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Time delay and resonances in potential scattering

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Abstract
We present stationary expressions for the on-shell time delay operator and for its trace in quantum-mechanical potential scattering. The trace of this operator is shown to represent the time delay for a monoenergetic and well-collimated beam of initial states. For exponentially decaying potentials the total scattering cross section and the trace of the on-shell time delay operator have analytic extensions to complex energies, with poles at most at the usual resonance poles (poles of the analytically continued S-matrix) in the lower half plane and at their mirror images with respect to the real axis. At real energies close to such a pole both the scattering cross section and the time delay are approximately of Breit–Wigner type, the sign of the time delay being related to that of the virial. These results corroborate the idea that a resonance should show up through a peak in the scattering cross section and a large (though positive) time delay.

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1. Introduction

The concept of scattering resonances has been developed and formalized in a very large number of publications. The principal characteristic of a resonance phenomenon is usually considered to reside in a sharp peak of the scattering cross section but, as pointed out in the literature (e.g. chapter 11 of [1], chapter 13 of [2]), this should be concurrent with a large positive time delay. This idea has been used in various calculations of resonance states or resonances (e.g. [3–5]). Our aim here is to show that, in situations where a resonance can be associated with a pole of the analytically continued S-matrix, there will be a strong correlation between peaks in the scattering cross and large (positive or negative) time delays. More precisely we shall prove that the time delay will also admit an analytic continuation having poles at the same points as the S-matrix.

We shall consider scattering theory for self-adjoint Schrödinger operators $H = H_0 + V$ in the complex Hilbert space $\mathcal{H} = L^2(\mathbf{R}^n)$. Here H_0 is the usual self-adjoint realization of the differential operator $-\Delta = -\sum_{k=1}^{n}(\partial/\partial x_k)^2$ and V is a short range potential. We assume that $n \geqslant 2$; with some care in the formulation our results are also valid for $n = 1$.

The notion of *time delay* for a scattering situation was introduced by Eisenbud [6] and Wigner [7]. In the Hilbert space approach it is described by a self-adjoint operator T commuting with H_0. It follows that T is decomposable in the spectral representation of H_0 (see equations (6) and (7)): there is a measurable family $\{T(\lambda)\}_{\lambda>0}$ of bounded operators acting in $L^2(S^{n-1})$ such that, if $f_\lambda \in L^2(S^{n-1})$ denotes the component at energy λ of a state vector f, then $(Tf)_\lambda = T(\lambda)f_\lambda$ for each f in the domain of T. The results of [6] suggest that the on-shell time delay operator $T(\lambda)$ should be related to the S-matrix $S(\lambda)$ by the formula $T(\lambda) = -\mathrm{i}S(\lambda)^*\,\mathrm{d}S(\lambda)/\mathrm{d}\lambda$. The decomposable operator determined by the family $\{-\mathrm{i}S(\lambda)^*\mathrm{d}S(\lambda)/\mathrm{d}\lambda\}_{\lambda>0}$ is usually called the *Eisenbud–Wigner time delay operator*.

We mention some other approaches to the question of time delay. Smith [8] proposed to define time delay as the difference of the sojourn times of the scattering state and of the initial state in balls of large radius ρ (more precisely one would finally take the limit $\rho \to \infty$). Thus, if f is a normalized state vector ($\|f\| = 1$) describing the initial state and $g = \Omega_- f$ the associated scattering state (with Ω_- the wave operator corresponding to the limit $t \to -\infty$), then the time delay for this state should be given by the expression

$$\langle f, Tf\rangle = \lim_{\rho\to\infty}\left[\int_{-\infty}^{\infty}\mathrm{d}t\int_{|x|\leqslant\rho}\mathrm{d}x\,|(\mathrm{e}^{-\mathrm{i}Ht}\Omega_- f)(x)|^2 - \int_{-\infty}^{\infty}\mathrm{d}t\int_{|x|\leqslant\rho}\mathrm{d}x\,|(\mathrm{e}^{-\mathrm{i}H_0t}f)(x)|^2\right]. \quad (1)$$

The existence of this limit and its relation with the Eisenbud–Wigner time delay operator has been investigated by various authors (see the references given in the review by Martin [9] and in [10]). In [10] it was proved, essentially for potentials decaying faster than $|x|^{-2}$, that the limit in (1) exists for a dense set of vectors f and coincides with the expectation value $\langle f, -\mathrm{i}S(\lambda)^*\,\mathrm{d}S(\lambda)/\mathrm{d}\lambda f\rangle$ of the Eisenbud–Wigner time delay operator.

A different time-dependent expression for time delay was given by Lavine [11], namely

$$\langle f, H_0Tg\rangle = \int_{-\infty}^{\infty}\langle\,\mathrm{e}^{-\mathrm{i}H_0t}f, \Omega_-^*\tilde{V}\Omega_-\,\mathrm{e}^{-\mathrm{i}H_0t}g\rangle\,\mathrm{d}t, \quad (2)$$

where

$$\tilde{V} = V + \frac{\mathrm{i}}{2}[D, V] = V + \frac{\mathrm{i}}{2}DV - \frac{\mathrm{i}}{2}VD \quad (3)$$

and $D = (2\mathrm{i})^{-1}(x\cdot\nabla + \nabla\cdot x)$ is the generator of the dilation group. Jensen [12] has studied the expression on the rhs of (2) and proved a theorem giving equality of T with the Eisenbud–Wigner time delay operator; his result applies to potentials decaying faster than $|x|^{-1}$.

In order to arrive at an expression for the differential and the total scattering cross section in the Hilbert space formulation of scattering, one has to introduce an appropriate description of an essentially monoenergetic and well-collimated beam of initial states. Under suitable hypotheses this leads to the usual expression for the differential scattering cross section at energy λ as the absolute square of the scattering amplitude $f(\lambda; \omega \to \omega')$ for scattering from the initial direction ω into the final direction ω'. Upon integration of the differential scattering cross section over all final directions and averaging over all initial directions, one finds that this averaged total scattering cross section $\bar{\sigma}(\lambda)$ is given by a multiple of the square of the Hilbert–Schmidt norm of the on-shell operator $R(\lambda) := S(\lambda) - I$. In discussing resonances it then seems natural to define in a similar way a time delay for a beam. The detailed calculation will be indicated in section 4. It will be found that the time delay for a beam, at energy λ, is proportional to the trace $\tau(\lambda)$ of the operator $T(\lambda)$. We note that the trace of $T(\lambda)$ has also been considered in a related context by Bollé and Gesztesy [13].

In situations where the S-matrix $S(\lambda)$ has an analytic continuation into some complex domain, its poles (and consequently those of the scattering amplitude) lie in the lower half complex plane. These poles are often referred to as *resonance poles*. It turns out that the averaged total scattering cross section $\bar{\sigma}(\lambda)$ and the time delay $\tau(\lambda)$ then have analytic continuations too. Since the scattering cross section also involves the complex-conjugate of the scattering amplitude (or the adjoint $S(\lambda)^*$ of the S-matrix), it will have poles also in the upper half plane. The poles in the upper half plane form conjugate pairs with the resonance poles in the lower half plane, a pair consisting of a resonance pole and its mirror image with respect to the real axis. Similarly one finds (see section 5) that the possible poles of the time delay $\tau(\lambda)$ are located at the points of these conjugate pairs. In certain situations one may expect the shape of $\bar{\sigma}(\lambda)$ and $\tau(\lambda)$, as functions of the energy λ near a resonance pole, to be approximately of Breit–Wigner type (see section 6 for details). For the time delay the sign of such a Breit–Wigner type approximation is related to the sign of $\tilde{V}$.

The paper is organized as follows. In section 2 we introduce our notations and present various preliminary results most of which can be found in the published literature. In section 3 we determine trace class properties of the on-shell time delay operator and continuity properties of its integral kernel for potentials with a power decay law. Section 4 is devoted to the derivation of the expression for the time delay of a beam, and in section 5 we discuss analyticity properties of the averaged total scattering cross section and of the time delay for exponentially decaying potentials. In section 6 we present an approximate treatment leading to Breit–Wigner type expressions for these quantities. In order to avoid burdening the derivation of properties of the time delay with technical details, we restrict our proofs in section 3 to situations where the potential V and the virial $\tilde{V}$ are bounded functions. In the appendix we indicate how to generalize these results to a class of potentials that may have local singularities.

