Anisotropic Lavine's formula and symmetrised time delay in scattering theory

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Abstract

We consider, in quantum scattering theory, symmetrised time delay defined in terms of sojourn times in arbitrary spatial regions symmetric with respect to the origin. For potentials decaying more rapidly than $|x|^{-4}$ at infinity, we show the existence of symmetrised time delay, and prove that it satisfies an anisotropic version of Lavine's formula. The importance of an anisotropic dilations-type operator is revealed in our study.

1 Introduction and main results

It is known for long that the definition of *time delay* (in terms of sojourn times) in scattering theory has to be *symmetrised* in the case of multichannel-type scattering processes (see *e.g.* [3, 4, 12, 13, 21, 22]). More recently [6] it has been shown that symmetrised time delay does exist, in two-body scattering processes, for arbitrary dilated spatial regions symmetric with respect to the origin (usual time delay does exist only for spherical spatial regions [20]). This leads to a generalised formula for time delay, which reduces to the usual one in the case of spherical spatial regions. The aim of the present paper is to provide a reasonable interpretation of this formula for potential scattering by proving its identity with an anisotropic version of Lavine's formula [11].

Let us recall the definition of symmetrised time delay for a two-body scattering process in $\mathbb{R}^d$, $d \geq 1$. Consider a bounded open set Σ in $\mathbb{R}^d$ containing the origin and the dilated spatial regions $\Sigma_r := \{rx \mid x \in \Sigma\}$, $r > 0$. Let $H_0 := -\frac{1}{2}\Delta$ be the kinetic energy operator in $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^d)$ (endowed with the norm $\|\cdot\|$ and scalar product $\langle\cdot,\cdot\rangle$). Let H be a selfadjoint perturbation of H_0 such that the wave operators $W_\pm := \text{s-}\lim_{t\to\pm\infty} \mathrm{e}^{itH}\,\mathrm{e}^{-itH_0}$ exist and are complete (so that the scattering operator $S := W_+^* W_-$ is unitary). Then one defines for some states $\varphi \in \mathcal{H}$ and $r > 0$ two sojourn times, namely:

$$T_r^0(\varphi) := \int_{-\infty}^{\infty} \mathrm{d}t \int_{x\in\Sigma_r} \mathrm{d}^d x \left|(\mathrm{e}^{-itH_0}\,\varphi)(x)\right|^2$$

and

$$T_r(\varphi) := \int_{-\infty}^{\infty} \mathrm{d}t \int_{x \in \Sigma_r} \mathrm{d}^d x \left|(\mathrm{e}^{-itH} W_- \varphi)(x)\right|^2 .$$

If the state φ is normalized to one the first number is interpreted as the time spent by the freely evolving state $\mathrm{e}^{-itH_0} \varphi$ inside the set Σ_r, whereas the second one is interpreted as the time spent by the associated scattering state $\mathrm{e}^{-itH} W_- \varphi$ within the same region. The usual time delay of the scattering process with incoming state φ for Σ_r is defined as

$$\tau_r^{\mathrm{in}}(\varphi) := T_r(\varphi) - T_r^0(\varphi),$$

and the corresponding symmetrised time delay for Σ_r is given by

$$\tau_r(\varphi) := T_r(\varphi) - \tfrac{1}{2}\left[T_r^0(\varphi) + T_r^0(S\varphi)\right].$$

If Σ is spherical and some abstract assumptions are verified, the limits of $\tau_r^{\mathrm{in}}(\varphi)$ and $\tau_r(\varphi)$ as $r \to \infty$ exist and satisfy [6, Sec. 4.3]

$$\lim_{r\to\infty} \tau_r(\varphi) = \lim_{r\to\infty} \tau_r^{\mathrm{in}}(\varphi) = -\tfrac{1}{2}\big\langle H_0^{-1/2}\varphi, S^*[D,S]H_0^{-1/2}\varphi\big\rangle, \tag{1.1}$$

where D is the generator of dilations. If Σ is not spherical the limit of $\tau_r^{\mathrm{in}}(\varphi)$ as $r \to \infty$ does not exist anymore [20], but the limit of $\tau_r(\varphi)$ as $r \to \infty$ does still exist, as soon as Σ is symmetric with respect to the origin [6, Rem. 4.8].

In this paper we study $\tau_r(\varphi)$ in the setting of potential scattering. For potentials decaying more rapidly than $|x|^{-4}$ at infinity, we prove the existence of $\lim_{r\to\infty} \tau_r(\varphi)$ by using the results of [6]. In a first step we show that the limit satisfies the equality

$$\lim_{r\to\infty} \tau_r(\varphi) = -\big\langle f(H_0)^{-1/2}\varphi, S^*[D_\Sigma, S] f(H_0)^{-1/2}\varphi\big\rangle, \tag{1.2}$$

where f is a real symbol of degree 1 and $D_\Sigma \equiv D_\Sigma(f)$ is an operator acting as an anisotropic generator of dilations. Then we prove that Formula (1.2) can be rewritten as an anisotropic Lavine's formula. Namely, one has (see Theorem 4.5 for a precise statement)

$$\lim_{r\to\infty} \tau_r(\varphi) = \int_{-\infty}^{\infty} \mathrm{d}s \,\big\langle \mathrm{e}^{-isH} W_- f(H_0)^{-1/2}\varphi, \mathsf{V}_{\Sigma,f}\, \mathrm{e}^{-isH} W_- f(H_0)^{-1/2}\varphi\big\rangle, \tag{1.3}$$

where the operator

$$\mathsf{V}_{\Sigma,f} = f(H) - f(H_0) - i[V, D_\Sigma]$$

generalises the virial $\widetilde{V} := 2V - i[V,D]$. Formula (1.3) provides an interesting relation between the potential V and symmetrised time delay, which we discuss.

Let us give a description of this paper. In section 2 we introduce the condition on the set Σ (see Assumption 2.1) under which our results are proved. We also define the anisotropic generator of dilations D_Σ and establish some of its properties. Section 3 is devoted to symmetrised time delay in potential scattering; the existence of symmetrised time delay for potentials decaying more rapidly than $|x|^{-4}$ at infinity is established in

Theorem 3.5. In Theorem 4.5 of Section 4 we prove the anisotropic Lavine's formula (1.3) for the same class of potentials. Remarks and examples are to be found at the end of Section 4.

We emphasize that the extension of Lavine's formula to non spherical sets Σ is not straightforward due, among other things, to the appearance of a singularity in the space of momenta not present in the isotropic case (see Equation (2.7) and the paragraphs that follow). The adjunction of the symbol f in the definition of the operator D_Σ (see Definition 2.2) is made to circumvent the difficulty.

Finally we refer to [9] (see also [8, 11, 15, 16, 17]) for a related work on Lavine's formula for time delay.

2 Anisotropic dilations

In this section we define the operator D_Σ and establish some of its properties in relation with the generator of dilations D and the shape of Σ. We start by recalling some notations.

Given two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, we write $\mathscr{B}(\mathcal{H}_1, \mathcal{H}_2)$ for the set of bounded operators from $\mathcal{H}_1$ to $\mathcal{H}_2$ with norm $\|\cdot\|_{\mathcal{H}_1\to\mathcal{H}_2}$, and put $\mathscr{B}(\mathcal{H}_1) := \mathscr{B}(\mathcal{H}_1, \mathcal{H}_1)$. We set $Q := (Q_1, Q_2, \ldots, Q_d)$ and $P := (P_1, P_2, \ldots, P_d)$, where Q_j (resp. P_j) stands for the j-th component of the position (resp. momentum) operator in $\mathcal{H}$. $\mathbb{N} := \{0, 1, 2, \ldots\}$ is the set of natural numbers. $\mathcal{H}^k$, $k \in \mathbb{N}$, are the usual Sobolev spaces over $\mathbb{R}^d$, and $\mathcal{H}^s_t(\mathbb{R}^d)$, $s, t \in \mathbb{R}$, are the weighted Sobolev spaces over $\mathbb{R}^d$ [1, Sec. 4.1], with the convention that $\mathcal{H}^s(\mathbb{R}^d) := \mathcal{H}^s_0(\mathbb{R}^d)$ and $\mathcal{H}_t(\mathbb{R}^d) := \mathcal{H}^0_t(\mathbb{R}^d)$. Given a set $\mathcal{M} \subset \mathbb{R}^d$ we write $\mathbb{1}_\mathcal{M}$ for the characteristic function for $\mathcal{M}$. We always assume that Σ is a bounded open set in $\mathbb{R}^d$ containing 0, with boundary $\partial\Sigma$ of class C^4. Often we even suppose that Σ satisfies the following stronger assumption (see [6, Sec. 2]).

