}{d\lambda}\right)^{\ell_3}(\mathscr{F}^*\gamma(\lambda^{1/2})^*)$$

 ℓ_1, ℓ_2, ℓ_3 non-negative integers satisfying $\ell_1 + \ell_2 + \ell_3 \leq k$. We now determine the condition under which these expressions make sense.

$$\begin{split} \left(\frac{d}{d\lambda}\right)^{\ell_3} \mathscr{F}^* \gamma(\lambda^{1/2})^* &\in B(\mathscr{P}, H^{1, -s}) \quad \text{for} \quad s > \ell_3 + \frac{1}{2}, \\ V &\in B(H^{1, -s}, H^{-1, \beta - s}), \\ \left(\frac{d}{d\lambda}\right)^{\ell_1} \gamma(\lambda^{1/2}) \mathscr{F} &\in B(H^{-1, \beta - s}, \mathscr{P}) \quad \text{for} \quad \beta - s > \ell_1 + \frac{1}{2}. \end{split}$$

Hence β must satisfy $\beta > \ell_1 + \ell_3 + 1$.

For the second term we have

$$\begin{split} \left(\frac{d}{d\lambda}\right)^{\ell_3} \mathscr{F}^* \gamma(\lambda^{1/2})^* &\in B(\mathscr{P}, H^{1, -s}) \quad \text{for} \quad s > \ell_3 + \frac{1}{2}, \\ V &\in B(H^{1, -s}, H^{-1, \beta - s}), \\ \left(\frac{d}{d\lambda}\right)^{\ell_2} R(\lambda + i0) &\in B(H^{-1, \beta - s}, H^{1, -s'}) \quad \text{for} \quad \beta > \ell_2 + 1, \\ & \text{and} \ \beta - s > \ell_2 + \frac{1}{2}, \ s' > \ell_2 + \frac{1}{2}. \\ V &\in B(H^{1, -s'}, H^{-1, \beta - s'}), \\ \left(\frac{d}{d\lambda}\right)^{\ell_1} \gamma(\lambda^{1/2}) \mathscr{F} &\in B(H^{-1, \beta - s'}, \mathscr{P}) \quad \text{for} \quad \beta - s' > \ell_1 + \frac{1}{2}. \end{split}$$

Hence β must satisfy

 $\beta > \ell_2 + \ell_3 + 1, \beta > \ell_2 + 1, \beta > \ell_1 + \ell_2 + 1.$

As $\ell_1 + \ell_2 + \ell_3 \leq k$, we must have $\beta > k + 1$. On the other hand, given $\beta > k + 1$, we can find *s*, *s'*, such that the terms exist as continuous functions of λ with values in $B(\mathcal{P})$. \Box

To prove the next result we use the dilation-group to relate a change in the energy to a change in the potential. This is a well known technique in scattering theory, see e.g. [12, Lemma 3.3] and for a recent application [6].

 $U(\theta)$ is given in (2.2). Define

$$V(\theta) = e^{-2\theta} U(-\theta) V U(\theta).$$

Let $S(\lambda; V)$ denote the scattering matrix for $H = H_0 + V$. Then

$$S(e^{2\theta}\lambda; V) = S(\lambda; V(\theta)).$$
(3.4)

This result can be proved using (3.3). It is interesting to note that (3.4) can be proved without using (3.3), see [6].

Theorem 3.6. Let V satisfy Assumption 3.2 for some $k \ge 0$. Then $S(\lambda)$ is k times continuously differentiable in $\lambda \in (0, \infty) \setminus \sigma_n(H)$.

Proof. Assumption 3.2 implies that $\theta \mapsto V(\theta)$ is differentiable k times from \mathbb{R} to $B(H^{1,-s}, H^{-1,s}), s > \frac{1}{2}$. Using (3.3) and (3.4) this gives the result. Notice that by taking θ small enough we can avoid possible eigenvalues for H. \Box

Theorem 3.7. Let V satisfy Assumption 3.1 a) for $\beta > 2$ or Assumption 3.2 for k = 1. Let T be defined by

$$\mathcal{D}(T) = \{ f \in \mathcal{H}_c | E_0([a, b]) f = f \quad \text{for some } a, b, [a, b] \subset (0, \infty) \setminus \sigma_p(H) \}$$
$$Tf = \left\{ -iS(\lambda)^* \frac{d}{d\lambda} S(\lambda) \right\} f \quad \text{for } f \in \mathcal{D}(T).$$

T is essentially selfadjoint on $\mathcal{D}(T)$, $\mathcal{D}(T) \subset \mathcal{D}(H_0)$, and T commutes with H_0 . E_0 denotes the spectral family for H_0 .

Proof. $S(\lambda)$ is differentiable by Theorems 3.5 or 3.6. $S(\lambda)^*S(\lambda) = 1$ implies

$$S(\lambda)^* \frac{d}{d\lambda} S(\lambda) + \left(\frac{d}{d\lambda} S(\lambda)\right)^* S(\lambda) = 0,$$

and hence for each $\lambda \in (0, \infty) \setminus \sigma_p(H)$, $-iS(\lambda)^* \frac{d}{d\lambda} S(\lambda)$ is a bounded selfadjoint operator in $B(\mathscr{P})$. Thus T is densely defined, symmetric, and for each $[a,b] \subset (0,\infty) \setminus \sigma_p(H)$, $TE_0([a,b])$ is a bounded selfadjoint operator. This implies the essential selfadjointness of T. Obviously T commutes with H_0 . \Box

T is called the Eisenbud-Wigner time-delay operator.

We have the following representation for TH_0 , which has a simple interpretation, see [23].

A. Jensen

Theorem 3.8.

$$H_0 T = -\frac{1}{2} S^* [D, S].$$
(3.5)

on the domain $\mathcal{D} = \{f \in \mathcal{H}_c | Ff \in C_0^1(0, \infty; \mathcal{P})\}$. (See Sect. 2 for the definition of F.)