2. Notations and preliminary results

We denote by $Q = (Q_1, \ldots, Q_n)$ and $P = (P_1, \ldots, P_n)$ the n-component position and momentum operator, by $D = (P \cdot Q + Q \cdot P)/2$ the self-adjoint generator of the dilation group and by $\langle Q \rangle$ the operator of multiplication in $L^2(\mathbf{R}^n)$ by the function $x \mapsto \langle x \rangle := (1 + |x|^2)^{1/2}$. We consider potentials $V : \mathbf{R}^n \to \mathbf{R}$ that can be expressed in the form of a product of three real-valued functions, $V = UA^2 = AUA$, satisfying the following conditions:

(C_κ) (i) A is a smooth function satisfying $A(x) > 0$ for all $x \in \mathbf{R}^n$ and $|A(x)| + |\nabla A(x)| + |\Delta A(x)| \leqslant c\langle x \rangle^{-\kappa}$ for some constant c;
(ii) $U = U_1 + U_2$ with real U_1 and U_2 satisfying $U_1 \in L^\infty(\mathbf{R}^n)$, $x \cdot \nabla U_1 \in L^\infty(\mathbf{R}^n)$, $\langle x \rangle U_2 \in L^\infty(\mathbf{R}^n) + L^q(\mathbf{R}^n)$ for some q satisfying $q \geqslant 2$ and $q > n/2$;
(iii) $U_1 x \cdot \frac{\nabla A}{A}$ belongs to $L^\infty(\mathbf{R}^n)$ and $U_2 x \cdot \frac{\nabla A}{A} \in L^\infty(\mathbf{R}^n) + L^q(\mathbf{R}^n)$ with q as in (ii).

Two cases of particular interest concern the functions $A(x) = \langle x \rangle^{-\kappa}$ and $A(x) = \mathrm{e}^{-\alpha\langle x \rangle}$, with $\kappa > 0$ and $\alpha > 0$. In the first case condition (iii) can be omitted, its validity follows from (ii). For technical reasons we shall make stronger assumptions on U_2 in various developments. In particular, we say that V satisfies condition ($C_{\kappa,n}$) if $q > n$ in (ii) and (iii).

We recall that a multiplication operator in $L^2(\mathbf{R}^n)$ by a function $\theta \in L^\infty(\mathbf{R}^n) + L^q(\mathbf{R}^n)$, with q as in (ii), is H_0-bounded as well as H-bounded. Except for lemma 1, where it suffices to have $\kappa > 0$, we shall always assume that (C_κ) is satisfied for some $\kappa > 1/2$. So, roughly speaking, the potential should decay faster than $\langle x \rangle^{-1}$, but the presence of U_2 allows for local singularities of V. Larger values of κ are necessary in order to obtain finer properties of the time delay operator $T(\lambda)$: if V decays faster than $\langle x \rangle^{-n}$, then $T(\lambda)$ is a trace class operator and its integral kernel is continuous. Further on, in section 5, the function A will be assumed to decay exponentially in order to allow for analytic continuation into the complex plane of various λ-dependent operators.

Unless otherwise stated, $\langle\cdot,\cdot\rangle$ and $\|\cdot\|$ denote the scalar product and the norm in various L^2-spaces. $\|\cdot\|$ will also be used for the norm of operators acting in a Hilbert space or between two Hilbert spaces. $\mathcal{B}(\mathcal{K})$ stands for the set of all bounded everywhere defined linear operators in a Hilbert space $\mathcal{K}$, $\mathcal{B}_1(\mathcal{K})$ for the trace class of operators in $\mathcal{K}$. The symbols $\|\cdot\|_1$ and $\|\cdot\|_2$ are used for the trace norm and the Hilbert–Schmidt norm, respectively. $\mathcal{D}(C)$ denotes the domain of a linear operator C, $\mathcal{R}(C)$ its range and $\mathcal{N}(C)$ its null space. I denotes the identity operator in various spaces. We set $\mathbf{R}^+ = (0,\infty)$, $\mathbf{C}^+ = \{z \in \mathbf{C} \mid \Im m\, z > 0\}$ and $\mathbf{C}^- = \{z \in \mathbf{C} \mid \Im m\, z < 0\}$. For $z \in \mathbf{C}^+ \cup \mathbf{C}^-$, we let $R_z^o = (H_0 - z)^{-1}$ and $R_z = (H - z)^{-1}$ be the resolvent of H_0 and H, respectively. We use the same symbol for functions defined on $\mathbf{R}^n$ and for the associated multiplication operators in $L^2(\mathbf{R}^n)$, e.g. $(\theta f)(x) = \theta(x) f(x)$.

Under the assumptions on V stated above ($\kappa > 1/2$) the usual properties of scattering theory are satisfied (see, e.g., theorem XIII.33 in [14]). The total Hamiltonian $H = H_0 + V$, defined as an operator sum on the domain $\mathcal{D}(H_0)$ of H_0, is self-adjoint on this domain and bounded from below. H has no singularly continuous spectrum, its spectrum $\sigma(H)$ consists of an absolutely continuous part covering the interval $[0,\infty)$ and possibly of a set of eigenvalues in $(-\infty, 0]$. In particular, H has no positive eigenvalues [15]. The wave operators $\Omega_+ = s - \lim_{t\to+\infty} \mathrm{e}^{\mathrm{i}Ht}\,\mathrm{e}^{-\mathrm{i}H_0 t}$ and $\Omega_- = s - \lim_{t\to-\infty} \mathrm{e}^{\mathrm{i}Ht}\,\mathrm{e}^{-\mathrm{i}H_0 t}$ exist, and the scattering theory is asymptotically complete: the range of each of the wave operators $\Omega_\pm$ is equal to the absolutely continuous subspace $\mathcal{H}_{\mathrm{ac}}(H)$ of the total Hamiltonian H. The scattering operator $S = \Omega_+^* \Omega_-$ is unitary. The existence of the Eisenbud–Wigner time delay operator T and the equality of the matrix elements $\langle f, H_0 T g\rangle$ with Lavine's expression (2) have been shown in [12] under the assumption that the supports of f and g in the spectral representation of H_0 belong to a compact interval in $(0,\infty)$.

The expression for the virial $\tilde{V}$ on the rhs of (3) determines a quadratic form on $\mathcal{D}(H) = \mathcal{D}(H_0)$, which may also be written as $\tilde{V} = A\tilde{U}A$ with

$$\tilde{U} = U + UQ\cdot\frac{\nabla A}{A} + \frac{1}{2}Q\cdot\nabla U_1 - \frac{n}{2}U_2 + \frac{\mathrm{i}}{2}P\cdot QU_2 - \frac{\mathrm{i}}{2}U_2 Q\cdot P. \tag{4}$$

Here, for example, ∇A denotes the multiplication operator by the function $\nabla A(\cdot)$ and $P\cdot Q = \sum_{j=1}^n P_j Q_j$.

The potentials considered here satisfy the hypotheses (H1) and (H2) of our earlier paper [10] on time delay. We shall use various estimates from that paper. In particular, by lemmas 2, 3 and 6 of [10], we have the following results:

Lemma 1. *Assume that V satisfies (C_κ) with $\kappa > 0$. Let $\varphi \in C_0^\infty(\mathbf{R})$ or let φ be the function $\varphi(\lambda) = (\lambda - z)^{-1}$ with $z \in \mathbf{C}\backslash\sigma(H)$, and let $\mathcal{W}$ be a H_0-bounded operator commuting with Q. Then, for each $s \in \mathbf{R}$, all of the following operators (taking closure if necessary) belong to $\mathcal{B}(L^2(\mathbf{R}^n))$:*

$\langle Q\rangle^s \varphi(H_0)\langle Q\rangle^{-s}$, $\quad\langle Q\rangle^s \varphi(H_0)\mathcal{W}\langle Q\rangle^{-s}$, $\quad\langle Q\rangle^s P_j\varphi(H_0)\langle Q\rangle^{-s}$,
$\langle Q\rangle^{s-1} D\varphi(H_0)\langle Q\rangle^{-s}$, $\quad\langle Q\rangle^s \varphi(H)\langle Q\rangle^{-s}$, $\quad\langle Q\rangle^s \varphi(H)\mathcal{W}\langle Q\rangle^{-s}$,
$\langle Q\rangle^s P_j\varphi(H)\langle Q\rangle^{-s}$ $\quad(j = 1,\ldots,n)$.

In what follows it will be important to know that various operators are smooth relative to H_0 or H. We recall that a closed operator C is said to be H-smooth on an interval J of $\mathbf{R}^+$ if there is a finite constant c_J such that $\int_{-\infty}^{\infty} \|C\,\mathrm{e}^{-\mathrm{i}Ht}E(J)f\|^2\,\mathrm{d}t \leqslant c_J\|f\|^2$ for each vector $f \in \mathcal{H}$, where $\{E(\cdot)\}$ denotes the spectral measure of H; an equivalent condition is that $\|C[(H-z)^{-1} - (H-\bar{z})^{-1}]C^*\| \leqslant c_j$ for all z with $\Re e\, z \in J$ and $0 < \Im m\, z < 1$. The operator C is said to be locally H-smooth on $\mathbf{R}^+$ if it is H-smooth on each compact $J \subset \mathbf{R}^+$. We refer to section XIII.7 of [14] or section 7.1 of [16] for details on the theory of smoothness.