Assumption 2.1. *Σ is a bounded open set in $\mathbb{R}^d$ containing 0, with boundary $\partial\Sigma$ of class C^4. Furthermore Σ satifies*

$$\int_0^\infty \mathrm{d}\mu \left[\mathbb{1}_\Sigma(\mu x) - \mathbb{1}_\Sigma(-\mu x)\right] = 0, \quad \forall x \in \mathbb{R}^d.$$

If $p \in \mathbb{R}^d$, then the number $\int_0^\infty \mathrm{d}t\, \mathbb{1}_\Sigma(tp)$ is the sojourn time in Σ of a free classical particle moving along the trajectory $t \mapsto x(t) := tp$, $t \geq 0$. Obviously Σ satisfies Assumption 2.1 if Σ is symmetric with respect to 0 (*i.e.* $\Sigma = -\Sigma$). Moreover if Σ is star-shaped with respect to 0 and satisfies Assumption 2.1, then $\Sigma = -\Sigma$.

We recall from [6, Lemma 2.2] that the limit

$$R_\Sigma(x) := \lim_{\varepsilon \searrow 0} \left(\int_\varepsilon^{+\infty} \frac{\mathrm{d}\mu}{\mu}\, \mathbb{1}_\Sigma(\mu x) + \ln \varepsilon \right) \tag{2.4}$$

exists for each $x \in \mathbb{R}^d \setminus \{0\}$, and we define the function $G_\Sigma : \mathbb{R}^d \setminus \{0\} \to \mathbb{R}$ by

$$G_\Sigma(x) := \tfrac{1}{2} \left[R_\Sigma(x) + R_\Sigma(-x)\right]. \tag{2.5}$$

The function $G_\Sigma : \mathbb{R}^d \setminus \{0\} \to \mathbb{R}$ is of class C^4 since $\partial\Sigma$ of class C^4. Let $x \in \mathbb{R}^d \setminus \{0\}$ and $t > 0$, then Formulas (2.4) and (2.5) imply that

$$G_\Sigma(tx) = G_\Sigma(x) - \ln(t).$$

From this one easily gets the following identities for the derivatives of G_Σ:

$$x \cdot (\nabla G_\Sigma)(x) = -1, \tag{2.6}$$

$$t^{|\alpha|}\big(\partial^\alpha G_\Sigma\big)(tx) = \big(\partial^\alpha G_\Sigma\big)(x), \tag{2.7}$$

where α is a d-dimensional multi-index with $|\alpha| \geq 1$ and $\partial^\alpha := \partial_1^{\alpha_1} \cdots \partial_d^{\alpha_d}$. The second identity suggests a way of regularizing the functions $\partial_j G_\Sigma$ which partly motivates the following definition. We use the notation $S^\mu(\mathbb{R};\mathbb{R})$, $\mu \in \mathbb{R}$, for the vector space of real symbols of degree μ on $\mathbb{R}$.

Definition 2.2. *Let $f \in S^1(\mathbb{R};\mathbb{R})$ be such that*

(i) $f(0) = 0$ and $f(u) > 0$ for each $u > 0$,

(ii) for each $j = 1, 2, \ldots, d$, the function $x \mapsto (\partial_j G_\Sigma)(x) f(x^2/2)$ (a priori only defined for $x \in \mathbb{R}^d \setminus \{0\}$) belongs to $C^3(\mathbb{R}^d;\mathbb{R})$.

Then we define $F_\Sigma : \mathbb{R}^d \to \mathbb{R}^d$ by $F_\Sigma(x) := -(\nabla G_\Sigma)(x) f(x^2/2)$.

Given a set Σ there are many appropriate choices for the function f. For instance if $\gamma > 0$ one can always take $f(u) = 2(u^2 + \gamma)^{-1} u^3$, $u \in \mathbb{R}$. But when Σ is equal to the open unit ball $\mathcal{B} := \{x \in \mathbb{R}^d \mid |x| < 1\}$ one can obviously make a simpler choice. Indeed in such case one has [6, Rem. 2.3.(b)] $(\partial_j G_{\mathcal{B}})(x) = -x_j x^{-2}$, and the choice $f(u) = 2u$, $u \in \mathbb{R}$, leads to the C^∞-function $F_\Sigma(x) = x$.

Remark 2.3. *One can associate to each set Σ a unique set $\widetilde{\Sigma}$ symmetric and star-shaped with respect to 0 such that $G_\Sigma = G_{\widetilde{\Sigma}}$ [6, Rem. 2.3.(c)]. The boundary $\partial\widetilde{\Sigma}$ of $\widetilde{\Sigma}$ satisfies*

$$\partial\widetilde{\Sigma} := \big\{ \mathrm{e}^{G_\Sigma(x)}\, x \mid x \in \mathbb{R}^d \setminus \{0\}\big\},$$

and $\widetilde{\Sigma}_r := \big\{rx \mid x \in \widetilde{\Sigma}\big\}$, $r > 0$. Thus the vector field $F_\Sigma = F_{\widetilde{\Sigma}}$ is orthogonal to the hypersurfaces $\partial\widetilde{\Sigma}_r$ in the following sense: if v belongs to the tangent space of $\partial\widetilde{\Sigma}_r$ at $y \in \partial\widetilde{\Sigma}_r$, then $F_\Sigma(y)$ is orthogonal to v. To see this let $s \mapsto y(s) \equiv r\,\mathrm{e}^{G_\Sigma(x(s))}\, x(s)$ be any differentiable curve on $\partial\widetilde{\Sigma}_r$. Then $\frac{\mathrm{d}}{\mathrm{d}s}\, y(s)$ belongs to the tangent space of $\partial\widetilde{\Sigma}_r$ at $y(s)$, and a direct calculation using Equations (2.6)-(2.7) *gives $F_\Sigma(y(s)) \cdot \frac{\mathrm{d}}{\mathrm{d}s}\, y(s) = 0$.*

In the rest of the section we give a meaning to the expression

$$D_\Sigma := \tfrac{1}{2}[F_\Sigma(P) \cdot Q + Q \cdot F_\Sigma(P)],$$

and we establish some properties of D_Σ in relation with the generator of dilations

$$D := \tfrac{1}{2}(P \cdot Q + Q \cdot P).$$

For the next lemma we emphasize that $\mathcal{H}^2$ is contained in the domain $\mathcal{D}\big(f(H_0)\big)$ of $f(H_0)$. The notation $\langle \cdot \rangle$ stands for $\sqrt{1 + |\cdot|^2}$, and $\mathscr{S}$ is the Schwartz space on $\mathbb{R}^d$.

Lemma 2.4. *Let Σ be a bounded open set in $\mathbb{R}^d$ containing 0, with boundary $\partial\Sigma$ of class C^4. Then*

(a) The operator D_Σ is essentially selfadjoint on $\mathscr{S}$. As a bounded operator, D_Σ extends to an element of $\mathscr{B}\big(\mathcal{H}^s_t, \mathcal{H}^{s-1}_{t-1}\big)$ for each $s \in \mathbb{R}$, $t \in [-2, 0] \cup [1, 3]$.

(b) One has for each $t \in \mathbb{R}$ and $\varphi \in \mathcal{D}(D_\Sigma) \cap \mathcal{D}\big(f(H_0)\big)$

$$\mathrm{e}^{-itH_0}\, D_\Sigma\, \mathrm{e}^{itH_0}\, \varphi = [D_\Sigma - tf(H_0)]\varphi. \tag{2.8}$$

In particular one has the equality

$$i[H_0, D_\Sigma] = f(H_0) \tag{2.9}$$

as sesquilinear forms on $\mathcal{D}(D_\Sigma) \cap \mathcal{H}^2$.

The second claim of point (a) is sufficient for our purposes, even if it is only a particular case of a more general result.

Proof. (a) The essential seladjointness of D_Σ on $\mathscr{S}$ follows from the fact that F_Σ is of class C^3 (see *e.g.* [1, Prop. 7.6.3.(a)]).

Due to the hypotheses on F_Σ one has for each $\varphi \in \mathscr{S}$ the bound

$$\big\|(\partial^\alpha F_{\Sigma j})(P)\varphi\big\| \leq \mathrm{Const.}\, \|\langle P\rangle\, \varphi\|\,, \tag{2.10}$$

where $F_{\Sigma j}$ is the j-th component of F_Σ and α is a d-dimensional multi-index with $|\alpha| \leq 3$. Furthermore

$$\|D_\Sigma\|_{\mathcal{H}^s_3 \to \mathcal{H}^{s-1}_2} \leq \sum_{j \leq d} \sup_{\varphi \in \mathscr{S}, \|\varphi\|_{\mathcal{H}^s_3} = 1} \Big\| \langle P\rangle^{s-1} \langle Q\rangle^2 \left[F_{\Sigma j}(P) Q_j + \tfrac{i}{2}(\partial_j F_{\Sigma j})(P)\right] \varphi \Big\|$$

for each $s \in \mathbb{R}$. Since $\langle Q\rangle^2$ acts as the operator $1 - \Delta$ after a Fourier transform, the inequalities above imply that D_Σ extends to an element of $\mathscr{B}(\mathcal{H}^s_3, \mathcal{H}^{s-1}_2)$. A similar argument shows that D_Σ extends to an element of $\mathscr{B}(\mathcal{H}^s_1, \mathcal{H}^{s-1})$ for each $s \in \mathbb{R}$. The second part of the claim follows then by using interpolation and duality.