Proof. We have
$$-\frac{1}{2}D = \left\{-i\lambda \frac{d}{d\lambda} - \frac{1}{2}i\right\}$$
, see Sect. 2. Let $g \in C_0^1(0, \infty; \mathscr{P})$. Then

$$\{(H_0 Tg)(\lambda)\} = \left\{-i\lambda S^*(\lambda)\frac{dS(\lambda)}{d\lambda}g(\lambda)\right\} = \left\{S^*(\lambda)\left[-i\lambda\frac{d}{d\lambda}-i\frac{1}{2},S(\lambda)\right]g(\lambda)\right\},$$

which proves (3.5).

4. Some Results Related to D

In this section we give various results on D to be used in the following sections. We refer to Sect. 2 for the definitions.

We have on $\mathscr{S}(\mathbb{R}^n)$ (in configuration space)

$$U(\theta)H_0U(-\theta)=e^{-2\theta}H_0,$$

which implies by differentiation on $\mathscr{S}(\mathbb{R}^n)$

$$i[H_0, D] = 2H_0$$

We also have

$$U(\theta)e^{-itH_0}U(-\theta) = \exp(-ite^{-2\theta}H_0).$$
(4.1)

Note that $U(\theta)$ and e^{-itH_0} map $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$.

Lemma 4.1. On $\mathscr{S}(\mathbb{R}^n)$ we have for k = 1, 2, 3

$$t^{k}H_{0}^{k}e^{-itH_{0}} = \sum_{j,j'=0}^{k} C_{jj'}^{k}D^{j}e^{-itH_{0}}D^{j'}, \qquad (4.2)$$

where $C_{ii'}^k$ are complex constants.

Proof. Let $f \in \mathscr{G}(\mathbb{R}^n)$. Differentiation of (4.1) with respect to θ gives

$$e^{i\theta D}i[D, e^{-itH_0}]e^{-i\theta D}f = 2itH_0e^{-2\theta}\exp(-ite^{-2\theta}H_0)f.$$
 (4.3)

Setting $\theta = 0$ in (4.3) gives (4.2) for k = 1. Differentiate (4.3) to obtain

$$e^{i\theta D}[D, [D, e^{-itH_0}]]e^{-i\theta D}f$$

= 4itH_0e^{-2\theta} exp(-ite^{-2\theta}H_0)f
+ 4t^2H_0^2e^{-4\theta} exp(-ite^{-2\theta}H_0)f.

Using (4.3) we obtain

$$-4t^2H_0^2e^{-4\theta}\exp(-ite^{-2\theta}H_0)f$$

= $-e^{i\theta D}[D, [D, e^{-itH_0}]]e^{-i\theta D}f + 2e^{i\theta D}i[D, e^{-itH_0}]e^{-i\theta D}f.$

444

Set $\theta = 0$ to obtain (4.2) for k = 2. The result for k = 3 is obtained by further differentiation. We omit the details. \Box

Remark 4.2. (4.2) is valid for any k. This can be seen from the proof using induction.

Lemma 4.3. Let $0 \leq \mu \leq 3$. We then have

$$|(1+x^2)^{-\mu/2}(H_0+1)^{-9/2}H_0^3e^{-itH_0}(1+D^2)^{-\mu/2}|| \leq c_{\mu}|t|^{-\mu}$$

for all $t \neq 0$. We also have

$$\|(1+D^2)^{-\mu/2}(1+H_0)^{-3}H_0^3e^{-itH_0}(1+D^2)^{-\mu/2}\| \leq c_{\mu}|t|^{-\mu}$$
(4.4)

for all $t \neq 0$. The norms are operator norm in $B(L^2)$.

Proof. The closure of $(1 + x^2)^{-3/2}(1 + H_0)^{-3/2}D^j$ [defined on $\mathscr{S}(\mathbb{R}^n)$] is a bounded operator, j = 0, 1, 2, 3. Let $f \in \mathscr{S}(\mathbb{R}^n)$. Lemma 4.1 implies

$$|t|^3 \|(1+x^2)^{-3/2}(1+H_0)^{-9/2}H_0^3 e^{-itH_0}f\| \leq C \|(1+D^2)^{3/2}f\|.$$

The first result now follows from this estimate and complex interpolation.

To prove the second result note that $i[H_0, D] = 2H_0$ implies

$$D(1+H_0)^{-1} = (1+H_0)^{-1} D - 2iH_0(1+H_0)^{-2}$$

Repeated application of this commutation-result leads to the result

$$t^{3}(1+H_{0})^{-3}H_{0}^{3}e^{-itH_{0}} = \sum_{j,j'=0}^{3} \tilde{C}_{jj'}^{3}D^{j}\psi(H_{0})e^{-itH_{0}}D^{j'},$$

where $\psi(H_0)$ is a bounded operator. The second result of the lemma is now proved using complex interpolation. \Box

We use the following result due to Mourre [21]. Let $\chi_+(t)(\chi_-(t))$ be the characteristic function for $[0, \infty)((-\infty, 0])$.

Lemma 4.4. Let $\phi \in C_0^{\infty}((0, \infty))$ and $0 \leq \mu' < \mu$. Then there exists a constant $c = c(\phi, \mu, \mu')$ such that for $t \in \mathbb{R}$

$$\|\chi_{\pm}(t)(D^{2}+1)^{-\mu/2}e^{-itH_{0}}\phi(H_{0})P_{\pm}\| \leq c(1+|t|)^{-\mu'}, \qquad (4.5)$$

where the norm is operator norm in $B(L^2)$.

Proof. See [21, Lemma 1].