Often locally H-smooth operators are constructed by proving a Mourre estimate on J [16]. In such a case one even obtains the existence in norm of the limits of $C(H-\lambda\pm\mathrm{i}\varepsilon)^{-1}C^*$ as $\varepsilon\to+0$ for $\lambda\in J$. A simple example is given by taking $C=\langle Q\rangle^{-\rho}$, $\rho\geqslant 1$, and $H=H_0$. In this case a very easy argument (see equation (7.0.3) of [16]) shows that, given $\delta>0$, there is a constant c_δ such that, for $\lambda>\delta$, $0<\varepsilon<1$ and f in the Schwartz space $\mathcal{S}(\mathbf{R}^n)$:

$$\left|\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\langle f,(H_0-\lambda\pm\mathrm{i}\varepsilon)^{-1}f\rangle\right|\leqslant c_\delta\varepsilon^{-1/2}(\|f\|^2+\|Df\|^2). \tag{5}$$

By taking functions f of the form $f=\varphi(H_0)\langle Q\rangle^{-\rho}g$, with $g\in\mathcal{S}(\mathbf{R}^n)$ and $\varphi\in C_0^\infty(\mathbf{R})$ such that $\varphi(\mu)=1$ in some neighbourhood of λ, and by using the boundedness of $D\varphi(H_0)\langle Q\rangle^{-\rho}$ (lemma 1), one obtains the convergence in norm of $\langle Q\rangle^{-\rho}(H_0-\lambda\pm\mathrm{i}\varepsilon)^{-1}\langle Q\rangle^{-\rho}$ as $\varepsilon\to+0$, uniformly in $\lambda>\delta$ (for $\rho\geqslant 1$). This result also holds for any $\rho>1/2$, and one has the estimate $\|\langle Q\rangle^{-\rho}(H_0-\lambda\pm\mathrm{i}\varepsilon)^{-1}\langle Q\rangle^{-\rho}\|\leqslant c\lambda^{-1/2}$ for all $\lambda>\delta>0$, where c is a constant depending on ρ and δ (see, for example, the proof of lemma 5 in section XIII.8 of [14] by considering also the λ-dependence of the occurring constants). For the class of Hamiltonians considered here (V satisfying (C_κ) for $\kappa>1/2$) it is well known (see, e.g., chapter 4 of [17]) that $\langle Q\rangle^{-\rho}(H-\lambda\pm\mathrm{i}\varepsilon)^{-1}\langle Q\rangle^{-\rho}$ converge in norm as $\varepsilon\to+0$ for each $\lambda>0$ and $\rho>1/2$, uniformly in λ on each compact $J\subset\mathbf{R}^+$, showing that $\langle Q\rangle^{-\rho}$ is locally H-smooth on $\mathbf{R}^+$ for these values of ρ.

Smooth operators relative to H_0 allow the construction of operators mapping between $\mathcal{H}=L^2(\mathbf{R}^n)$ and $L^2(S^{n-1})$, where S^{n-1} denotes the unit sphere in $\mathbf{R}^n$: $S^{n-1}=\{x\in\mathbf{R}^n\,||x|=1\}$. The space $L^2(S^{n-1})$ occurs naturally in the spectral representation of H_0: one identifies $L^2(\mathbf{R}^n)$ with the space $\mathcal{K}=L^2(\mathbf{R}^+;L^2(S^{n-1}))$, the Hilbert space of $L^2(S^{n-1})$-valued functions defined on $\mathbf{R}^+=(0,\infty)$, by the unitary mapping F_0 given as follows:

$$(F_0f)(\lambda;\omega)=2^{-1/2}\lambda^{(n-2)/4}(\mathcal{F}f)(\sqrt{\lambda}\omega),\qquad \lambda\in\mathbf{R}^+,\quad \omega\in S^{n-1}, \tag{6}$$

where $\mathcal{F}$ denotes Fourier transformation. For simplicity, we shall write $f_\lambda(\omega)$ for $(F_0f)(\lambda;\omega)$. If $f\in L^2(\mathbf{R}^n)$, then the family $\{f_\lambda\}$ ($f_\lambda\in L^2(S^{n-1})$ for a.a. $\lambda\in\mathbf{R}^+$) gives the representative of f in the spectral representation of H_0:

$$(H_0f)_\lambda=\lambda f_\lambda\qquad\text{if}\quad f\in\mathcal{D}(H_0),\qquad\text{and}\qquad \|f\|^2_{L^2(\mathbf{R}^n)}=\int_0^\infty\|f_\lambda\|^2_{L^2(S^{n-1})}\,\mathrm{d}\lambda. \tag{7}$$

The norm in $L^2(S^{n-1})$ is defined in terms of the induced Lebesgue measure on S^{n-1}. We shall denote this measure by $\mathrm{d}\omega$.

If C is a closed operator such that its adjoint C^* is locally H_0-smooth on $\mathbf{R}^+$, then there exists a measurable family of bounded operators $\{M_C(\lambda)\}_{\lambda>0}$ from $L^2(\mathbf{R}^n)$ to $L^2(S^{n-1})$ such that $\sup_{\lambda\in J}\|M_C(\lambda)\|<\infty$ for each compact $J\subset\mathbf{R}^+$,

$$(Cf)_\lambda=M_C(\lambda)f\qquad\text{for}\quad\text{a.a. }\lambda>0,\quad\forall f\in\mathcal{D}(C) \tag{8}$$

and

$$C^*f=\int_{\mathbf{R}^+}M_C(\lambda)^*f_\lambda\,\mathrm{d}\lambda\qquad\text{if}\quad F_0f\text{ has compact support in }\mathbf{R}^+. \tag{9}$$

The proof can be found in section 17.1.2 of [18] (and essentially also in the original paper by Kato [19] or in lemma 10.20 of [20]). In many situations encountered here the operator C will in fact be bounded.

We mention a few simple consequences of (8) and (9):

$$M_{CZ}(\lambda)=M_C(\lambda)Z\qquad\text{if}\quad Z\in\mathcal{B}(L^2(\mathbf{R}^n)), \tag{10}$$

$$M_{\varphi(H_0)C}(\lambda)=M_C(\lambda)\qquad\text{if}\quad\varphi\in C_0^\infty(\mathbf{R}^+)\quad\text{with}\quad\varphi(\lambda)=1. \tag{11}$$

Also, if C_1 is a second operator satisfying the conditions imposed on C, and if $\varphi \in L^\infty(\mathbf{R})$ has compact support in $\mathbf{R}^+$, then for $f \in \mathcal{D}(C)$ and $g \in \mathcal{D}(C_1)$

$$\langle f, C^*\varphi(H_0)C_1 g\rangle = \int_{\mathbf{R}^+} \varphi(\lambda)\big\langle M_C(\lambda)f, M_{C_1}(\lambda)g\big\rangle_{L^2(S^{n-1})}\,\mathrm{d}\lambda,$$

which implies that

$$C^*\varphi(H_0)C_1 = \int_{\mathbf{R}^+} \varphi(\lambda)M_C(\lambda)^*M_{C_1}(\lambda)\,\mathrm{d}\lambda. \tag{12}$$

If C_1 is unbounded, the left-hand side of (12) should be interpreted as the (bounded) closure of the densely defined operator $C^*\varphi(H_0)C_1$. In general, the integrals in (9) and (12) are Bochner integrals. In most applications the integrand in (12) will be (at least strongly) continuous in λ and the integral may be interpreted in the sense of Riemann.

The following consequence of (12) will be important. Assume that, for $\mu > 0$, the limits of $C^*R^o_{\mu+\mathrm{i}\varepsilon}C_1$ and $C^*R^o_{\mu-\mathrm{i}\varepsilon}C_1$ as $\varepsilon \to +0$ exist, or more generally that $\lim_{\varepsilon\to+0} C^*\big[R^o_{\mu+\mathrm{i}\varepsilon} - R^o_{\mu-\mathrm{i}\varepsilon}\big]C_1$ exists (e.g. in the norm of $\mathcal{B}(\mathcal{H})$). Assume also that $\lambda \mapsto M_C(\lambda)$ and $\lambda \mapsto M_{C_1}(\lambda)$ are continuous (e.g. in norm) on $\mathbf{R}^+$. Let $\varphi \in C_0^\infty(\mathbf{R})$ with $\varphi(\lambda) = 1$ in some neighbourhood of μ. Then

$$\begin{aligned}\lim_{\varepsilon\to+0} C^*\big[R^o_{\mu+\mathrm{i}\varepsilon} - R^o_{\mu-\mathrm{i}\varepsilon}\big]C_1 &= \lim_{\varepsilon\to+0} C^*\big[R^o_{\mu+i\varepsilon} - R^o_{\mu-i\varepsilon}\big]\varphi(H_0)C_1\\ &= \lim_{\varepsilon\to+0}\int_{\mathbf{R}^+}\left[\frac{1}{\lambda-\mu-\mathrm{i}\varepsilon} - \frac{1}{\lambda-\mu+\mathrm{i}\varepsilon}\right]\varphi(\lambda)M_C(\lambda)^*M_{C_1}(\lambda)\,\mathrm{d}\lambda\\ &= 2\pi\mathrm{i}M_C(\mu)^*M_{C_1}(\mu),\end{aligned}$$

i.e.,

$$M_C(\mu)^*M_{C_1}(\mu) = \frac{1}{2\pi\mathrm{i}}\lim_{\varepsilon\to+0} C^*\big[R^o_{\mu+\mathrm{i}\varepsilon} - R^o_{\mu-\mathrm{i}\varepsilon}\big]C_1. \tag{13}$$

We consider some special cases that are important in our applications. The results of examples 2 and 5 will be needed only in the appendix.