(b) Let $\varphi \in \mathrm{e}^{-itH_0}\, \mathscr{S}$. Since $\mathrm{e}^{-itH_0}\, Q_j\, \mathrm{e}^{itH_0}\, \varphi = (Q_j - tP_j)\varphi$, it follows by Formula (2.6) that

$$\mathrm{e}^{-itH_0}\, D_\Sigma\, \mathrm{e}^{itH_0}\, \varphi = [D_\Sigma + tP \cdot (\nabla G_\Sigma)(P) f(H_0)]\varphi = [D_\Sigma - tf(H_0)]\varphi.$$

This together with the essential selfajointness of $\mathrm{e}^{-itH_0}\, D_\Sigma\, \mathrm{e}^{itH_0}$ on $\mathrm{e}^{-itH_0}\, \mathscr{S}$ implies the first part of the claim. Relation (2.9) follows by taking the derivative of (2.8) w.r.t. t in the form sense and then posing $t = 0$. □

Remark 2.5. *If $\Sigma = \mathcal{B}$ and $f(u) = 2u$, then $F_\Sigma(x) = x$ for each $x \in \mathbb{R}^d$, and the operators D_Σ and D coincide. If Σ is not spherical it is still possible to determine part of* *the behaviour of the group $W_t := \mathrm{e}^{itD_\Sigma}$. Indeed let $\mathbb{R}\times\mathbb{R}^d \ni (t,x) \mapsto \xi_t(x) \in \mathbb{R}^d$ be the flow associated to the vector field $-F_\Sigma$, that is, the solution of the differential equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\xi_t(x) = (\nabla G_\Sigma)(\xi_t(x))f\big(\xi_t(x)^2/2\big), \quad \xi_0(x) = x. \tag{2.11}$$

Then it is known (see e.g. *the proof of [1, Prop. 7.6.3.(a)]) that the group W_t acts in the Fourier space as*

$$\big(\widehat{W_t}\varphi\big)(x) := \sqrt{\eta_t(x)}\varphi(\xi_t(x)), \tag{2.12}$$

where $\eta_t(x) \equiv \det(\nabla\xi_t(x))$ is the Jacobian at x of the mapping $x \mapsto \xi_t(x)$. Taking the scalar product of Equation (2.11) *with $\xi_t(x)$ and then using Formula* (2.6) *leads to the equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\xi_t(x)^2 = -2f\big(\xi_t(x)^2/2\big), \quad \xi_0(x) = x.$$

If $t<0$ and $x\neq 0$, then $\xi_t(x)^2 \geq x^2 > 0$, and $\xi_t(x)^2$ is given by the implicit formula

$$2t + \int_{x^2}^{\xi_t(x)^2} \mathrm{d}u\, f(u/2)^{-1} = 0.$$

This, together with the facts that $x \mapsto f(x^2/2)$ belongs to $S^2(\mathbb{R};\mathbb{R})$ and $f(u) > 0$ for $u>0$, implies the estimate $\langle\xi_t(x)\rangle \leq \mathrm{e}^{-\mathrm{c}t}\langle x\rangle$ for some constant $\mathrm{c}>0$. Since $\langle\xi_t(x)\rangle \leq \langle x\rangle$ for each $t\geq 0$ it follows that

$$\langle\xi_t(x)\rangle \leq (1+\mathrm{e}^{-\mathrm{c}t})\,\langle x\rangle \tag{2.13}$$

for all $t\in\mathbb{R}$ and $x\in\mathbb{R}^d$ (the case $x=0$ is covered since $\xi_t(0)=0$ for all $t\in\mathbb{R}$). Equation (2.13) *implies that the domain $\mathcal{H}^2$ of H_0 is left invariant by the group W_t.*

The results of Remarks 2.3 and 2.5 suggest that W_t may be interpreted as an anisotropic version of the dilations group, which reduces to the usual dilations group in the case $\Sigma = \mathcal{B}$ and $f(u) = 2u$.

In the next lemma we show some properties of the mollified resolvent

$$R_\lambda := i\lambda(D_\Sigma + i\lambda)^{-1}, \quad \lambda \in \mathbb{R}\setminus\{0\}.$$

We refer to [18, Lemma 6.2] for the same results in the case of the usual dilations generator D, that is, when $\Sigma = \mathcal{B}$ and $f(u) = 2u$. See also [5, Lemma 4.5] for a general result.

Lemma 2.6. *Let Σ be a bounded open set in $\mathbb{R}^d$ containing 0, with boundary $\partial\Sigma$ of class C^4. Then*

(a) One has for each $t\in\mathbb{R}$ and $\varphi\in\mathcal{D}\big(\xi_t(P)^2\big)$

$$\mathrm{e}^{itD_\Sigma}\,H_0\,\mathrm{e}^{-itD_\Sigma}\,\varphi = \tfrac{1}{2}\,\xi_t(P)^2\varphi. \tag{2.14}$$

(b) For each $\lambda \in \mathbb{R}$ with $|\lambda|$ large enough, R_λ belongs to $\mathscr{B}(\mathcal{H}^2)$, and R_λ extends to an element of $\mathscr{B}(\mathcal{H}^{-2})$. Furthermore we have for each $\varphi \in \mathcal{H}^2$ and each $\psi \in \mathcal{H}^{-2}$

$$\lim_{|\lambda|\to\infty} \|(1-R_\lambda)\varphi\|_{\mathcal{H}^2} = 0 \quad \text{and} \quad \lim_{|\lambda|\to\infty} \|(1-R_\lambda)\psi\|_{\mathcal{H}^{-2}} = 0.$$

Proof. (a) Let $\varphi \in \mathrm{e}^{itD_\Sigma}\mathscr{S}$. A direct calculation using Formula (2.12) gives

$$(\mathscr{F}\,\mathrm{e}^{itD_\Sigma} H_0\,\mathrm{e}^{-itD_\Sigma}\varphi)(k) = \tfrac{1}{2}\,\xi_t(k)^2(\mathscr{F}\varphi)(k),$$

where $\mathscr{F}$ is the Fourier transform. This together with the essential selfajointness of $\mathrm{e}^{itD_\Sigma} H_0\,\mathrm{e}^{-itD_\Sigma}$ on $\mathrm{e}^{itD_\Sigma}\mathscr{S}$ implies the claim.

(b) Let $\varphi \in \mathcal{H}^2$ and take $\lambda \in \mathbb{R}$ with $|\lambda| > \mathrm{C}$, where C is the constant in the inequality (2.13). Using the (strong) integral formula

$$(D_\Sigma + i\lambda)^{-1} = i\int_0^{\mp\infty} \mathrm{d}t\ \mathrm{e}^{\lambda t}\,\mathrm{e}^{-itD_\Sigma}, \quad \operatorname{sgn}(\lambda) = \pm 1,$$

and Relation (2.14) we get the equalities

$$\begin{aligned}
(D_\Sigma + i\lambda)^{-1}\varphi &= (H_0+1)^{-1}(D_\Sigma+i\lambda)^{-1}(H_0+1)\varphi \\
&\quad + i\int_0^{\mp\infty} \mathrm{d}t\ \mathrm{e}^{\lambda t}\left[\mathrm{e}^{-itD_\Sigma}, (H_0+1)^{-1}\right](H_0+1)\varphi \\
&= (H_0+1)^{-1}(D_\Sigma+i\lambda)^{-1}(H_0+1)\varphi \\
&\quad - i\int_0^{\mp\infty} \mathrm{d}t\ \mathrm{e}^{\lambda t}(H_0+1)^{-1}\,\mathrm{e}^{-itD_\Sigma}\left[H_0 - \tfrac{1}{2}\xi_t(P)^2\right]\varphi \\
&= (H_0+1)^{-1}(D_\Sigma+i\lambda)^{-1}\varphi + \tfrac{i}{2}(H_0+1)^{-1}\int_0^{\mp\infty} \mathrm{d}t\ \mathrm{e}^{\lambda t}\,\mathrm{e}^{-itD_\Sigma}\,\xi_t(P)^2\varphi.
\end{aligned}$$

It follows that

$$H_0 R_\lambda \varphi = -\tfrac{\lambda}{2}\int_0^{\mp\infty} \mathrm{d}t\ \mathrm{e}^{\lambda t}\,\mathrm{e}^{-itD_\Sigma}\,\xi_t(P)^2\varphi, \quad \operatorname{sgn}(\lambda) = \pm 1.$$