Lemma 4.5. Let $f \in \mathscr{H}_c = L^2(\mathbb{R}^n)$ and $1 \leq q < \infty$. Assume for some $\phi \in C_0^{\infty}((0, \infty))\phi(H_0)f = f$, and for some $\mu > 1/q ||(D^2 + 1)^{\mu/2}f|| < \infty$. Then we have

$$\int_{0}^{\infty} \|P_{-}e^{-itH_{0}}f\|^{q}dt < \infty$$
(4.6)

and

$$\int_{-\infty}^{0} \|P_{+}e^{-itH_{0}}f\|^{q} dt < \infty.$$
(4.7)

Proof. We prove (4.6). The proof of (4.7) is similar. Taking adjoints we obtain from (4.5) the following estimate. Let $\frac{1}{a} < \mu' < \mu$. For t > 0 we have

$$\begin{split} \|P_{-}e^{-itH_{0}}f\| \\ &\leq \|P_{-}e^{-itH_{0}}\phi(H_{0})(D^{2}+1)^{-\mu/2}\|\cdot\|(D^{2}+1)^{\mu/2}f\| \\ &\leq c(1+t)^{-\mu'}, \end{split}$$

which implies (4.6).

The following lemma gives a result on the wave operators which could be obtained directly from the usual stationary phase argument for a dense set of f, see e.g. [25]. The following lemma is useful, because it gives a condition on f, which can also be verified for Sf.

Lemma 4.6. Let V satisfy Assumption 3.1 b) for some $\beta > 2$. Let $f \in \mathscr{H}_c$ satisfy $\phi(H_0)f = f$ for some $\phi \in C_0^{\infty}((0, \infty))$, and $\|(D^2 + 1)^{\mu/2}f\| < \infty$ for some $\mu > 2$. We then have

$$\int_{0}^{\infty} \|(W_{+} - 1)e^{-itH_{0}}f\|\,dt < \infty$$
(4.8)

and

$$\int_{-\infty}^{0} \|(W_{-}-1)e^{-itH_{0}}f\|\,dt < \infty \,.$$
(4.9)

Proof. Consider first (4.8). We have for $f \in \mathcal{D}(H) = \mathcal{D}(H_0)$

$$(W_+-1)f=i\int_0^\infty e^{isH}Ve^{-isH_0}fds,$$

where the integral is strongly convergent, and for any $t \in \mathbb{R}$

$$(W_{+}-1)e^{-itH_{0}}f = ie^{-itH}\int_{t}^{\infty}e^{isH}Ve^{-isH_{0}}fds.$$

Hence to prove (4.8) it suffices to prove

$$\int_{0}^{\infty} \int_{t}^{\infty} \|Ve^{-isH_0}f\| \, ds \, dt < \infty$$

for f satisfying the assumptions of the lemma. (Such f's are obviously in the domain of H_0 .) The result follows if we prove

$$||Ve^{-isH_0}f|| \leq cs^{-\mu}, \quad s > 0$$

for some $\mu > 2$.

Let f satisfy $\phi(H_0)f = f$ for some $\phi \in C_0^{\infty}((0, \infty))$ and $||(1+D^2)^{\mu/2}f|| < \infty$. We can assume $2 < \mu \leq \beta$. Let $\tilde{\phi}(\lambda) = \phi(\lambda)(1+\lambda)^{11/2}\lambda^{-3}$, and define $g = \tilde{\phi}(H_0)f$.

Then $f = (1 + H_0)^{-11/2} H_0^3 g$. We have $||(1 + D^2)^{\mu/2} g|| < \infty$ since $||(1 + D^2)^{\mu/2} \tilde{\phi}(H_0) (1 + D^2)^{-\mu/2} ||_{B(L^2)} < \infty$, see [31] for a proof.

$$\begin{split} \| Ve^{-isH_0} f \| &= \| Ve^{-isH_0} (1+H_0)^{-11/2} H_0^3 g \| \\ &\leq \| V(1+H_0)^{-1} (1+x^2)^{\mu/2} \| \\ &\cdot \| (1+x^2)^{-\mu/2} (1+H_0)^{-9/2} H_0^3 e^{-isH_0} (1+D^2)^{-\mu/2} \| \\ &\cdot \| (1+D^2)^{\mu/2} g \| \leq c |s|^{-\mu} \,. \end{split}$$

We used Lemma 4.3 and the result that $V(1+H_0)^{-1}(1+x^2)^{\mu/2}$ is bounded on L^2 by assumption and $\mu \leq \beta$. Thus we have proved (4.8).

(4.9) is proved using

$$(W_{-}-1)e^{-itH_{0}}f = -ie^{-itH}\int_{-\infty}^{t}e^{isH}Ve^{-isH_{0}}fds,$$

and the estimate given above. \Box

Remark 4.7. (4.8) and (4.9) are valid for any $f \in \mathcal{D}(H_0)$ satisfying for some $\varepsilon > 0$

$$||Ve^{-isH_0}f|| = O(|s|^{-2-\varepsilon})$$

as $|s| \to \infty$. Such an estimate can be proved in the following manner. Let f satisfy $\phi(H_0)f = f$ for some $\phi \in C_0^{\infty}(0, \infty)$. Let $\delta = \frac{1}{2} \operatorname{dist}(0, \operatorname{supp} \phi)$. $F(|x| \ge \delta |s|)$ is multiplication by the characteristic function for $\{x | |x| \ge \delta |s|\}$ in \mathscr{H}_c

$$||Ve^{-isH_0}f|| \le ||V(H_0+1)^{-1}F(|x| \ge \delta|s|)|| \cdot ||(H_0+1)f|| + ||V(H_0+1)^{-1}|| \cdot ||F(|x| < \delta|s|)e^{-isH_0}(H_0+1)f||.$$

The first term is $O(|s|^{-\beta})$ by Assumption 3.1 b). We can obtain estimates

$$||F(|x| < \delta |s|)e^{-isH_0}(H_0 + 1)f|| = O(|s|^{-2-\varepsilon})$$

using stationary phase arguments, see e.g. [8, 25]. The conditions on f have a form that makes it very hard to verify them for Sf. Hence we prefer to give the above arguments.