Example 1. $C = \langle Q\rangle^{-\rho}$, with $\rho > 1/2$. Then C is H_0-smooth on (δ, ∞) for each $\delta > 0$. Thus (at least formally)

$$M_C(\lambda)f = (Cf)_\lambda = 2^{-1/2}(2\pi)^{-n/2}\lambda^{(n-2)/4}\int_{\mathbf{R}^n} \mathrm{e}^{-\mathrm{i}\sqrt{\lambda}\omega\cdot x}\langle x\rangle^{-\rho}f(x)\,\mathrm{d}x. \tag{14}$$

In this case $M_C(\lambda)$ is an integral operator with kernel given by

$$K(\lambda;\omega,x) = 2^{-1/2}(2\pi)^{-n/2}\lambda^{(n-2)/4}\,\mathrm{e}^{-\mathrm{i}\sqrt{\lambda}\omega\cdot x}\langle x\rangle^{-\rho}.$$

By (13) and the bound for $\|\langle Q\rangle^{-\rho}(H_0 - \lambda \pm \mathrm{i}\varepsilon)^{-1}\langle Q\rangle^{-\rho}\|$ given below equation (5), one has $\|M_{\langle Q\rangle^{-\rho}}(\lambda)\| \leqslant c\lambda^{-1/4}$ for $\lambda \geqslant 1$. If $\rho > n/2, K(\lambda;\omega,x)$ is a Hilbert–Schmidt kernel, so in this case $M_{\langle Q\rangle^{-\rho}}(\lambda)$ is a Hilbert–Schmidt operator. Also, by using the inequality $|\mathrm{e}^{\mathrm{i}\alpha} - \mathrm{e}^{\mathrm{i}\beta}| \leqslant 2^{1-\nu}|\alpha-\beta|^\nu$ $(0 \leqslant \nu \leqslant 1, \alpha, \beta \in \mathbf{R})$, one easily finds that $\lambda \mapsto M_{\langle Q\rangle^{-\rho}}(\lambda)$ is then Hölder continuous in Hilbert–Schmidt norm on $\mathbf{R}^+$, with Hölder index given by $\min(1, \rho - n/2)$. In particular, if A is as in (C_κ) and $\kappa > n/2$, then $M_A(\lambda) \equiv M_{\langle Q\rangle^{-\kappa}}(\lambda)[\langle Q\rangle^\kappa A]$ is a Hilbert–Schmidt operator, the mapping $\lambda \mapsto M_A(\lambda)$ is Hölder continuous in Hilbert–Schmidt norm and $\|M_A(\lambda)\| \leqslant c\lambda^{-1/4}$ for $\lambda \geqslant 1$.

Example 2. If (C_κ) is satisfied with $\kappa > 1/2$, one can also give a meaning to $M_{AU}(\lambda)$ and more generally to $M_{A\theta}(\lambda)$ if θ is the multiplication operator by a function $\theta \in L^\infty(\mathbf{R}^n) + L^q(\mathbf{R}^n)$ with $q \geqslant 2$ and $q > n/2$. The operator $(A\theta)^*$ is locally H_0-smooth on $\mathbf{R}^+$: if J is a compact interval in $\mathbf{R}^+$ and $E_0(J)$ the associated spectral projection of H_0, write $(A\theta)^*E_0(J)$

as $A\bar{\theta}\psi(H_0)\langle Q\rangle^{\kappa} \times \langle Q\rangle^{-\kappa} E_0(J)$ with $\psi \in C_0^\infty(\mathbf{R}^+)$ such that $\psi(H_0)E_0(J) = E_0(J)$, observe from lemma 1 that $A\bar{\theta}\psi(H_0)\langle Q\rangle^{\kappa}$ is bounded and that $\langle Q\rangle^{-\kappa}$ is locally H_0-smooth on $\mathbf{R}^+$. For $f \in \mathcal{D}(\theta)$ one has

$$M_{A\theta}(\lambda)f = (A\theta f)_\lambda = 2^{-1/2}(2\pi)^{-n/2}\lambda^{(n-2)/4}\int_{\mathbf{R}^n} \mathrm{e}^{-\mathrm{i}\sqrt{\lambda}\omega\cdot x}A(x)\theta(x)f(x)\,\mathrm{d}x.$$

Since $(A\theta)(\cdot)$ belongs to $L^2(\mathbf{R}^n)$ if $\kappa > n/2$ by the Hölder inequality, $M_{A\theta}(\lambda)$ is a Hilbert–Schmidt operator if $\kappa > n/2$ and depends continuously on λ in Hilbert–Schmidt norm.

Example 3. Let C be a closed operator such that C^* is locally H_0-smooth on $\mathbf{R}^+$ and such that the closure of $\langle Q\rangle^s\psi(H_0)C$ belongs to $\mathcal{B}(\mathcal{H})$ for some $s > 1/2$ and some bounded continuous function ψ on $\mathbf{R}^+$. Then, if $\lambda \in \mathbf{R}^+$ is such that $\psi(\lambda) \neq 0$, one has, for $f \in \mathcal{D}(\langle Q\rangle^s\psi(H_0)C)$,

$$M_C(\lambda)f = \frac{1}{\psi(\lambda)}[\langle Q\rangle^{-s}\langle Q\rangle^s\psi(H_0)Cf]_\lambda = \frac{1}{\psi(\lambda)}M_{\langle Q\rangle^{-s}}(\lambda)\langle Q\rangle^s\psi(H_0)Cf.$$

So

$$M_C(\lambda) = \frac{1}{\psi(\lambda)}M_{\langle Q\rangle^{-s}}(\lambda)[\langle Q\rangle^s\psi(H_0)C]. \tag{15}$$

If, furthermore, $s > n/2$, $M_C(\lambda)$ is Hilbert–Schmidt and depends continuously on λ in Hilbert–Schmidt norm.

Example 4. $C = \Omega_\pm^*\langle Q\rangle^{-\rho}$, $\rho > 1/2$. By using the intertwining relation $\Omega_\pm\varphi(H_0) = \varphi(H)\Omega_\pm$ and the fact that $\langle Q\rangle^{-\rho}$ is locally H-smooth on $\mathbf{R}^+$, one sees that $\langle Q\rangle^{-\rho}\Omega_\pm$ are locally H_0-smooth on $\mathbf{R}^+$. So $M_{(\langle Q\rangle^{-\rho}\Omega_\pm)^*}(\lambda)$ exist for each $\lambda > 0$ as bounded operators from $L^2(\mathbf{R}^n)$ to $L^2(S^{n-1})$. In particular, if A is as in (C_κ) and $\kappa > 1/2$, then $M_{(A\Omega_\pm)^*}(\lambda) = M_{(\langle Q\rangle^{-\kappa}\Omega_\pm)^*}(\lambda)[\langle Q\rangle^\kappa A]$ are well defined. If $\kappa > n/2$, these operators are Hilbert–Schmidt. The continuity in Hilbert–Schmidt norm of the mappings $\lambda \mapsto M_{(A\Omega_\pm)^*}(\lambda)$ can be obtained by using mapping properties of the wave operators between weighted L^2-spaces. For example, if $\kappa > n/2$ and $n \geqslant 3$, it is known [21] that $\langle Q\rangle^\kappa\psi(H_0)\Omega_\pm^*A \in \mathcal{B}(\mathcal{H})$ if $\psi \in C_0^\infty(\mathbf{R}^+)$, so that one can apply example 3 to obtain the above-mentioned continuity property. Alternatively the continuity in Hilbert–Schmidt norm of $\lambda \mapsto M_{(A\Omega_\pm)^*}(\lambda)$, with $\kappa > n/2$, follows from the expression (33) for $M_{(A\Omega_\pm)^*}(\lambda)$.

Example 5. If θ is as in example 2, one can define $M_{(A\Omega_\pm)^*\theta}(\lambda)$ by proceeding as in example 2. If J and ψ are as in example 2, one may write $A\bar{\theta}\Omega_\pm E_0(J) = A\bar{\theta}\psi(H)\langle Q\rangle^\kappa \times \langle Q\rangle^{-\kappa}\Omega_\pm E_0(J)$. It follows that $A\bar{\theta}\Omega_\pm$ are locally H_0-smooth because $\langle Q\rangle^{-\kappa}\Omega_\pm$ are locally H_0-smooth as already pointed out in example 4 and $A\bar{\theta}\psi(H)\langle Q\rangle^\kappa \in \mathcal{B}(\mathcal{H})$ by lemma 1.