Now $|\lambda| > \mathrm{C}$, and $\left\|\xi_t(P)^2\varphi\right\| \le (1+\mathrm{e}^{-\mathrm{C}t})\|\varphi\|_{\mathcal{H}^2}$ due to the bound (2.13). Thus

$$\begin{aligned}
\|H_0 R_\lambda\varphi\| &\le \tfrac{|\lambda|}{2}\int_0^\infty \mathrm{d}t\ \mathrm{e}^{-|\lambda|t}\left\|\xi_{-\operatorname{sgn}(\lambda)t}(P)^2\varphi\right\| \\
&\le \tfrac{|\lambda|}{2}\int_0^\infty \mathrm{d}t\left(\mathrm{e}^{-|\lambda|t} + \mathrm{e}^{(\operatorname{sgn}(\lambda)\mathrm{C}-|\lambda|)t}\right)\|\varphi\|_{\mathcal{H}^2} \\
&\le \text{Const.}\,\|\varphi\|_{\mathcal{H}^2}.
\end{aligned} \tag{2.15}$$

Using the estimate (2.15) and a duality argument one gets the bounds

$$\|R_\lambda\|_{\mathcal{H}^2\to\mathcal{H}^2} \le \text{Const.} \qquad \text{and} \qquad \|R_\lambda\|_{\mathcal{H}^{-2}\to\mathcal{H}^{-2}} \le \text{Const.}, \tag{2.16}$$

which imply the first part of the claim. For the second part we remark that

$$1 - R_\lambda = (i\lambda)^{-1} D_\Sigma R_\lambda$$

on $\mathcal{H}$. Using this together with the bounds (2.16) one easily shows that $\lim_{|\lambda|\to\infty} \|(1 - R_\lambda)\varphi\|_{\mathcal{H}^2} = 0$ for each $\varphi \in \mathcal{H}^2$ and that $\lim_{|\lambda|\to\infty} \|(1 - R_\lambda)\psi\|_{\mathcal{H}^{-2}} = 0$ for each $\psi \in \mathcal{H}^{-2}$. □

3 Symmetrised time delay

In this section we collect some facts on short-range scattering theory in connection with the existence of symmetrised time delay. We always assume that the potential V satisfies the usual Agmon-type condition:

Assumption 3.1. *V is a multiplication operator by a real-valued function such that V defines a compact operator from $\mathcal{H}^2$ to $\mathcal{H}_\kappa$ for some $\kappa > 1$.*

By using duality, interpolation and the fact that V commutes with the operator $\langle Q\rangle^t$, $t \in \mathbb{R}$, one shows that V also defines a bounded operator from $\mathcal{H}_t^{2s}$ to $\mathcal{H}_{t+\kappa}^{2(s-1)}$ for any $s \in [0,1]$, $t \in \mathbb{R}$. Furthermore the operator sum $H := H_0 + V$ is selfadjoint on $\mathcal{D}(H) = \mathcal{H}^2$, the wave operators $W_\pm$ exist and are complete, and the projections $1\!\!1_{\Sigma_r}(Q)$ are locally H-smooth on $(0,\infty) \setminus \sigma_{\rm pp}(H)$ (see *e.g.* [7, Sec. 3] and [19, Sec. XIII.8]).

Since the first two lemmas are somehow standard, we give their proofs in the appendix.

Lemma 3.2. *Let V satisfy Assumption 3.1 with $\kappa > 1$, and take $z \in \mathbb{C}\setminus\{\sigma(H_0)\cup\sigma(H)\}$. Then the operator $(H - z)^{-1}$ extends to an element of $\mathscr{B}\big(\mathcal{H}_t^{-2s}, \mathcal{H}_t^{2(1-s)}\big)$ for each $s \in [0,1]$, $t \in \mathbb{R}$.*

Alternate formulations of the next lemma can be found in [7, Lemma 4.6] and [22, Lemma 3.9]. For each $s \geq 0$ we define the dense set

$$\mathscr{D}_s := \big\{\varphi \in \mathcal{D}(\langle Q\rangle^s) \mid \eta(H_0)\varphi = \varphi \text{ for some } \eta \in C_0^\infty((0,\infty) \setminus \sigma_{\rm pp}(H))\big\}.$$

Lemma 3.3. *Let V satisfy Assumption 3.1 with $\kappa > 2$. Then one has for each $\varphi \in \mathscr{D}_s$ with $s > 2$*

$$\big\|(W_- - 1)\,\mathrm{e}^{-itH_0}\,\varphi\big\| \in \mathsf{L}^1(\mathbb{R}_-, \mathrm{d}t) \tag{3.17}$$

and

$$\big\|(W_+ - 1)\,\mathrm{e}^{-itH_0}\,\varphi\big\| \in \mathsf{L}^1(\mathbb{R}_+, \mathrm{d}t). \tag{3.18}$$

Lemma 3.4. *Let V satisfy Assumption 3.1 with $\kappa > 4$, and let $\varphi \in \mathscr{D}_s$ for some $s > 2$. Then there exists $s' > 2$ such that $S\varphi \in \mathscr{D}_{s'}$, and the following conditions are satisfied:*

$$\big\|(W_- - 1)\,\mathrm{e}^{-itH_0}\,\varphi\big\| \in \mathsf{L}^1(\mathbb{R}_-, \mathrm{d}t) \quad \text{and} \quad \big\|(W_+ - 1)\,\mathrm{e}^{-itH_0}\,S\varphi\big\| \in \mathsf{L}^1(\mathbb{R}_+, \mathrm{d}t).$$

Proof. The first part of the claim follows by [10, Thm. 1.4.(ii)]. Since $\varphi \in \mathscr{D}_s$ and $S\varphi \in \mathscr{D}_{s'}$ with $s, s' > 2$, the second part of the claim follows by Lemma 3.3. $\square$

Theorem 3.5. *Let Σ satisfy Assumption 2.1. Suppose that V satisfies Assumption 3.1 with $\kappa > 4$. Let $\varphi \in \mathscr{D}_s$ with $s > 2$. Then the limit of $\tau_r(\varphi)$ as $r \to \infty$ exists, and one has*

$$\lim_{r\to\infty} \tau_r(\varphi) = -\big\langle f(H_0)^{-1/2}\varphi, S^*[D_\Sigma, S] f(H_0)^{-1/2}\varphi\big\rangle. \tag{3.19}$$

Proof. Due to Lemma 3.4 all the assumptions for the existence of $\lim_{r\to\infty} \tau_r(\varphi)$ are verified (see [6, Sec. 4]), and we know by Theorem [6, Thm. 4.6] that

$$\lim_{r\to\infty} \tau_r(\varphi) = -\tfrac{1}{2} \left\langle \varphi, S^* \left[i[Q^2, G_\Sigma(P)], S\right] \varphi\right\rangle .$$

It follows that

$$\begin{aligned}
\lim_{r\to\infty} \tau_r(\varphi) &= \tfrac{1}{2} \left\langle \varphi, S^*[Q \cdot (\nabla G_\Sigma)(P) + (\nabla G_\Sigma)(P) \cdot Q, S]\varphi\right\rangle \\
&= \tfrac{1}{2}\big\langle f(H_0)^{-1/2}\varphi, S^*\big[f(H_0)^{1/2}\big(Q \cdot (\nabla G_\Sigma)(P) \\
&\qquad\qquad + (\nabla G_\Sigma)(P) \cdot Q\big) f(H_0)^{1/2}, S\big] f(H_0)^{-1/2}\varphi\big\rangle \\
&= -\big\langle f(H_0)^{-1/2}\varphi, S^*[D_\Sigma, S] f(H_0)^{-1/2}\varphi\big\rangle.
\end{aligned}$$

$\square$

Note that Theorem 3.5 can be proved with the function $f(u) = 2u$, even if Σ is not spherical. Indeed, in such a case, point (ii) of Definition 2.2 is the only assumption not satisfied by f, and a direct inspection shows that this assumption does not play any role in the proof of Theorem 3.5.

Remark 3.6. *Some results of the literature suggest that Theorem 3.5 may be proved under a less restrictive decay assumption on V if one modifies some of the previous definitions. Typically one proves the existence of (usual) time delay for potentials decaying more rapidly than $|x|^{-2}$ (or even $|x|^{-1}$) at infinity by using smooth cutoff in configuration space and by considering particular potentials. The reader is referred to [2, 14, 15, 23, 24] for more informations on this issue.*

4 Anisotropic Lavine's formula

In this section we prove the anisotropic Lavine's formula (1.3). We first give a precise meaning to some commutators.

Lemma 4.1. *Let Σ be a bounded open set in $\mathbb{R}^d$ containing 0 with boundary $\partial\Sigma$ of class C^4. Let V satisfy Assumption 3.1 with $\kappa > 1$. Then*

(a) The commutator $[V, D_\Sigma]$, defined as a sesquilinear form on $\mathcal{D}(D_\Sigma) \cap \mathcal{H}^2$, extends uniquely to an element of $\mathscr{B}(\mathcal{H}^2, \mathcal{H}^{-2})$.