5. Time-Delay and the Subspace of Incoming (Outgoing) States

In this section we establish a connection between the time-delay operator and the projection P_{-} onto the subspace of incoming states. P_{-} (and P_{+} , the projection onto outgoing states) was introduced by Mourre [21]. Roughly, our result states that the time-delay equals the difference of the times $f(t) = e^{-itH_0}f$ and $(Sf)(t) = e^{-itH_0}Sf$ spend in the incoming subspace. A similar result is true for P_{+} , with the obvious reversal of sign.

The result is based on a representation of $S^*[P_-, S]$ in \mathscr{H}_s as an integral operator with an operator-valued kernel $\kappa(\lambda, \mu) \in B(\mathscr{P}), \ \lambda, \mu \in (0, \infty) \setminus \sigma_p(H)$. For $g \in \mathscr{H}_s$ with g having compact support in $(0, \infty)$

$$(S^*[P_-,S]g)(\lambda) = \int_0^\infty \kappa(\lambda,\mu) g(\mu) d\mu.$$

Lemma 5.1. Let V satisfy Assumption 3.1 a) with $\beta > 2$ or Assumption 3.2 with k = 1. Then $S^*[P_-, S]$ is given by the kernel $\kappa(\lambda, \mu)$; $\lambda, \mu \in (0, \infty) \setminus \sigma_p(H)$:

$$\kappa(\lambda,\mu) = \frac{1}{2\pi i} \frac{1}{\lambda^{1/2} \mu^{1/2}} S^*(\lambda) \frac{S(\lambda) - S(\mu)}{\ln \lambda - \ln \mu}, \quad \lambda \neq \mu,$$

$$\kappa(\lambda,\mu) = \frac{1}{2\pi i} S^*(\lambda) \frac{d}{d\lambda} S(\lambda), \quad \lambda = \mu.$$
(5.1)

 $\kappa(\lambda,\mu)$ is continuous in $\lambda,\mu\in(0,\infty)\setminus\sigma_p(H)$.

Proof. Let $g \in \mathscr{H}_s$ have compact support in $(0, \infty) \setminus \sigma_p(H)$. (2.4) implies

$$\begin{split} (S^*[P_-,S]g)(\lambda) &= \lim_{\delta \downarrow 0} \left(\int_0^{\lambda-\delta} + \int_{\lambda+\delta}^{\infty} \right) S^*(\lambda) \frac{-1}{2\pi i} \frac{1}{\lambda^{1/2} \mu^{1/2}} \frac{1}{\ln \lambda - \ln \mu} \\ & \cdot \left(S(\mu)g(\mu) - S(\lambda) \frac{1}{\ln \lambda - \ln \mu} g(\mu) \right) d\mu \\ &= \lim_{\delta \downarrow 0} \left(\int_0^{\lambda-\delta} + \int_{\lambda+\delta}^{\infty} \right) \frac{1}{2\pi i} \frac{1}{\lambda^{1/2} \mu^{1/2}} S^*(\lambda) \frac{S(\lambda) - S(\mu)}{\ln \lambda - \ln \mu} g(\mu) d\mu . \end{split}$$

Theorems 3.5 or 3.6 implies that $S(\lambda)$ is continuously differentiable in operator norm. Hence

$$\frac{1}{\lambda^{1/2}\mu^{1/2}} \frac{S(\lambda) - S(\mu)}{\ln \lambda - \ln \mu} \to \frac{d}{d\lambda} S(\lambda) \quad \text{as} \quad \lambda \to \mu \,.$$

Since g has compact support, the result follows using dominated convergence. \Box

Theorem 5.2. Let V satisfy Assumption 3.1 a) with $\beta > 2$ or Assumption 3.2 with k = 1. Let $f \in \mathscr{H}_c$ satisfy $Ff \in C_0^1((0, \infty) \setminus \sigma_p(H); \mathscr{P})$. Then

$$\langle f, Tf \rangle = \int_{-\infty}^{\infty} (\|P_{-}e^{-itH_{0}}Sf\|^{2} - \|P_{-}e^{-itH_{0}}f\|^{2})dt,$$
 (5.2)

where the integral is absolutely convergent.

Proof. First we show absolute convergence of the integral. Let f satisfy our assumptions. In the spectral representation D is given by $D = \left\{2i\lambda \frac{d}{d\lambda} + i\right\}$, so we have $\|Df\| < \infty$ which is equivalent to $\|(D^2+1)^{1/2}f\| < \infty$. Since $S = \{S(\lambda)\}$ is continuously differentiable (Theorems 3.5 or 3.6), a computation in the spectral representation shows that $\|(D^2+1)^{1/2}Sf\| < \infty$. We can now use Lemma 4.5 with $q=2, \mu=1$ to conclude that the integral over $(0, \infty)$ in (5.2) converges absolutely. For $t \leq 0$ we use the identity

$$\|P_{-}e^{-itH_{0}}Sf\|^{2} - \|P_{-}e^{-itH_{0}}f\|^{2} = \|P_{+}e^{-itH_{0}}f\|^{2} - \|P_{+}e^{-itH_{0}}Sf\|^{2},$$
(5.3)

which follows from the unitarity of *S* and e^{-itH_0} together with $P_+ + P_- = 1$, P_+ and P_- both orthogonal projections. (5.3) and (4.7) show that the integral converges absolutely for $t \leq 0$.