We now introduce the operators $K_z^o = AR_z^oA$, $K_z = AR_zA$, $W_z^o = UK_z^o$ and $W_z = UK_z$. This defines four families of compact operators in $\mathbf{C}\backslash\sigma(H)$ each of which is norm analytic. The compactness of K_z^o and W_z^o, for $z \notin [0,\infty)$, is obtained by noticing that the function $\mathbf{R}^n \ni k \mapsto (k^2 - z)^{-1}$ belongs to $L^p(\mathbf{R}^n)$ for each $p > n/2$, that $A \in L^{2n}(\mathbf{R}^n)$ and $UA \in [L^{2n}(\mathbf{R}^n) + L^q(\mathbf{R}^n)]$ with q as in (ii) of (C_κ) (remember that $\kappa > 1/2$, and take into account lemma 3.13 of [22]). The compactness of K_z and W_z follows from that of K_z^o and W_z^o respectively by observing that, by the second resolvent equation (I denotes the identity operator), one has for $z \in \mathbf{C}\backslash\sigma(H)$

$$K_z = K_z^o\big(I + W_z^o\big)^{-1} = \big(I + W_{\bar{z}}^o\big)^{-1*}K_z^o, \qquad W_z = W_z^o\big(I + W_z^o\big)^{-1}. \tag{16}$$

Here the operator $\big(I + W_z^o\big)^{-1}$ belongs to $\mathcal{B}(\mathcal{H})$ for each $z \notin \sigma(H)$ by the analytic Fredholm theorem (theorem VI.14 of [23]) and by the fact that the eigenvalues of H are real (if $W_z^o f = -f$ for some $f \in \mathcal{H}$, with $z \notin [0, \infty)$), then $VR_z^o Af = AW_z^o f = -Af = -(H_0 - z)R_z^o Af$; hence $R_z^o Af$ is an eigenvector of H associated with the eigenvalue z).

The operators K_z^o, K_z, W_z^o and W_z can also be defined for z on the positive real axis $\mathbf{R}^+$ by a suitable limiting procedure from the upper or the lower half plane. This can be achieved for example by using a Mourre estimate and the fact that there are no positive eigenvalues for H_0 and for H. For a different approach, let us consider a pair of H-bounded operators C, N having the following properties, for some $\rho > 1/2$: (i) the closures of CR_zN and $\langle Q\rangle^{-\rho}R_zN$ are in $\mathcal{B}(\mathcal{H})$ for each non-real z, (ii) the closure $C_{m,\rho}$ of $C(H+m)^{-1}\langle Q\rangle^{\rho}$ is in $\mathcal{B}(\mathcal{H})$ for $m < \inf\sigma(H)$. By the first resolvent equation one has

$$CR_{\lambda\pm\mathrm{i}\varepsilon}N = CR_{-m}N + (m + \lambda \pm \mathrm{i}\varepsilon)C_{m,\rho}\langle Q\rangle^{-\rho}R_{\lambda\pm\mathrm{i}\varepsilon}N. \tag{17}$$

Suppose that $\langle Q\rangle^{-\rho}R_{\lambda\pm\mathrm{i}\varepsilon}N$ converge in norm as $\varepsilon \to +0$. Then (17) implies that the norm limits of $CR_{\lambda\pm\mathrm{i}\varepsilon}N$ as $\varepsilon \to +0$ exist. We shall use the notation $CR_{\lambda\pm\mathrm{i}0}N$ for these limits and sometimes write $C(R_{\lambda+\mathrm{i}0} - R_{\lambda-\mathrm{i}0})N$ for $CR_{\lambda+\mathrm{i}0}N - CR_{\lambda-\mathrm{i}0}N$. Some simple consequences of (17) are collected in the following lemma, and further applications are given in the appendix.

Lemma 2. *(a) For each $\lambda > 0$, the operators $K_{\lambda\pm\mathrm{i}0}^o$, $W_{\lambda\pm\mathrm{i}0}^o$, $K_{\lambda\pm\mathrm{i}0}$ and $W_{\lambda\pm\mathrm{i}0}$ exist as norm limits and are compact. Furthermore $\left(I + W_{\lambda\pm\mathrm{i}0}^o\right)^{-1} \in \mathcal{B}(\mathcal{H})$.*

(b) All operators defined in (a) depend continuously on λ in norm.

(c) One has $\mathcal{R}\left(K_{\lambda\pm\mathrm{i}0}^o\right) \subseteq \mathcal{D}(U)$, $\mathcal{R}(K_{\lambda\pm\mathrm{i}0}) \subseteq \mathcal{D}(U)$ and $UK_{\lambda\pm\mathrm{i}0}^o = W_{\lambda\pm\mathrm{i}0}^o$, $UK_{\lambda\pm\mathrm{i}0} = W_{\lambda\pm\mathrm{i}0}$.

(d) For $j = 1, \ldots, n$ one has $\mathcal{R}\left(K_{\lambda\pm\mathrm{i}0}^o\right) \subseteq \mathcal{D}(P_j)$ and $\mathcal{R}(K_{\lambda\pm\mathrm{i}0}) \subseteq \mathcal{D}(P_j)$. The operators $P_jK_{\lambda\pm\mathrm{i}0}^o$ and $P_jK_{\lambda\pm\mathrm{i}0}$ belong to $\mathcal{B}(\mathcal{H})$.

Proof. (a), (b) The existence of $K_{\lambda\pm\mathrm{i}0}^o$ and $W_{\lambda\pm\mathrm{i}0}^o$ and their continuity as functions of λ are obtained from (17) by setting $H = H_0$, $C = A$ or $C = UA$, $N = A$ and $\rho = \kappa$ (then the closure of $C(H_0+m)^{-1}\langle Q\rangle^{\kappa}$ is bounded by lemma 1). To see that $\left(I + W_{\lambda\pm\mathrm{i}0}^o\right)^{-1} \in \mathcal{B}(\mathcal{H})$, it suffices to know that -1 is not an eigenvalue of $W_{\lambda\pm\mathrm{i}0}^o$ (by the compactness of $W_{\lambda\pm\mathrm{i}0}^o$). If $W_{\lambda\pm\mathrm{i}0}^o f = -f$ for some f in $\mathcal{H}$, one can show that $R_{\lambda\pm\mathrm{i}0}^o Af$ (suitably interpreted, see, e.g., lemma 8 in section XIII.8 of [14]) defines an eigenvector of H with eigenvalue λ, and we have seen that such eigenvalues do not exist if $\lambda > 0$.

The continuity in norm of $z \mapsto \left(I + W_z^o\right)^{-1}$ on $\mathbf{C}^+ \cup \mathbf{R}^+$ and on $\mathbf{C}^- \cup \mathbf{R}^+$ is now a consequence of the compactness of W_z^o (see, e.g., lemma 9.5 of [20]). Finally, the existence and properties of $K_{\lambda\pm\mathrm{i}0}$ and $W_{\lambda\pm\mathrm{i}0}$ follow by setting $z = \lambda \pm \mathrm{i}\varepsilon$ in (16) and letting $\varepsilon \to +0$.

(c) Let $f \in \mathcal{H}$ and set $f_\varepsilon = AR_{\lambda+\mathrm{i}\varepsilon}Af$. Then $f_\varepsilon \in \mathcal{D}(U)$, $f_\varepsilon \to K_{\lambda+\mathrm{i}0}f$ and $Uf_\varepsilon \equiv W_{\lambda+\mathrm{i}\varepsilon}f \to W_{\lambda+\mathrm{i}0}f$ strongly as $\varepsilon \to +0$. Since U is a closed operator, one has $UK_{\lambda+\mathrm{i}0}f = W_{\lambda+\mathrm{i}0}f$.