(b) *For each $t \in \mathbb{R}$ the commutator $[D_\Sigma, \mathrm{e}^{-itH}]$, defined as a sesquilinear form on $\mathcal{D}(D_\Sigma) \cap \mathcal{H}^2$, extends uniquely to an element $[D_\Sigma, \mathrm{e}^{-itH}]^a$ of $\mathscr{B}(\mathcal{H}^2, \mathcal{H}^{-2})$ which satisfies*
$$\big\|[D_\Sigma, \mathrm{e}^{-itH}]^a\big\|_{\mathcal{H}^2 \to \mathcal{H}^{-2}} \le \mathrm{Const.}\,|t|.$$

(c) *For each $\eta \in C_0^\infty(\mathbb{R})$ the commutator $[D_\Sigma, \eta(H)]$, defined as a sesquilinear form on $\mathcal{D}(D_\Sigma) \cap \mathcal{H}^2$, extends uniquely to an element of $\mathscr{B}(\mathcal{H})$. In particular, the operator $\eta(H)$ leaves $\mathcal{D}(D_\Sigma)$ invariant.*

Proof. Point (a) follows easily from Lemma 2.4.(a) and the hypotheses on V. Given point (a) and Lemma 2.6.(b), one shows points (b) and (c) as in [18, Lemma 7.4]. □

If V satisfies Assumption 3.1 with $\kappa > 2$, then the result of Lemma 4.1.(a) can be improved by using Lemma 2.4.(a). Namely, there exists $\delta > \frac{1}{2}$ such that the commutator $[V, D_\Sigma]$, defined as a sesquilinear form on $\mathcal{D}(D_\Sigma) \cap \mathcal{H}^2$, extends uniquely to an element $[V, D_\Sigma]^a$ of $\mathscr{B}\big(\mathcal{H}^2_{-\delta}, \mathcal{H}^{-2}_\delta\big)$.

Next Lemma is a generalisation of [9, Lemmas 2.5 & 2.7]. It is proved under the following assumption on the function f.

Assumption 4.2. *For each $t \in \mathbb{R}$ there exists $\rho > 1$ such that the operator $f(H) - f(H_0)$, defined on $\mathcal{H}^2$, extends to an element of $\mathscr{B}\big(\mathcal{H}^2_t, \mathcal{H}_{t+\rho}\big)$.*

We refer to Remark 4.4 for examples of admissible functions f. Here we only note that the operator

$$\mathsf{V}_{\Sigma,f} := f(H) - i[H, D_\Sigma]^a = f(H) - f(H_0) - i[V, D_\Sigma]^a.$$

belongs to $\mathscr{B}(\mathcal{H}^2_{-\delta}, \mathcal{H}^{-2}_\delta)$ for some $\delta > \frac{1}{2}$ as soon as f satisfies Assumption 4.2.

Lemma 4.3. *Let Σ be a bounded open set in $\mathbb{R}^d$ containing 0, with boundary $\partial\Sigma$ of class C^4. Let V satisfy Assumption 3.1 with $\kappa > 2$. Suppose that Assumption 4.2 is verified. Then*

(a) *One has for each $\eta \in C_0^\infty((0,\infty) \setminus \sigma_{\rm pp}(H))$ and each $t \in \mathbb{R}$ the inequality*
$$\big\|(D_\Sigma + i)^{-1}\,\mathrm{e}^{-itH}\,\eta(H)(D_\Sigma + i)^{-1}\big\| \le \mathrm{Const.}\,\langle t\rangle^{-1}.$$

(b) *For each $\eta \in C_0^\infty((0,\infty)\setminus\sigma_{\rm pp}(H))$ the operators $[D_\Sigma, W_\pm \eta(H_0)]$ and $[D_\Sigma, W_\pm^* \eta(H)]$, defined as sesquilinear forms on $\mathcal{D}(D_\Sigma)$, extend uniquely to elements of $\mathscr{B}(\mathcal{H})$. In particular, the operators $W_\pm \eta(H_0)$ and $W_\pm^* \eta(H)$ leave $\mathcal{D}(D_\Sigma)$ invariant.*

Proof. (a) Since the case $t = 0$ is trivial, we can suppose $t \neq 0$. Let $\varphi, \psi \in \mathcal{D}(D_\Sigma) \cap \mathcal{H}^2$, then

$$\big\langle D_\Sigma\varphi, \mathrm{e}^{-itH}\,\psi\big\rangle - \big\langle \varphi, \mathrm{e}^{-itH}\,D_\Sigma\psi\big\rangle = \lim_{\lambda\to\infty}\int_0^t \mathrm{d}s\,\big\langle \varphi, \mathrm{e}^{i(s-t)H}\,i[H, D_\Sigma R_\lambda]\,\mathrm{e}^{-isH}\,\psi\big\rangle$$

due to Lemma 2.6.(b). By using Lemma 2.4.(b) and Lemma 4.1.(b) we get in $\mathscr{B}(\mathcal{H}^2, \mathcal{H}^{-2})$ the equalities

$$\begin{aligned}[D_\Sigma, \mathrm{e}^{-itH}]^a &= \mathrm{e}^{-itH} \int_0^t \mathrm{d}s \; \mathrm{e}^{isH} \, i[H, D_\Sigma]^a \, \mathrm{e}^{-isH} \\ &= t \, \mathrm{e}^{-itH} \, f(H) - \mathrm{e}^{-itH} \int_0^t \mathrm{d}s \; \mathrm{e}^{isH} \, \mathsf{V}_{\Sigma,f} \, \mathrm{e}^{-isH} \, . \end{aligned} \tag{4.20}$$

Take $\eta, \vartheta \in C_0^\infty((0,\infty) \setminus \sigma_{\rm pp}(H))$ with ϑ identically one on the support of η, and let $\zeta \in C_0^\infty((0,\infty) \setminus \sigma_{\rm pp}(H))$ be defined by $\zeta(u) := f(u)^{-1}\vartheta(u)$. Then $\eta(H) = f(H)\zeta(H)\eta(H)$ and

$$\begin{aligned}\mathrm{e}^{-itH} \, \eta(H) &= \frac{1}{t}\zeta(H) t \, \mathrm{e}^{-itH} \, f(H)\eta(H) \\ &= \frac{1}{t}\zeta(H) \, \mathrm{e}^{-itH} \int_0^t \mathrm{d}s \; \mathrm{e}^{isH} \, \mathsf{V}_{\Sigma,f} \, \mathrm{e}^{-isH} \, \eta(H) + \frac{1}{t}\zeta(H)[D_\Sigma, \mathrm{e}^{-itH}]^a \eta(H). \end{aligned}$$

Since $\mathsf{V}_{\Sigma,f}$ belongs to $\mathscr{B}(\mathcal{H}^2_{-\delta}, \mathcal{H}^{-2}_\delta)$ for some $\delta > \frac{1}{2}$, a local H-smoothness argument shows that the first term is bounded by $\mathrm{Const.}|t|^{-1}$ in $\mathcal{H}$. Furthermore by using Lemma 4.1.(c) one shows that $(D_\Sigma + i)^{-1}\zeta(H)[D_\Sigma, \mathrm{e}^{-itH}]^a \eta(H)(D_\Sigma + i)^{-1}$ is bounded in $\mathcal{H}$ by a constant independent of t. Thus

$$\big\|(D_\Sigma + i)^{-1} \, \mathrm{e}^{-itH} \, \eta(H)(D_\Sigma + i)^{-1}\big\| \le \mathrm{Const.} \, |t|^{-1},$$

and the claim follows.