Let $I(\varepsilon)$, $\varepsilon > 0$ be defined by

$$I(\varepsilon) = \int_{-\infty}^{\infty} e^{-\varepsilon |t|} \langle f, e^{itH_0} S^*[P_-, S] e^{-itH_0} f \rangle dt.$$

We have by the first part of the proof

$$\lim_{\varepsilon \downarrow 0} I(\varepsilon) = \int_{-\infty}^{\infty} (\|P_{-}e^{-itH_{0}}Sf\|^{2} - \|P_{-}e^{-itH_{0}}f\|^{2}) dt.$$

The time-integral in $I(\varepsilon)$ can be computed in the spectral representation. Let g = Ff. Using Lemma 5.1 we have

$$I(\varepsilon) = \int_{-\infty}^{\infty} dt \, e^{-\varepsilon |t|} \int_{0}^{\infty} d\lambda \int_{0}^{\infty} d\mu \, e^{it(\lambda-\mu)} \langle g(\lambda), \kappa(\lambda,\mu)g(\mu) \rangle \, dx$$

Since *g* has support in an interval $[a, b] \in (0, \infty) \setminus \sigma_p(H)$, (5.1) implies $\|\kappa(\lambda, \mu)\|_{B(\mathscr{P})} \leq C$ for all $\lambda, \mu \in [a, b]$, and we can interchange the order of integration

$$I(\varepsilon) = \int_{0}^{\infty} d\lambda \int_{0}^{\infty} d\mu \langle g(\lambda), \kappa(\lambda, \mu) g(\mu) \rangle \int_{-\infty}^{\infty} dt \, e^{-\varepsilon |t|} e^{it(\lambda - \mu)}$$
$$= \int_{0}^{\infty} d\lambda \int_{0}^{\infty} d\mu \langle g(\lambda), \kappa(\lambda, \mu) g(\mu) \rangle \frac{2\varepsilon}{\varepsilon^{2} + (\lambda - \mu)^{2}}.$$

For a.e. λ the following integral exists:

$$\psi_{\varepsilon}(\lambda) = \int_{0}^{\infty} d\mu \langle g(\lambda), \kappa(\lambda, \mu) g(\mu) \rangle \frac{2\varepsilon}{\varepsilon^{2} + (\lambda - \mu)^{2}}.$$

 $P_{\varepsilon}(v) = \frac{1}{\pi} \frac{\varepsilon}{\varepsilon^2 + v^2}$ is the Poisson kernel, so we have

$$\psi_{\varepsilon}(\lambda) \rightarrow 2\pi \langle g(\lambda), \kappa(\lambda, \lambda)g(\lambda) \rangle$$
 as $\varepsilon \downarrow 0$

for a.e. λ . The Poisson kernel has the property that this convergence is dominated, see [28, p. 63]. Hence

$$\begin{aligned} |\psi_{\varepsilon}(\lambda)| &\leq c \, \|g(\lambda)\|_{\mathscr{P}} \cdot (P_{\varepsilon}^{*} \|g(\cdot)\|_{\mathscr{P}}) \, (\lambda) \\ &\leq c \, \|g(\lambda)\|_{\mathscr{P}} \cdot h(\lambda) \end{aligned}$$

for some $h \in L^2(0, \infty)$. This gives the result

$$\lim_{\varepsilon \downarrow 0} I(\varepsilon) = \int_{0}^{\infty} 2\pi \langle g(\lambda), \kappa(\lambda, \lambda) g(\lambda) \rangle d\lambda.$$

(5.1) and the definition of T show that we have proved (5.2). \Box

Remark 5.3. (5.3) shows that under the assumptions of the theorem we have

$$\langle f, Tf \rangle = - \int_{-\infty}^{\infty} dt (\|P_+ e^{-itH_0} Sf\|^2 - \|P_+ e^{-itH_0} f\|^2).$$

Remark 5.4. Other choices for projections P_{-} and P_{+} on incoming and outgoing states have been proposed, see [8, 30]. One can prove that (5.2) is true for the projection P_{-} from [30]. The proof is similar to the one given above. We omit the details.

6. Phase-Space Description of Time-Delay

In this section we state and prove the results on the phase-space description of time-delay mentioned in the introduction. Several of our results require finiteness of integrals of the form

$$\int_{-\infty}^{\infty} \|Qe^{-itH_0}f\|^2 dt$$

for a dense set of f. In many cases this can be proved by showing local H_0 -smoothness of Q. See [14, 15, 17, 18, 26] for the definition of smoothness and local smoothness. For the moment we assume finiteness of such integrals for $f \in \mathcal{D}$, \mathcal{D} dense.

Definition 6.1. Let $\{P_r\}$ be a sequence of orthogonal projections such that $s-\lim_{r\to\infty} P_r = 1$. $\{P_r\}$ is said to satisfy condition (E), if there exists a dense set $\mathcal{D} \subset \mathcal{H}_c$ such that for all $f \in \mathcal{D}$ and all r the integrals

$$\int_{-\infty}^{\infty} \|P_r e^{-itH_0} f\|^2 dt$$

and

$$\int_{-\infty}^{\infty} \|P_r e^{-itH} W_- f\|^2 dt$$

are finite.

Theorem 6.2. Let $\{P_r\}$ satisfy condition (E).

(i) Let V satisfy Assumption 3.1 b) with $\beta > 2$. Let $f \in \mathcal{D}$ satisfy $\phi(H_0) f = f$ for some $\phi \in C_0^{\infty}((0, \infty))$ and $||(D^2 + 1)^{\mu/2} f|| < \infty$ for some $\mu > 2$. For any $T_0 \in \mathbb{R}$ we have

$$\lim_{r \to \infty} \int_{-\infty}^{\infty} dt (\|P_r e^{-itH} W_- f\|^2 - \|P_r e^{-itH_0} f\|^2)$$
$$= \lim_{r \to \infty} \int_{T_0}^{\infty} dt (\|P_r e^{-itH} W_- f\|^2 - \|P_r e^{-itH_0} f\|^2),$$
(6.1)

where both limits either exist or are infinite.