(d) We take $C = P_jA$, $N = A$ and $\rho = \kappa$ in (17). After writing $CR_z = AP_jR_z - \mathrm{i}(\partial_jA)R_z$, and by taking into account lemma 1, one sees that all conditions for obtaining the existence of the limit in (17) are satisfied. So $P_jAR_{\lambda\pm\mathrm{i}\varepsilon}A$ have norm limits as $\varepsilon \to +0$. As in (c), one finds that $\mathcal{R}(K_{\lambda\pm\mathrm{i}0}) \subseteq \mathcal{D}(P_j)$ by using the closedness of the operator P_j. The fact that $P_jK_{\lambda\pm\mathrm{i}0} \in \mathcal{B}(\mathcal{H})$ follows from the closed graph theorem (problem III.5.22 in [24]). □

Lemma 3. *Assume that V satisfies (C_κ) with $\kappa > 1/2$. Then one has, for each $\lambda > 0$,*

$$M_{(A\Omega_+)^*}(\lambda)^* M_{(A\Omega_+)^*}(\lambda) = M_{(A\Omega_-)^*}(\lambda)^* M_{(A\Omega_-)^*}(\lambda) = \frac{1}{2\pi\mathrm{i}}[K_{\lambda+\mathrm{i}0} - K_{\lambda-\mathrm{i}0}] \tag{18}$$

and

$$K_{\lambda+\mathrm{i}0} - K_{\lambda-\mathrm{i}0} = \left(I + W_{\lambda+\mathrm{i}0}^o\right)^{-1*}\left[K_{\lambda+\mathrm{i}0}^o - K_{\lambda-\mathrm{i}0}^o\right]\left(I + W_{\lambda+\mathrm{i}0}^o\right)^{-1}. \tag{19}$$

Proof. (i) By taking $C = C_1 = (A\Omega)^*$ in (13), with Ω either Ω_+ or Ω_-, we get for $\lambda > 0$

$$2\pi \mathrm{i} M_{(A\Omega)^*}(\lambda)^* M_{(A\Omega)^*}(\lambda) = \lim_{\varepsilon\to+0} A\Omega\big[R^o_{\lambda+\mathrm{i}\varepsilon} - R^o_{\lambda-\mathrm{i}\varepsilon}\big]\Omega^* A$$
$$= \lim_{\varepsilon\to+0} A[R_{\lambda+\mathrm{i}\varepsilon} - R_{\lambda-\mathrm{i}\varepsilon}]\Omega\Omega^* A = \lim_{\varepsilon\to+0} A[R_{\lambda+\mathrm{i}\varepsilon} - R_{\lambda-\mathrm{i}\varepsilon}]E_{\mathrm{ac}}(H)A.$$

Here $E_{\mathrm{ac}}(H) = I - E_p(H)$ is the spectral projection of H onto its absolutely continuous subspace, with $E_p(H)$ being the projection onto the subspace spanned by the eigenvectors of H. Since H has no positive eigenvalues, one has $\lim_{\varepsilon\to 0}(R_{\lambda+\mathrm{i}\varepsilon} - R_{\lambda-\mathrm{i}\varepsilon})E_p(H) = 0$ for $\lambda > 0$. So

$$2\pi \mathrm{i} M_{(A\Omega)^*}(\lambda)^* M_{(A\Omega)^*}(\lambda) = \lim_{\varepsilon\to+0}[K_{\lambda+\mathrm{i}\varepsilon} - K_{\lambda-\mathrm{i}\varepsilon}] = K_{\lambda+\mathrm{i}0} - K_{\lambda-\mathrm{i}0}.$$

(ii) By (16) we have $K_{\bar z} = \big(I + W^o_z\big)^{-1*} K^o_{\bar z}$. Hence

$$K_z - K_{\bar z} = K^o_z\big(I + W^o_z\big)^{-1} - \big(I + W^o_z\big)^{-1*} K^o_{\bar z}$$
$$= \big(I + W^o_z\big)^{-1*}\big[\big(I + W^o_z\big)^* K^o_z - K^o_{\bar z}\big(I + W^o_z\big)\big]\big(I + W^o_z\big)^{-1}. \qquad (20)$$

By observing that $K^o_{\bar z} W^o_z = A R^o_{\bar z} V R^o_z A = W^{o*}_z K^o_z$, this leads to the relation

$$K_z - K_{\bar z} = \big(I + W^o_z\big)^{-1*}\big(K^o_z - K^o_{\bar z}\big)\big(I + W^o_z\big)^{-1}. \qquad (21)$$

Equation (19) follows from (21) by setting $z = \lambda + \mathrm{i}\varepsilon$ and taking the limit $\varepsilon \to +0$. □

Proposition 1. *Assume that V satisfies (C_κ) with $\kappa > n/2$. Then, for each $\lambda > 0$, the following operators are of trace class : $K^o_{\lambda+\mathrm{i}0} - K^o_{\lambda-\mathrm{i}0}$, $W^o_{\lambda+\mathrm{i}0} - W^o_{\lambda-\mathrm{i}0}$, $K_{\lambda+\mathrm{i}0} - K_{\lambda-\mathrm{i}0}$ and $W_{\lambda+\mathrm{i}0} - W_{\lambda-\mathrm{i}0}$. As functions of λ, all of these operators are continuous in trace norm.*

Proof. (i) By (13) we have, for $\lambda > 0$,

$$K^o_{\lambda+\mathrm{i}0} - K^o_{\lambda-\mathrm{i}0} = \lim_{\varepsilon\to+0} A\big(R^o_{\lambda+\mathrm{i}\varepsilon} - R^o_{\lambda-\mathrm{i}\varepsilon}\big)A = 2\pi \mathrm{i} M_A(\lambda)^* M_A(\lambda). \qquad (22)$$

Since $M_A(\lambda)$ is Hilbert–Schmidt if $\kappa > n/2$, the operator $K^o_{\lambda+\mathrm{i}0} - K^o_{\lambda-\mathrm{i}0}$ is trace class. Its continuity in trace norm follows from the continuity in Hilbert–Schmidt norm of the mapping $\lambda \mapsto M_A(\lambda)$ (using the inequality $\|YZ\|_1 \leqslant \|Y\|_2\|Z\|_2$).

Similarly one finds from (18) and example 4 that $K_{\lambda+\mathrm{i}0} - K_{\lambda-\mathrm{i}0}$ is trace class. Its continuity in trace norm follows from that of $K^o_{\lambda+\mathrm{i}0} - K^o_{\lambda-\mathrm{i}0}$ and the fact that $\big(I + W^o_{\lambda+\mathrm{i}0}\big)^{-1}$ is a $\mathcal{B}(\mathcal{H})$-valued norm continuous function of λ on $\mathbf{R}^+$ (use equation (19) and the inequality $\|YZ\|_1 \leqslant \|Y\|_1\|Z\|$).

(ii) From a relation analogous to (22) one finds that $\langle Q\rangle^{-\kappa}\big[R^o_{\lambda+\mathrm{i}0} - R^o_{\lambda-\mathrm{i}0}\big]A$ is trace class. Now, if $\varphi \in C_0^\infty(\mathbf{R})$ is such that $\varphi(\mu) = 1$ in a neighbourhood of λ, then $\big(R^o_{\lambda+\mathrm{i}\varepsilon} - R^o_{\lambda-\mathrm{i}\varepsilon}\big)[I - \varphi(H_0)]$ converges to zero as $\varepsilon \to +0$, so that $W^o_{\lambda+\mathrm{i}0} - W^o_{\lambda-\mathrm{i}0} = [UA\varphi(H_0)\langle Q\rangle^\kappa] \times \big[\langle Q\rangle^{-\kappa}\big(R^o_{\lambda+\mathrm{i}0} - R^o_{\lambda-\mathrm{i}0}\big)A\big]$. Since $UA\varphi(H_0)\langle Q\rangle^\kappa$ extends to an operator in $\mathcal{B}(\mathcal{H})$ (see lemma 1), it follows that $W^o_{\lambda+\mathrm{i}0} - W^o_{\lambda-\mathrm{i}0}$ is trace class. Its continuity in trace norm follows from the continuity in Hilbert–Schmidt norm of the mappings $\lambda \mapsto M_A(\lambda)$ and $\lambda \mapsto M_{\langle Q\rangle^{-\kappa}}(\lambda)$. (iii) To treat the operator $W_{\lambda+\mathrm{i}0} - W_{\lambda-\mathrm{i}0}$, we choose φ as in part (ii) above and have $W_{\lambda+\mathrm{i}0} - W_{\lambda-\mathrm{i}0} = B_1 \times \langle Q\rangle^{-\kappa}[R_{\lambda+\mathrm{i}0} - R_{\lambda-\mathrm{i}0}]\langle Q\rangle^{-\kappa} \times B_2$, where $B_1 = UA\varphi(H)\langle Q\rangle^\kappa$ and $B_2 = \langle Q\rangle^\kappa A$ belong to $\mathcal{B}(\mathcal{H})$. Setting $\mathcal{W}^o_z = \langle Q\rangle^\kappa V R^o_z\langle Q\rangle^{-\kappa}$, $\mathcal{K}_z = \langle Q\rangle^{-\kappa} R_z\langle Q\rangle^{-\kappa}$ and $\mathcal{K}^o_z = \langle Q\rangle^{-\kappa} R^o_z\langle Q\rangle^{-\kappa}$, one finds from the first resolvent equation that $\mathcal{K}_z = \mathcal{K}^o_z\big(I + \mathcal{W}^o_z\big)^{-1} = \big(I + \mathcal{W}^o_{\bar z}\big)^{-1*}\mathcal{K}^o_z$. All equations given in part (ii) of the proof of lemma 3 remain valid if one replaces K_z, K^o_z and W^o_z by $\mathcal{K}_z$, $\mathcal{K}^o_z$ and $\mathcal{W}^o_z$, respectively, so that

$$\langle Q\rangle^{-\kappa}[R_{\lambda+\mathrm{i}0} - R_{\lambda-\mathrm{i}0}]\langle Q\rangle^{-\kappa} = \mathcal{K}_{\lambda+\mathrm{i}0} - \mathcal{K}_{\lambda-\mathrm{i}0} = \big(I + \mathcal{W}^o_{\lambda+\mathrm{i}0}\big)^{-1*}\big(\mathcal{K}^o_{\lambda+\mathrm{i}0} - \mathcal{K}^o_{\lambda-\mathrm{i}0}\big)\big(I + \mathcal{W}^o_{\lambda+\mathrm{i}0}\big)^{-1}.$$