(b) Consider first $[D_\Sigma, W_+\eta(H_0)]$. Given $\eta \in C_0^\infty((0,\infty) \setminus \sigma_{\rm pp}(H))$ let $\zeta \in C_0^\infty((0,\infty) \setminus \sigma_{\rm pp}(H))$ be identically one on the support of η. Due to Lemma 4.1.(c) one has on $\mathcal{D}(D_\Sigma)$

$$\begin{aligned}&[D_\Sigma, \zeta(H) \, \mathrm{e}^{itH} \, \eta(H) \, \mathrm{e}^{-itH_0} \, \zeta(H_0)] \\ &= \zeta(H)[D_\Sigma, \mathrm{e}^{itH} \, \eta(H) \, \mathrm{e}^{-itH_0}]\zeta(H_0) + [D_\Sigma, \zeta(H)] \, \mathrm{e}^{itH} \, \eta(H) \, \mathrm{e}^{-itH_0} \, \zeta(H_0) \\ &\quad + \zeta(H) \, \mathrm{e}^{itH} \, \eta(H) \, \mathrm{e}^{-itH_0} [D_\Sigma, \zeta(H_0)], \end{aligned}$$

and the last two operators belong to $\mathscr{B}(H)$ with norm uniformly bounded in t. Let $\varphi, \psi \in \mathcal{D}(D_\Sigma)$. Using Lemma 2.4.(b) and Lemma 2.6.(b) one gets for the first operator the following equalities

$$
\begin{aligned}
&\big\langle \varphi, \zeta(H)[D_\Sigma, \mathrm{e}^{itH}\,\eta(H)\,\mathrm{e}^{-itH_0}]\zeta(H_0)\psi\big\rangle \\
&= \big\langle \varphi, \zeta(H)[D_\Sigma, \mathrm{e}^{itH}]\eta(H)\,\mathrm{e}^{-itH_0}\,\zeta(H_0)\psi\big\rangle \\
&\quad + \big\langle \varphi, \zeta(H)\,\mathrm{e}^{itH}[D_\Sigma, \eta(H)]\,\mathrm{e}^{-itH_0}\,\zeta(H_0)\psi\big\rangle \\
&\quad + \big\langle \varphi, \zeta(H)\,\mathrm{e}^{itH}\,\eta(H)[D_\Sigma, \mathrm{e}^{-itH_0}]\zeta(H_0)\psi\big\rangle \\
&= -\int_0^t \mathrm{d}s\,\big\langle \varphi, \zeta(H)\,\mathrm{e}^{i(t-s)H}\,i[H, D_\Sigma]^a\,\mathrm{e}^{isH}\,\eta(H)\,\mathrm{e}^{-itH_0}\,\zeta(H_0)\big\rangle \\
&\quad + \big\langle \varphi, \zeta(H)\,\mathrm{e}^{itH}[D_\Sigma, \eta(H)]\,\mathrm{e}^{-itH_0}\,\zeta(H_0)\psi\big\rangle \\
&\quad + t\,\big\langle \varphi, \zeta(H)\,\mathrm{e}^{itH}\,\eta(H)\,\mathrm{e}^{-itH_0}\,f(H_0)\zeta(H_0)\psi\big\rangle \\
&= \int_0^t \mathrm{d}s\,\big\langle \varphi, \zeta(H)\,\mathrm{e}^{i(t-s)H}\,\mathsf{V}_{\Sigma,f}\,\mathrm{e}^{isH}\,\eta(H)\,\mathrm{e}^{-itH_0}\,\zeta(H_0)\big\rangle \\
&\quad + \big\langle \varphi, \zeta(H)\,\mathrm{e}^{itH}[D_\Sigma, \eta(H)]\,\mathrm{e}^{-itH_0}\,\zeta(H_0)\psi\big\rangle \\
&\quad - t\,\big\langle \varphi, \eta(H)\,\mathrm{e}^{itH}\{f(H) - f(H_0)\}\,\mathrm{e}^{-itH_0}\,\zeta(H_0)\psi\big\rangle\,.
\end{aligned}
$$

The first two terms are bounded by $\mathrm{c}\,\|\varphi\|\cdot\|\psi\|$ with $\mathrm{c} > 0$ independent of φ, ψ and t (use the local H-smoothness of $\mathsf{V}_{\Sigma,f}$ for the first term). Furthermore due to the local H- and H_0-smoothness of $f(H) - f(H_0)$ one can find a sequence $t_n \to \infty$ as $n \to \infty$ such that

$$\lim_{n\to\infty} t_n\,\big\langle \varphi, \eta(H)\,\mathrm{e}^{it_nH}\{f(H) - f(H_0)\}\,\mathrm{e}^{-it_nH_0}\,\zeta(H_0)\psi\big\rangle = 0.$$

This together with the previous remarks implies that

$$\lim_{n\to\infty} \big\langle \varphi, [D_\Sigma, \zeta(H)\,\mathrm{e}^{it_nH}\,\eta(H)\,\mathrm{e}^{-it_nH_0}\,\zeta(H_0)]\psi\big\rangle \le \mathrm{c}'\|\varphi\|\cdot\|\psi\|,$$

with $\mathrm{c}' > 0$ independent of φ, ψ and t. Thus using the intertwining relation and the identity $\eta(H_0) = \zeta(H_0)\eta(H_0)\zeta(H_0)$ one finds that

$$
\begin{aligned}
&\big|\,\langle D_\Sigma\varphi, W_+\eta(H_0)\psi\rangle - \langle \varphi, W_+\eta(H_0)\psi\rangle\,\big| \\
&= \lim_{n\to\infty} \big|\,\big\langle \varphi, [D_\Sigma, \zeta(H)\,\mathrm{e}^{it_nH}\,\eta(H)\,\mathrm{e}^{-it_nH_0}\,\zeta(H_0)]\psi\big\rangle\,\big| \\
&\le \mathrm{c}'\|\varphi\|\cdot\|\psi\|.
\end{aligned}
$$

This proves the result for $[D_\Sigma, W_+\eta(H_0)]$. A similar proof holds for $[D_\Sigma, W_-\eta(H_0)]$. Since the wave operators are complete, one has $W_\pm^*\eta(H) = \text{s-}\lim_{t\to\pm\infty} \mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,\eta(H)$, and an analogous proof can be given for the operators $[D_\Sigma, W_\pm^*\eta(H)]$. □

Remark 4.4. *In the case $\Sigma = \mathcal{B}$ the requirements of Definition 2.2 and Assumption 4.2 are satisfied by many functions f. A natural choice is $f(u) = 2u$, $u \in \mathbb{R}$, since in such a case $f(H) - f(H_0) = 2V \in \mathscr{B}\big(\mathcal{H}_t^2, \mathcal{H}_{t+\kappa}\big)$, $t \in \mathbb{R}$, $\kappa > 1$. If Σ is not spherical there are still many appropriate choices for f. For instance if $\gamma > 0$, then the function*

$f(u) = 2(u^2+\gamma)^{-1}u^3$, $u \in \mathbb{R}$, *satisfies all the desired requirements. Indeed in such a case one has on* $\mathcal{H}^2$ *the following equalities*

$$
\begin{aligned}
&f(H) - f(H_0)\\
&= 2V - 2\gamma\big[(H^2+\gamma)^{-1}H - (H_0^2+\gamma)^{-1}H_0\big]\\
&= 2V - 2\gamma(H^2+\gamma)^{-1}V + 2\gamma(H^2+\gamma)^{-1}(H_0V + VH_0 + V^2)(H_0^2+\gamma)^{-1}H_0,
\end{aligned}
$$

and thus $f(H)-f(H_0)$ *also extends to an element of* $\mathscr{B}\big(\mathcal{H}_t^2,\mathcal{H}_{t+\kappa}\big)$, $t\in\mathbb{R}$, $\kappa>1$, *due to Lemma 3.2 and the assumptions on* V.

Next Theorem provides a rigorous meaning to the anisotropic Lavine's formula (1.3).

Theorem 4.5. *Let* Σ *satisfy Assumption 2.1. Let* V *satisfy Assumption 3.1 with* $\kappa > 4$. *Suppose that Assumption 4.2 is verified. Then one has for each* $\varphi \in \mathscr{D}_s$ *with* $s > 2$

$$
\lim_{r\to\infty}\tau_r(\varphi) = \int_{-\infty}^{\infty}\mathrm{d}s\,\big\langle \mathrm{e}^{-isH}\,W_- f(H_0)^{-1/2}\varphi, \mathsf{V}_{\Sigma,f}\,\mathrm{e}^{-isH}\,W_- f(H_0)^{-1/2}\varphi\big\rangle_{2,-2}, \tag{4.21}
$$

where $\langle\,\cdot\,,\,\cdot\,\rangle_{2,-2} : \mathcal{H}^2\times\mathcal{H}^{-2}\to\mathbb{C}$ *is the anti-duality map between* $\mathcal{H}^2$ *and* $\mathcal{H}^{-2}$.

Proof. (i) Set $W(t) := \mathrm{e}^{itH}\,\mathrm{e}^{-itH_0}$, and let $\psi := \eta(H)\widetilde{\psi}$, where $\eta \in C_0^\infty((0,\infty)\setminus\sigma_{\rm pp}(H))$ and $\widetilde{\psi}\in\mathcal{D}(D_\Sigma)$. We shall prove that $\|D_\Sigma W(t)^*\psi\| \le \mathrm{c}$, with c independent of t. Due to Lemma 2.4.(b) and Lemma 4.1.(c) one has

$$
\begin{aligned}
\|D_\Sigma W(t)^*\psi\| &= \big\|\,\mathrm{e}^{-itH_0}\,D_\Sigma\,\mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,\eta(H)(D_\Sigma+i)^{-1}\psi_1\big\|\\
&\le |t|\big\|\{f(H)-f(H_0)\}\,\mathrm{e}^{-itH}\,\eta(H)(D_\Sigma+i)^{-1}\psi_1\big\|\\
&\quad + \big\|\{D_\Sigma - tf(H)\}\,\mathrm{e}^{-itH}\,\eta(H)(D_\Sigma+i)^{-1}\psi_1\big\|,
\end{aligned}\tag{4.22}
$$

where $\psi \equiv \eta(H)(D_\Sigma+i)^{-1}\psi_1$. Let $z\in\mathbb{C}\setminus\{\sigma(H_0)\cup\sigma(H)\}$ and set $\widetilde{\eta}(H) := (H-z)^2\eta(H)$. Then Lemmas 2.4.(a), 3.2, and 4.3.(a) imply that

$$
\begin{aligned}
&|t|\big\|\{f(H)-f(H_0)\}\,\mathrm{e}^{-itH}\,\eta(H)(D_\Sigma+i)^{-1}\psi_1\big\|\\
&\le |t|\big\|\{f(H)-f(H_0)\}(H-z)^{-2}(D_\Sigma+i)\big\|\cdot\big\|(D_\Sigma+i)^{-1}\,\mathrm{e}^{-itH}\,\widetilde{\eta}(H)(D_\Sigma+i)^{-1}\big\|\\
&\le \mathrm{Const.}
\end{aligned}
$$

Calculations similar to those of Lemma 4.3.(a) show that the second term of (4.22) is also bounded uniformly in t.