(ii) Let V satisfy Assumption 3.1 b) with $\beta > 2$. Let $f \in \mathcal{D}$ satisfy $\phi(H_0) f = f$ for some $\phi \in C_0^{\infty}((0, \infty) \setminus \sigma_p(H))$ and $||(D^2 + 1)^{\mu/2} f|| + ||(D^2 + 1)^{\mu/2} Sf|| < \infty$ for some $\mu > 2$. Assume for each r

$$\int_0^\infty \|P_r e^{-itH_0} Sf\|^2 dt < \infty \,.$$

Then we have

$$\lim_{r \to \infty} \int_{-\infty}^{\infty} dt (\|P_r e^{-itH} W_- f\|^2 - \|P_r e^{-itH_0} f\|^2) = \lim_{r \to \infty} \int_{0}^{\infty} dt (\|P_r e^{-itH_0} Sf\|^2 - \|P_r e^{-itH_0} f\|^2),$$
(6.2)

where both limits either exist or are infinite.

Remark 6.3. (i) A result similar to (6.2) has been proved in [1, Proposition 7.11] in an abstract framework.

(ii) The assumption $||(D^2 + 1)^{\mu/2} Sf|| < \infty$, $\mu > 2$ can be verified under additional assumptions on V and f. Let V satisfy 3.1 b) with $\beta > 4$, and let $||(D^2 + 1)^{3/2} f|| < \infty$. The assumption on f is equivalent to $||D^j f|| < \infty$ for j = 0, 1, 2, 3. Theorem 3.5 now implies $||D^j Sf|| < \infty$, j = 0, 1, 2, 3, cf. the proof of Theorem 5.2. Hence the assumption is verified with $\mu = 3$.

(iii) For any T_1 , T_2 , $-\infty < T_1 < T_2 < \infty$, we have

$$\lim_{r \to \infty} \int_{T_1}^{T_2} dt (\|P_r e^{-itH} W_- f\|^2 - \|P_r e^{-itH_0} f\|^2) = 0$$

and

$$\lim_{r \to \infty} \int_{T_1}^{T_2} dt (\|P_r e^{-itH_0} Sf\|^2 - \|P_r e^{-itH_0} f\|^2) = 0$$

Hence the important contributions to the limits in (6.1), (6.2) come from the behavior of the integrand near $t = +\infty$, as expected.

Proof of (i). It suffices to prove

$$\lim_{r \to \infty} \int_{-\infty}^{0} (\|P_r e^{-itH} W_f\|^2 - \|P_r e^{-itH_0} f\|^2) dt = 0.$$

For each r the integral exists by assumption. Using the intertwining relation we have

$$\int_{-\infty}^{0} (\|P_r e^{-itH} W_{-} f\|^2 - \|P_r e^{-itH_0} f\|^2) dt$$
$$= \int_{-\infty}^{0} \langle e^{-itH_0} f, (W_{-}^* P_r W_{-} - P_r) e^{-itH_0} f \rangle dt.$$

Define

$$g_r(t) = \langle e^{-itH_0}f, (W_-^*P_rW_- - P_r)e^{-itH_0}f \rangle.$$

Clearly $g_r(t) \rightarrow 0$ as $r \rightarrow \infty$ for each t.

$$g_{r}(t) = \langle W_{-}e^{-itH_{0}}f, P_{r}(W_{-}-1)e^{-itH_{0}}f \rangle + \langle (W_{-}-1)e^{-itH_{0}}f, P_{r}e^{-itH_{0}}f \rangle.$$

Hence

$$|g_{\mathbf{r}}(t)| \leq 2 \|f\| \cdot \|(W_{-}-1)e^{-itH_{0}}f\|.$$

Using the assumptions on V and f we have by Lemma 4.6 that the right hand side is integrable over $(-\infty, 0]$. Dominated convergence gives

$$\lim_{r\to\infty}\int_{-\infty}^{0}g_r(t)dt=0.$$

Proof of (ii). Using the first part we see that it suffices to prove

$$\lim_{r\to\infty} \int_{0}^{\infty} dt (\|P_{r}e^{-itH}W_{-}f\|^{2} - \|P_{r}e^{-itH_{0}}Sf\|^{2}) = 0.$$

By assumption the integral exists for each r. We have

$$\int_{0}^{\infty} dt (\|P_{r}e^{-itH}W_{-}f\|^{2} - \|P_{r}e^{-itH_{0}}Sf\|^{2})$$
$$= \int_{0}^{\infty} dt \langle e^{-itH_{0}}f, (W_{-}^{*}P_{r}W_{-} - S^{*}P_{r}S)e^{-itH_{0}}f \rangle.$$

Let

$$h_r(t) = \langle e^{-itH_0} f, (W_-^* P_r W_- - S^* P_r S) e^{-itH_0} f \rangle$$

For each t we clearly have $\lim_{r\to\infty} h_r(t) = 0$. S is unitary and commutes with H_0 , so we have

$$h_r(t) = \langle e^{-itH_0} Sf, (SW_-^*P_rW_- - P_rS)e^{-itH_0}f \rangle.$$

Now use $SW_{-}^{*} = W_{+}^{*}$ and $W_{+}S = W_{-}$.

$$\begin{split} h_r(t) &= \langle (W_+ - 1)e^{-itH_0}Sf, P_r W_- e^{-itH_0}f \rangle \\ &+ \langle e^{-itH_0}Sf, (P_r W_- - P_r S)e^{-itH_0}f \rangle \\ &= \langle (W_+ - 1)e^{-itH_0}Sf, P_r W_- e^{-itH_0}f \rangle \\ &+ \langle e^{-itH_0}Sf, P_r (W_+ - 1)e^{-itH_0}Sf \rangle, \\ &|h_r(t)| \leq 2 \|f\| \cdot \|(W_+ - 1)e^{-itH_0}Sf\|. \end{split}$$