Now, as in part (i) above, $\mathcal{K}_{\lambda+i0} - \mathcal{K}_{\lambda-i0}$ is trace class and depends continuously on λ in trace norm, and $\left(I + \mathcal{W}^o_{\lambda+i0}\right)^{-1}$ exists and is norm continuous in λ ($\mathcal{W}^o_z$ plays the role of the operator W^o_z for the potential $V' = A'U'A'$ with $A' = \langle Q\rangle^{-\kappa}$ and $U' = UA^2\langle Q\rangle^{2\kappa}$). □

3. Time delay operators

In this section we present stationary expressions for the time delay operator and for its trace. The results are valid for potentials satisfying the condition (C_κ) for suitable values of the parameters κ and q. In order to avoid certain technicalities occurring when $\tilde{U}$ is an unbounded operator (i.e. when $U_2 \neq 0$), we shall restrict the proofs here to potentials for which $U_2 = 0$, and we shall indicate in the appendix how to treat the general case and how to interpret our equations in that case.

We first derive from Lavine's formula (2) a stationary expression for the time delay operator $T(\lambda)$ (this expression has been given in [12] in a somewhat different language). As pointed out in [12], the integral in (2) is absolutely convergent if $\{f_\lambda\}$ and $\{g_\lambda\}$ have compact support in $\mathbf{R}^+$.

Proposition 2. *Assume that V satisfies (C_κ) with $\kappa > 1/2$. Then*

$$T(\lambda) = \frac{2\pi}{\lambda} M_{(A\Omega_-)^*}(\lambda)\tilde{U} M_{(A\Omega_-)^*}(\lambda)^*. \tag{23}$$

Proof (assuming $U_2 = 0$)**.** Let J be a closed interval in $\mathbf{R}^+$ and denote by $E_0(J)$ the spectral projection of H_0 for this interval. By (2) we have, for $f, g \in \mathcal{R}(E_0(J))$,

$$\langle f, H_0Tg\rangle = \int_{-\infty}^{\infty} \langle \mathrm{e}^{-\mathrm{i}H_0t} f, \Omega_-^* A\tilde{U} A\Omega_- \mathrm{e}^{-\mathrm{i}H_0t} g\rangle \, \mathrm{d}t. \tag{24}$$

We use (9) to rewrite (24) in terms of the operators $M_{(A\Omega_-)^*}(\lambda)$ and then apply Parseval's formula:

$$\begin{aligned}\langle f, H_0Tg\rangle &= \int_{-\infty}^{\infty} \mathrm{d}t \int_J \mathrm{d}\lambda \int_J \mathrm{d}\mu \, \mathrm{e}^{\mathrm{i}t(\lambda-\mu)} \langle M_{(A\Omega_-)^*}(\lambda)^* f_\lambda, \tilde{U} M_{(A\Omega_-)^*}(\mu)^* g_\mu\rangle \\ &= 2\pi \int_J \mathrm{d}\lambda \langle M_{(A\Omega_-)^*}(\lambda)^* f_\lambda, \tilde{U} M_{(A\Omega_-)^*}(\lambda)^* g_\lambda\rangle \equiv \int_J \mathrm{d}\lambda \langle f_\lambda, \lambda T(\lambda) g_\lambda\rangle,\end{aligned}$$

which shows that (23) holds for almost all λ in J. □

By proceeding as in the preceding proof, it is easy to derive a stationary expression for the S-matrix $S(\lambda)$. The scattering operator S in $L^2(\mathbf{R}^n)$ satisfies the following relation:

$$S - I = (\Omega_+^* - \Omega_-^*)\Omega_- = -\mathrm{i}\int_{-\infty}^{\infty} (\mathrm{e}^{\mathrm{i}H_0t} AUA \, \mathrm{e}^{-\mathrm{i}Ht})\Omega_- \, \mathrm{d}t.$$

This leads to

$$R(\lambda) := S(\lambda) - I = -2\pi \mathrm{i} M_{AU}(\lambda) M_{(A\Omega_-)^*}(\lambda)^*. \tag{25}$$

Proposition 3. *Assume that V satisfies $(C_{\kappa,n})$ with $\kappa > n/2$. Then $T(\lambda)$ is a trace class operator in $L^2(S^{n-1})$. Its trace $\tau(\lambda)$ is a continuous function of λ ($\lambda > 0$) given as follows:*

$$\tau(\lambda) \equiv \operatorname{Tr} T(\lambda) = \frac{-\mathrm{i}}{\lambda} \operatorname{Tr} \tilde{U}(K_{\lambda+i0} - K_{\lambda-i0}). \tag{26}$$

Alternatively one has the following expressions for $\tau(\lambda)$*:*

$$\tau(\lambda) = \frac{-\mathrm{i}}{\lambda}\operatorname{Tr}\big\{\tilde{U}\big(I + W^{o}_{\lambda+\mathrm{i}0}\big)^{-1*}\big(K^{o}_{\lambda+\mathrm{i}0} - K^{o}_{\lambda-\mathrm{i}0}\big)\big(I + W^{o}_{\lambda+\mathrm{i}0}\big)^{-1}\big\} \tag{27}$$

$$= \frac{2\pi}{\lambda}\operatorname{Tr}\big\{M_A(\lambda)\big(I + W^{o}_{\lambda+\mathrm{i}0}\big)^{-1}\tilde{U}\big(I + W^{o}_{\lambda+\mathrm{i}0}\big)^{-1*}M_A(\lambda)^*\big\}. \tag{28}$$

Note that the trace on the lhs of (26) and that in (28) are taken in $L^2(S^{n-1})$ whereas the one on the rhs of (26) and that in (27) are in $L^2(\mathbf{R}^n)$.

Proof (with $U_2 = 0$, hence $\tilde{U} \in \mathcal{B}(\mathcal{H})$)**.** By example 4, $M_{(A\Omega_-)^*}(\lambda)$ is a Hilbert–Schmidt operator. So $T(\lambda)$ belongs to the trace class (see (23)). By the cyclicity of the trace we deduce from (23) that

$$\tau(\lambda) = \frac{2\pi}{\lambda}\operatorname{Tr}\{\tilde{U}M_{(A\Omega_-)^*}(\lambda)^*M_{(A\Omega_-)^*}(\lambda)\}. \tag{29}$$

By virtue of (18), this implies (26). Equation (27) now follows by taking into account equation (19), and (28) is obtained from (27) by using (22). □

In the situation described in proposition 3, $T(\lambda)$ is an integral operator in $L^2(S^{n-1})$: there is a square-integrable function $T(\lambda;\cdot,\cdot)$ on $S^{n-1}\times S^{n-1}$ such that

$$[T(\lambda)h](\omega) = \int_{S^{n-1}} T(\lambda;\omega,\omega')h(\omega')\,\mathrm{d}\omega' \qquad (\omega \in S^{n-1}) \tag{30}$$

for $h \in L^2(S^{n-1})$. We shall express $T(\lambda)$ in the form $T(\lambda) = T_1(\lambda)T_2(\lambda)^*$, where $T_1(\lambda)$ and $T_2(\lambda)$ are Hilbert–Schmidt operators from $L^2(\mathbf{R}^n)$ to $L^2(S^{n-1})$. We denote the integral kernel of the Hilbert–Schmidt operator $T_1(\lambda)$ by $T_1(\lambda;\omega,x)$ and that of $T_2(\lambda)$ by $T_2(\lambda;\omega,x)$, with $x \in \mathbf{R}^n$ and $\omega \in S^{n-1}$. Since the kernel of $T_2(\lambda)^* : L^2(S^{n-1}) \to L^2(\mathbf{R}^n)$ is just $\overline{T_2(\lambda;\omega,x)}$, we have

$$T(\lambda;\omega,\omega') = \int_{\mathbf{R}^n} T_1(\lambda;\omega,x)\overline{T_2(\lambda;\omega',x)}\,\mathrm{d}x. \tag{31}$$

In terms of this expression for $T(\lambda;\omega,\omega')$, the trace of $T(\lambda)$ is given as follows (see example X.1.18 in [24]):

$$\tau(\lambda) \equiv \operatorname{Tr} T(\lambda) = \int_{S^{n-1}} T(\lambda;\omega,\omega)\,\mathrm{d}\omega. \tag{32}$$

We now show that the kernel $T(\lambda;\omega,\omega')$ is continuous in all three arguments. More precisely, as $T(\lambda;\omega,\omega')$ is defined only for almost all ω,ω' in S^{n-1}, given a realization $T(\lambda;\omega,\omega')$ of this kernel, it can be modified (for each fixed λ) on a set of measure zero in ω,ω' such as to become continuous in these two variables (continuity in λ is already contained in proposition 3).