(ii) Let $W(t)$ and ψ be as in point (i). Lemma 2.4.(b), Lemma 4.1.(c), and commutator calculations as in (4.20) lead to

$$
\begin{aligned}
\langle W(t)^*\psi, D_\Sigma W(t)^*\psi\rangle &= \big\langle\psi, \mathrm{e}^{itH}\,D_\Sigma\,\mathrm{e}^{-itH}\,\psi\big\rangle - t\,\big\langle\psi, \mathrm{e}^{itH}\,f(H_0)\,\mathrm{e}^{-itH}\,\psi\big\rangle\\
&= \langle\psi, D_\Sigma\psi\rangle - \int_0^t \mathrm{d}s\,\big\langle\,\mathrm{e}^{-isH}\,\psi, \mathsf{V}_{\Sigma,f}\,\mathrm{e}^{-isH}\,\psi\big\rangle_{2,-2}\\
&\quad + t\,\big\langle\psi, \mathrm{e}^{itH}\{f(H)-f(H_0)\}\,\mathrm{e}^{-itH}\,\psi\big\rangle\,.
\end{aligned}
$$

The local H-smoothness of $f(H)-f(H_0)$ implies the existence of a sequence $t_n \to \infty$ as $n \to \infty$ such that

$$\lim_{n\to\infty} t_n \left\langle \psi, \mathrm{e}^{it_nH}\{f(H)-f(H_0)\}\, \mathrm{e}^{-it_nH}\, \psi\right\rangle = 0.$$

This together with point (i) and the local H-smoothness of $\mathsf{V}_{\Sigma,f}$ implies that

$$\left\langle W_+^*\psi, D_\Sigma W_+^*\psi\right\rangle = \langle \psi, D_\Sigma\psi\rangle - \int_0^\infty \mathrm{d}s \left\langle \mathrm{e}^{-isH}\,\psi, \mathsf{V}_{\Sigma,f}\,\mathrm{e}^{-isH}\,\psi\right\rangle_{2,-2}.$$

Similarly, one finds

$$\left\langle W_-^*\psi, D_\Sigma W_-^*\psi\right\rangle = \langle \psi, D_\Sigma\psi\rangle + \int_{-\infty}^0 \mathrm{d}s \left\langle \mathrm{e}^{-isH}\,\psi, \mathsf{V}_{\Sigma,f}\,\mathrm{e}^{-isH}\,\psi\right\rangle_{2,-2},$$

and thus

$$\left\langle W_+^*\psi, D_\Sigma W_+^*\psi\right\rangle - \left\langle W_-^*\psi, D_\Sigma W_-^*\psi\right\rangle = -\int_{-\infty}^\infty \mathrm{d}s \left\langle \mathrm{e}^{-isH}\,\psi, \mathsf{V}_{\Sigma,f}\,\mathrm{e}^{-isH}\,\psi\right\rangle_{2,-2}. \tag{4.23}$$

Let $\varphi \in \mathscr{D}_s$ with $s > 2$. Due to Lemma 4.3.(b) the vector $W_- f(H_0)^{-1/2}\varphi$ is of the form $\eta(H)\widetilde{\psi}$, with $\eta \in C_0^\infty((0,\infty)\setminus\sigma_{\rm pp}(H))$ and $\widetilde{\psi} \in \mathcal{D}(D_\Sigma)$. Thus one can put $\psi = W_- f(H_0)^{-1/2}\varphi$ in Formula (4.23). This gives

$$\begin{aligned}&\left\langle Sf(H_0)^{-1/2}\varphi, D_\Sigma Sf(H_0)^{-1/2}\varphi\right\rangle - \left\langle f(H_0)^{-1/2}\varphi, D_\Sigma f(H_0)^{-1/2}\varphi\right\rangle\\ &= -\int_{-\infty}^\infty \mathrm{d}s \left\langle \mathrm{e}^{-isH}\,W_- f(H_0)^{-1/2}\varphi, \mathsf{V}_{\Sigma,f}\,\mathrm{e}^{-isH}\,W_- f(H_0)^{-1/2}\varphi\right\rangle_{2,-2},\end{aligned}$$

and the claim follows by Theorem 3.5. □

Remark 4.6. *Symmetrised time delay and usual time delay are equal when* Σ *is spherical (see Formula* (1.1)*). Therefore in such a case Formula* (4.21) *must reduces to the usual Lavine's formula. This turns out to be true. Indeed if* $\Sigma = \mathcal{B}$ *and* $f(u) = 2u$*, then* $f(H_0) = 2H_0$, $\mathsf{V}_{\Sigma,f}$ *is equal to the virial* $\widetilde{V} := 2V - i[V,D]^a$*, and Formula* (4.21) *takes the usual form*

$$\lim_{r\to\infty} \tau_r(\varphi) = \int_{-\infty}^\infty \mathrm{d}s \left\langle \mathrm{e}^{-isH}\,W_- H_0^{-1/2}\varphi, \left\{V - \tfrac{i}{2}[V,D]^a\right\}\mathrm{e}^{-isH}\,W_- H_0^{-1/2}\varphi\right\rangle_{2,-2}.$$

In the following remark we give some insight on the meaning of Formula (4.21) when Σ is not spherical. Then we present two simple examples as an illustration.

Remark 4.7. *Let* V *satisfy Assumption 3.1 with* $\kappa > 4$*, and choose a set* $\Sigma \neq \mathcal{B}$ *satisfying Assumption 2.1. In such a case the function* $f_\gamma(u) := 2(u^2+\gamma)^{-1}u^3$, $u \in \mathbb{R}$*, fulfills the* *requirements of Definition 2.2 and Assumption 4.2 (see Remark 4.4). Thus Theorem 4.5 applies, and one has for $\varphi \in \mathscr{D}_s$ with $s > 2$*

$$\begin{aligned}&\lim_{r\to\infty} \tau_r(\varphi)\\ &= \lim_{\gamma \searrow 0} \int_{-\infty}^{\infty} \mathrm{d}s \left\langle \mathrm{e}^{-isH} W_- f_\gamma(H_0)^{-1/2}\varphi, \mathsf{V}_{\Sigma,f_\gamma} \mathrm{e}^{-isH} W_- f_\gamma(H_0)^{-1/2}\varphi \right\rangle_{2,-2}.\end{aligned}$$

Now $f_\gamma(H_0)\varphi$ converges in norm to $2H_0\varphi$ as $\gamma \searrow 0$, so formally one gets the identity

$$\lim_{r\to\infty} \tau_r(\varphi) = \tfrac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}s \left\langle \mathrm{e}^{-isH} W_- H_0^{-1/2}\varphi, \mathsf{V}_\Sigma \, \mathrm{e}^{-isH} W_- H_0^{-1/2}\varphi \right\rangle_{2,-2}, \qquad (4.24)$$

where

$$\mathsf{V}_\Sigma := 2V - i[V, D_\Sigma]^a = 2V - \tfrac{i}{2} \sum_{j\le d} \big\{ \big[V, F_{\Sigma j}(P)\big] \cdot Q_j + Q_j \cdot \big[V, F_{\Sigma j}(P)\big] \big\},$$

and

$$F_{\Sigma j}(P) = -(\partial_j G_\Sigma)(P) P^2. \qquad (4.25)$$

The pseudodifferential operator V_Σ generalises the virial $\widetilde{V}$ of the isotropic case. It furnish a measure of the variation of the potential V along the vector field $-F_\Sigma$, which is orthogonal to the hypersurfaces $\partial\Sigma_r$ due to Remark 2.3. Therefore Formula (4.24) *establishes a relation between symmetrised time delay and the variation of V along $-F_\Sigma$. Moreover one can rewrite V_Σ as*

$$\begin{aligned}\mathsf{V}_\Sigma &= \widetilde{V} + i[V, D - D_\Sigma]^a\\ &= \widetilde{V} + \tfrac{i}{2} \sum_{j\le d} \big\{ \big[V, \big(P_j - F_{\Sigma j}(P)\big)\big] \cdot Q_j + Q_j \cdot \big[V, \big(P_j - F_{\Sigma j}(P)\big)\big] \big\}.\end{aligned}$$

where $P - F_\Sigma(P)$ is orthogonal to P due to Formulas (4.25) *and* (2.6)*. Consequently there are two distinct contributions to symmetrised time delay. The first one is standard; it is associated to the term $\widetilde{V}$, and it is due to the variation of the potential V along the radial coordinate (see [11, Sec. 6] for details). The second one is new; it is associated to the term $i[V, D - D_\Sigma]^a$ and it is due to the variation of V along the vector field $x \mapsto x - F_\Sigma(x)$.*