The assumptions on V and Sf together with Lemma 4.6 imply that the right hand side is integrable over $(0, \infty)$. Dominated convergence gives

$$\lim_{r\to\infty}\int_0^\infty h_r(t)dt=0.$$

Theorem 6.4. Let V satisfy Assumption 3.1 a) with $\beta > 2$ or Assumption 3.2 with k=1. Let $\{P_r\}$ satisfy condition (E). Assume P_r given by an integral kernel $\kappa_r(\lambda, \mu) \in B(\mathcal{P})$ in the spectral representation. For each $[a, b] \subset (0, \infty) \setminus \sigma_p(H)$ assume

ess sup
$$\|\kappa_r(\lambda,\mu)\|_{B(\mathscr{P})} < \infty$$
.

452

For each r assume in $B(\mathcal{P})$

$$S(\lambda)\kappa_r(\lambda,\mu) = \kappa_r(\lambda,\mu)S(\lambda) \tag{6.3}$$

for a.e. λ, μ .

Let $f \in \mathscr{D}$ satisfy $\phi(H_0)f = f$ for some $\phi \in C_0^{\infty}((0, \infty) \setminus \sigma_p(H))$, and for each r

$$\int_0^\infty \|P_r e^{-itH_0} Sf\|^2 dt < \infty \,.$$

Then the following limit exists and is expressed as follows

$$\lim_{r \to \infty} \int_{0}^{\infty} (\|P_{r}e^{-itH_{0}}Sf\|^{2} - \|P_{r}e^{-itH_{0}}f\|^{2})dt = \langle f, Tf \rangle.$$
(6.4)

Here T is the Eisenbud-Wigner time-delay operator.

Proof. Write g = Ff. There exist $a, b, 0 < a < b < \infty$, such that g has support in [a, b]. By assumption the integral in (6.4) exists for each r

$$\int_{0}^{\infty} (\|P_{r}e^{-itH_{0}}Sf\|^{2} - \|P_{r}e^{-itH_{0}}f\|^{2})dt$$
$$= \lim_{\epsilon \downarrow 0} \int_{0}^{\infty} e^{-\epsilon t} (\|P_{r}e^{-itH_{0}}Sf\|^{2} - \|P_{r}e^{-itH_{0}}f\|^{2})dt$$

The integral on the right hand side is denoted $I(\varepsilon, r)$. In the spectral representation we have

$$I(r,\varepsilon) = \int_{0}^{\infty} e^{-\varepsilon t} \int_{0}^{\infty} d\lambda \int_{0}^{\infty} d\mu e^{it(\lambda-\mu)} .$$

 $\cdot \langle g(\lambda), (S(\lambda)^* \kappa_r(\lambda,\mu) S(\mu) - \kappa_r(\lambda,\mu)) g(\mu) \rangle dt .$

g has support in [a, b] and $\|\kappa_r(\lambda, \mu)\| < C$ for a.e. $\lambda, \mu \in [a, b]$, so we can change the order of integration, and carry out the *t*-integral.

$$I(r,\varepsilon) = \int_{0}^{\infty} d\lambda \int_{0}^{\infty} d\mu \frac{i}{\lambda - \mu + i\varepsilon} \langle g(\lambda), (S(\lambda)^{*} \kappa_{r}(\lambda, \mu) S(\mu) - \kappa_{r}(\lambda, \mu)) g(\mu) \rangle.$$

Using (6.3) we have

$$\begin{split} h_{r,\varepsilon}(\lambda,\mu) &= \frac{i}{\lambda-\mu+i\varepsilon} \langle g(\lambda), (S(\lambda)^*\kappa_r(\lambda,\mu)S(\mu)-\kappa_r(\lambda,\mu))g(\mu) \rangle \\ &= -i \left\langle g(\lambda), S(\lambda)^*\kappa_r(\lambda,\mu) \frac{S(\lambda)-S(\mu)}{\lambda-\mu+i\varepsilon}g(\mu) \right\rangle. \end{split}$$

 $S(\lambda)$ is continuously differentiable in norm by Theorems 3.5 or 3.6. We have

$$|h_{r,\varepsilon}(\lambda,\mu)| \leq C_r \|g(\lambda)\|_{\mathscr{P}} \|g(\mu)\|_{\mathscr{P}}$$

for $\lambda, \mu \in (0, \infty)$.

$$h_{r,\varepsilon}(\lambda,\mu) \rightarrow h_{r,0}(\lambda,\mu)$$
 as $\varepsilon \downarrow 0$

for $\lambda, \mu \in (0, \infty)$, where

$$h_{r,0}(\lambda,\mu) = \begin{cases} -i\left\langle g(\lambda), S(\lambda)^* \kappa_r(\lambda,\mu) \frac{S(\lambda) - S(\mu)}{\lambda - \mu} g(\mu) \right\rangle, & \lambda \neq \mu \\ -i\left\langle g(\lambda), S^*(\lambda) \kappa_r(\lambda,\mu) \left(\frac{d}{d\lambda} S(\lambda)\right) g(\lambda) \right\rangle, & \lambda = \mu. \end{cases}$$

Hence

$$I(r,0) = \lim_{\varepsilon \to 0} I(r,\varepsilon)$$

= $\int_{0}^{\infty} d\lambda \int_{0}^{\infty} d\mu(-i) \left\langle g(\lambda), S(\lambda)^{*} \kappa_{r}(\lambda,\mu) \frac{S(\lambda) - S(\mu)}{\lambda - \mu} g(\mu) \right\rangle.$

By assumption

$$\int_{0}^{\infty} \kappa_{r}(\lambda,\mu)\xi(\mu)d\mu \rightarrow \xi(\lambda) \quad \text{as} \quad r \rightarrow \infty$$

in $L^2(0, \infty; \mathscr{P})$. Hence

$$\lim_{r \to \infty} I(r, 0) = \int_{0}^{\infty} d\lambda \left\langle g(\lambda), -iS(\lambda)^{*} \left(\frac{d}{d\lambda} S(\lambda) \right) g(\lambda) \right\rangle,$$

or, using g = Ff and the definition of T,

$$\lim_{r \to \infty} I(r, 0) = \langle f, Tf \rangle. \quad \Box$$

In applications condition (6.3) seems to be difficult to verify. In two cases it is trivially verified: When either $S(\lambda)$ or $\kappa_r(\lambda, \mu)$ is scalar. The first case is the one dealt with in [20], simple scattering. Thus we have given a new proof of Martin's result. Notice that in this case P_r is multiplication by the characteristic function for $\{x | |x| < r\}$. Condition (E) is satisfied, because P_r is H_0 - and H-smooth locally. Our main application here is to the case where $\kappa_r(\lambda, \mu)$ is scalar.

Let $P_r = \chi_r(D)$, the spectral projection for D for the interval [-r, r].

Lemma 6.5. Let V satisfy assumption 3.1 b) with $\beta > 4$. Then $\{P_r\}$ satisfies condition (E) with

 $\mathcal{D} = \{ f | \phi(H_0) f = f \quad \text{for some} \quad \phi \in C_0^{\infty}((0,\infty) \setminus \sigma_p(H)) \quad \text{and} \quad \|(1+D^2)^{3/2} f \| < \infty \} \,.$

Furthermore, for each r and each $f \in \mathcal{D}$ we have

$$\int_0^\infty \|P_r e^{-itH_0} Sf\|^2 dt < \infty.$$

 P_r is given in \mathscr{H}_s by $\kappa_r(\lambda, \mu)$ defined in (2.5). It satisfies

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$$\|\kappa_r(\lambda,\mu)\|_{B(\mathscr{P})}$$

for each $[a, b] \in (0, \infty) \setminus \sigma_p(H)$. $\kappa_r(\lambda, \mu)$ satisfies (6.3).

Proof. Since $||P_r(1+D^2)^{\mu/2}|| \leq (1+r^2)^{\mu/2}$, Lemma 4.3 gives for $\mu > 1/2$

$$\|P_r e^{-itH_0} (1+H_0)^{-3} H_0^3 (1+D^2)^{-\mu/2}\| \leq c(1+|t|)^{-\mu}.$$

Let $f \in \mathcal{D}$, \mathcal{D} defined in the lemma. Then we have

$$\int_{-\infty}^{\infty} \|P_r e^{-itH_0}f\|^2 dt < \infty$$

The proof of Theorem 5.2 and Remark 6.3(ii) show $f \in \mathcal{D}$ implies $Sf \in \mathcal{D}$ under our assumptions on V. Hence we also have

$$\int_0^\infty \|P_r e^{-itH_0} Sf\|^2 dt < \infty.$$

We have

$$\|P_r e^{-itH} W_- f\| \leq \|(W_- - 1)e^{-itH_0} f\| + \|P_r e^{-itH_0} f\|.$$

(4.8) and the above result imply that $||P_r e^{-itH} W_- f||$ is square integrable over $(-\infty, 0]$. Using $W_- = W_+ S$ we have

$$||P_{r}e^{-itH}W_{-}f|| \leq ||(W_{+}-1)e^{-itH_{0}}Sf|| + ||P_{r}e^{-itH_{0}}Sf||,$$

so $||P_r e^{-itH} W_f||$ is square integrable over $[0, \infty)$ by (4.9) and the above result. The remaining results in the lemma follow from results given in Sect. 2.

Theorem 6.6. Let $\{P_r\}$ be the sequence defined above. Let V satisfy Assumption 3.1 b) with $\beta > 4$. Let $f \in \mathscr{H}_c = L^2(\mathbb{R}^n)$ satisfy $Ff \in C_0^3((0, \infty) \setminus \sigma_n(H); \mathscr{P})$. We then have

$$\langle f, Tf \rangle = \lim_{r \to \infty} \int_{-\infty}^{\infty} dt (\|P_r e^{-itH} W_- f\|^2 - \|P_r e^{-itH_0} f\|^2).$$

Proof. The result follows from Lemma 6.5, Theorem 6.2(ii), Remark 6.3(ii), and Theorem 6.4. \Box

Remark 6.7. (i) The conclusions of the theorem are true under the following assumptions: V satisfies 3.1 b) with $\beta > 3$ and $f \in \mathscr{H}_c$, $\phi(H_0)f = f$, $\phi \in C_0((0,\infty) \setminus \sigma_p(H))$, $\|(1+D^2)^{\mu/2}f\| + \|(1+D^2)^{\mu/2}Sf\| < \infty$ for some $\mu > 2$. If V satisfies 3.1 b) with $\beta > 3$, we expect $\|(1+D^2)^{\mu/2}f\| < \infty$ to imply $\|(1+D^2)^{\mu/2}Sf\| < \infty$, but we have not been able to prove this result.

(ii) The conclusions of the theorem are also true under the following assumptions: V satisfies 3.1 b) with $\beta > 2$ and 3.2 with k=3, and f satisfies $||(1+D^2)^{3/2}f|| < \infty$. This result is true, because 3.1 b) with $\beta > 2$ is enough to apply all the results except the one requiring $||(1+D^2)^{\mu/2}Sf|| < \infty$ for some $\mu > 2$. But 3.2 with k=3 implies $S(\lambda)$ three times differentiable, so we get $||(1+D^2)^{3/2}Sf|| < \infty$. This result also requires an obvious modification in the definition of \mathcal{D} .

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