Example 4.8 (Examples in $\mathbb{R}^2$)**.** *Set $d = 2$, suppose that V satisfies Assumption 3.1 with $\kappa > 4$, and let Σ be equal to the superellipse $\mathcal{E} := \big\{(x_1, x_2) \in \mathbb{R}^2 \mid x_1^4 + x_2^4 < 1\big\}$. Then one has $G_\mathcal{E}(x) = -\frac{1}{4}\ln\big(x_1^4 + x_2^4\big)$ and $(\partial_j G_\mathcal{E})(x) = -x_j^3\big(x_1^4 + x_2^4\big)^{-1}$. Thus due to Remark 4.7 the symmetrised time delay associated to $\mathcal{E}$ is (formally) caracterised by the pseudodifferential operator*

$$\mathsf{V}_\mathcal{E} = 2V - \tfrac{i}{2} \sum_{j\le d} \big\{ \big[V, F_{\mathcal{E} j}(P)\big] \cdot Q_j + Q_j \cdot \big[V, F_{\mathcal{E} j}(P)\big] \big\},$$

where $F_{\mathcal{E} j}(P) = P_j^3 P^2 \big(P_1^4 + P_2^4\big)^{-1}$ (see Figure 1).

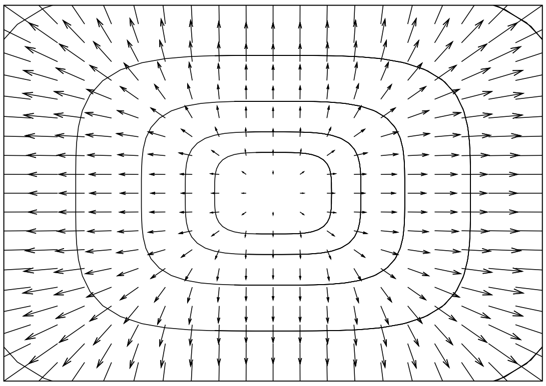

Figure 1: The vector field $F_{\mathcal{E}}$ and the sets $\partial\mathcal{E}_r$

When Σ is equal to the star-type set

$$\mathcal{S} := \Big\{\ell(\theta)\,\mathrm{e}^{i\theta} \in \mathbb{R}^2 \mid \theta \in [0,2\pi),\ \ell(\theta) < \big[\cos(2\theta)^8 + \sin(2\theta)^8\big]^{-1/2}\Big\},$$

one has $G_{\mathcal{S}}(x) = \frac{7}{2}\ln(x_1^2+x_2^2) - \frac{1}{2}\ln\big[(x_1^2-x_2^2)^8 + 2^8(x_1x_2)^8\big]$, and a direct calculation using Formula (4.25) *gives the vector field $F_{\mathcal{S}}$. The result is plotted in Figure 2.*

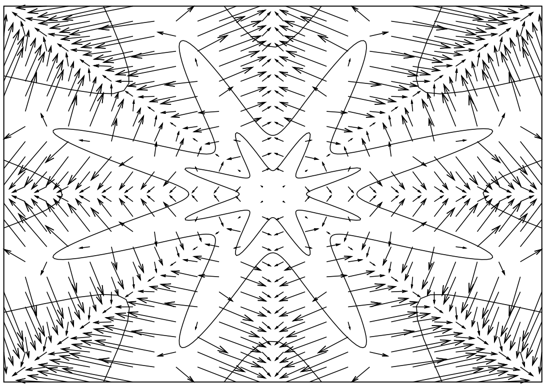

Figure 2: The vector field $F_{\mathcal{S}}$ and the sets $\partial\mathcal{S}_r$

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Appendix

Proof of Lemma 3.2. We first prove that $(H-z)^{-1}$ extends to an element of $\mathscr{B}\big(\mathcal{H}_t^{-2},\mathcal{H}_t\big)$ for each $t \geq 0$. This clearly holds for $t = 0$. Since $(H_0 - z)^{-1}\langle P\rangle^2 = 2+(1+2z)(H_0 - z)^{-1}$ one has by virtue of the second resolvent equation

$$\begin{aligned}
&\langle Q\rangle^t (H-z)^{-1} \langle P\rangle^2 \langle Q\rangle^{-t} \qquad (4.26)\\
&= 2 + (1+2z)\langle Q\rangle^t (H_0-z)^{-1} \langle Q\rangle^{-t}\\
&\quad - \langle Q\rangle^t (H_0-z)^{-1}(\langle Q\rangle V)\langle Q\rangle^{-t}\cdot\langle Q\rangle^{t-1}(H-z)^{-1}\langle P\rangle^2\langle Q\rangle^{-t}.
\end{aligned}$$

If we take $t = 1$ we find that each term on the r.h.s. of (4.26) is in $\mathscr{B}(\mathcal{H})$ due to [2, Lemmas 1 & 2]. Hence, by interpolation, $\langle Q\rangle^t (H-z)^{-1}\langle P\rangle^2\langle Q\rangle^{-t} \in \mathscr{B}(\mathcal{H})$ for each $t \in [0,1]$. Next we choose $t \in (1,2]$ and obtain, by using the preceding result and (4.26), that $\langle Q\rangle^t (H-z)^{-1}\langle P\rangle^2\langle Q\rangle^{-t} \in \mathscr{B}(\mathcal{H})$ for these values of t. By iteration (take $t \in (2,3]$, then $t \in (3,4]$, etc.) one obtains that $\langle Q\rangle^t (H-z)^{-1}\langle P\rangle^2\langle Q\rangle^{-t} \in \mathscr{B}(\mathcal{H})$ for each $t > 0$. Thus $(H-z)^{-1}$ extends to an element of $\mathscr{B}\big(\mathcal{H}_t^{-2},\mathcal{H}_t\big)$ for each $t \geq 0$. A similar argument shows that $(H-z)^{-1}$ also extends to an element of $\mathscr{B}\big(\mathcal{H}_t^{-2},\mathcal{H}_t\big)$ for each $t < 0$. The claim follows then by using duality and interpolation. □

Proof of Lemma 3.3. For $\varphi \in \mathscr{D}_s$ and $t \in \mathbb{R}$, we have (see the proof of [7, Lemma 4.6])

$$(W_- - 1)\,\mathrm{e}^{-itH_0}\varphi = -i\,\mathrm{e}^{-itH}\int_{-\infty}^t \mathrm{d}\tau\ \mathrm{e}^{i\tau H}\, V\,\mathrm{e}^{-i\tau H_0}\varphi,$$

where the integral is strongly convergent. Hence to prove (3.17) it is enough to show that

$$\int_{-\infty}^{-\delta}\mathrm{d}t\int_{-\infty}^{t}\mathrm{d}\tau\,\big\|V\,\mathrm{e}^{-i\tau H_0}\varphi\big\| < \infty \qquad (4.27)$$

for some $\delta > 0$. If $\zeta := \min\{\kappa, s\}$, then $\big\|\langle Q\rangle^\zeta\varphi\big\| < \infty$, and $V\langle P\rangle^{-2}\langle Q\rangle^\zeta$ belongs to $\mathscr{B}(\mathcal{H})$ due to Assumption 3.1. Since $\eta(H_0)\varphi = \varphi$ for some $\eta \in C_0^\infty((0,\infty)\setminus\sigma_{\rm pp}(H))$, this implies that

$$\big\|V\,\mathrm{e}^{-i\tau H_0}\varphi\big\| \leq \text{Const.}\,\big\|\langle Q\rangle^{-\zeta}\langle P\rangle^2\eta(H_0)\,\mathrm{e}^{-i\tau H_0}\langle Q\rangle^{-\zeta}\big\|.$$

For each $\varepsilon > 0$, it follows from [2, Lemma 9] that there exists a constant $\mathrm{c} > 0$ such that $\big\|V\,\mathrm{e}^{-i\tau H_0}\varphi\big\| \leq \mathrm{c}\,(1+|\tau|)^{-\zeta+\varepsilon}$. Since $\zeta > 2$, this implies (3.17). The proof of (3.18) is similar. □

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