To prove the preceding assertion, we interpret the rhs of (31) as the scalar product in $L^2(\mathbf{R}^n)$ between $T_2(\lambda;\omega',\cdot)$ and $T_1(\lambda;\omega,\cdot)$. We observe that, for $j = 1,2$ and fixed $\lambda > 0$, $T_j(\lambda;\omega,\cdot)$ defines an element of $L^2(\mathbf{R}^n)$ for almost all $\omega \in S^{n-1}$, so that each of these two kernels can be viewed as defining an $L^2(\mathbf{R}^n)$-valued function on $S^{n-1}\backslash N_j$, where N_j is a null set in S^{n-1} (depending on λ). In the proof of the next proposition we establish the fact that, after modification of these $L^2(\mathbf{R}^n)$-valued functions on a null set in S^{n-1}, they become (strongly) continuous in ω and λ. Consequently, after these modifications, the scalar product in (31) is continuous in λ, ω and ω'.

Proposition 4. *Assume that V satisfies $(C_{\kappa,n})$ with $\kappa > n/2$. Then, for each $\lambda > 0$, the time delay operator $T(\lambda)$ can be represented as an integral operator $T(\lambda; \omega, \omega')$, and this representation can be chosen in such a way that the map $(\lambda; \omega, \omega') \mapsto T(\lambda; \omega, \omega')$ is continuous on $\mathbf{R}^+ \times S^{n-1} \times S^{n-1}$. Furthermore, the map $(\lambda, \omega) \mapsto T(\lambda; \omega, \omega)$ is then continuous on $\mathbf{R}^+ \times S^{n-1}$.*

Proof (with $U_2 = 0$)**.** As in proposition 10.5 of [20], one may use a stationary expression for $\Omega_\pm$ to find that, for $\kappa > n/2$,

$$M_{(A\Omega_\pm)^*}(\lambda) = M_A(\lambda)\big(I + W^o_{\lambda \pm \mathrm{i}0}\big)^{-1}. \tag{33}$$

This gives the following expression for the time delay operator (23):

$$T(\lambda) = \frac{2\pi}{\lambda} M_A(\lambda)\big(I + W^o_{\lambda-\mathrm{i}0}\big)^{-1} \tilde{U} \big(I + W^o_{\lambda-\mathrm{i}0}\big)^{-1*} M_A(\lambda)^*. \tag{34}$$

The idea of the proof is explained in the comments preceding the proposition. We take $T_1(\lambda) = 2\pi\lambda^{-1} M_A(\lambda)\big(I + W^o_{\lambda-\mathrm{i}0}\big)^{-1}\tilde{U}$, $T_2(\lambda) = M_A(\lambda)\big(I + W^o_{\lambda-\mathrm{i}0}\big)^{-1}$. To prove the first assertion of the proposition, we have to verify the following claim: the $L^2(\mathbf{R}^n)$-valued functions determined by the integral kernels of $T_j(\lambda)$ become strongly continuous after modification on a suitable null set in S^{n-1}.

(i) Let F be a bounded operator in $L^2(\mathbf{R}^n)$ (in our application $F = I$ or $F = \tilde{U}$). For $\lambda > 0$, fix a function $G(\lambda; \omega, x)$ representing the integral kernel of the Hilbert–Schmidt operator $M_A(\lambda)\big(I + W^o_{\lambda-\mathrm{i}0}\big)^{-1} F : L^2(\mathbf{R}^n) \to L^2(S^{n-1})$. Then $G(\lambda; \omega, \cdot)$ defines an element of $L^2(\mathbf{R}^n)$ for almost all $\omega \in S^{n-1}$: there is a null set N_λ in S^{n-1} such that, for $\omega \notin N_\lambda$, $G(\lambda; \omega, \cdot)$ determines a continuous mapping $\Psi^\lambda_\omega : L^2(\mathbf{R}^n) \to \mathbf{C}$, namely

$$\Psi^\lambda_\omega(f) = \int_{\mathbf{R}^n} G(\lambda; \omega, x) f(x)\,\mathrm{d}x, \tag{35}$$

with

$$\big|\Psi^\lambda_\omega(f)\big| \leqslant \left[\int_{\mathbf{R}^n} |G(\lambda; \omega, x)|^2\,\mathrm{d}x\right]^{1/2} \|f\|.$$

We introduce another continuous mapping $\Phi^\lambda_\omega : L^2(\mathbf{R}^n) \to \mathbf{C}$ by setting

$$\Phi^\lambda_\omega(f) = \frac{1}{\sqrt{2(2\pi)^n}} \lambda^{(n-2)/4} \int_{\mathbf{R}^n} \mathrm{e}^{-\mathrm{i}\sqrt{\lambda}\omega\cdot x} A(x)(Y_\lambda f)(x)\,\mathrm{d}x, \tag{36}$$

with $Y_\lambda = \big(I + W^o_{\lambda-\mathrm{i}0}\big)^{-1} F$. Since $A(\cdot)(Y_\lambda f)(\cdot)$ belongs to $L^1(\mathbf{R}^n)$, Φ^λ_ω is defined for all $\omega \in S^{n-1}$ and depends continuously on ω and λ in the sense that, for each $f \in L^2(\mathbf{R}^n)$,

$$\begin{aligned}\big|\Phi^\lambda_\omega(f) - \Phi^{\lambda'}_{\omega'}(f)\big| &\leqslant \frac{\lambda^{(n-2)/4}}{\sqrt{2(2\pi)^n}} \|A(\cdot)\|_{L^2} \|Y_\lambda - Y_{\lambda'}\| \|f\| + \frac{1}{\sqrt{2(2\pi)^n}} \\ &\quad\times \left[\int_{\mathbf{R}^n} |(\lambda^{(n-2)/4}\,\mathrm{e}^{-\mathrm{i}\sqrt{\lambda}\omega\cdot x} - \lambda'^{(n-2)/4}\,\mathrm{e}^{-\mathrm{i}\sqrt{\lambda'}\omega'\cdot x}) A(x)|^2\,\mathrm{d}x\right]^{1/2} \|Y_{\lambda'}\| \|f\|. \end{aligned} \tag{37}$$

(ii) For fixed f in $L^2(\mathbf{R}^n)$ one has $\Psi^\lambda_\omega(f) = \Phi^\lambda_\omega(f)$ for almost all $\omega \in S^{n-1} \backslash N_\lambda$, since both $\Psi^\lambda_\omega(f)$ and $\Phi^\lambda_\omega(f)$, viewed as functions of ω, are representatives of the equivalence class in $L^2(S^{n-1})$ of the vector $M_A(\lambda)\big(I + W^o_{\lambda-\mathrm{i}0}\big)^{-1} F f$. So, for each f in $L^2(\mathbf{R}^n)$, there is a null set $N_\lambda(f)$ in S^{n-1} such that $\Psi^\lambda_\omega(f) = \Phi^\lambda_\omega(f)$ for all $\omega \notin N_\lambda(f)$ (note that $N_\lambda(f)$ contains the null set N_λ introduced in (i) above).

Let $\mathcal{V}$ be a countable dense subset of $L^2(\mathbf{R}^n)$ and let $\mathcal{M}_\lambda = \bigcup_{f\in\mathcal{V}} N_\lambda(f)$. $\mathcal{M}_\lambda$ is a null set in S^{n-1} and

$$\Psi_\omega^\lambda(f) = \Phi_\omega^\lambda(f) \qquad \forall f \in \mathcal{V}, \forall\omega \notin \mathcal{M}_\lambda.$$

By continuity we then have $\Psi_\omega^\lambda(f) = \Phi_\omega^\lambda(f)$ for all $f \in L^2(\mathbf{R}^n)$ and all $\omega \notin \mathcal{M}_\lambda$. Since, by (37), $(\lambda,\omega) \mapsto \Phi_\omega^\lambda$ is strongly continuous as a $L^2(\mathbf{R}^n)$-valued mapping, we have completed the verification of the claim made at the beginning of the proof. The remaining assertions of the proposition are now straightforward consequences of (37). □

4. Time delay for scattering of a beam

As pointed out in the introduction, in order to relate the behaviour of the time delay to that of the scattering cross section, one should define the time delay for an essentially monoenergetic and well-collimated beam of initial states. This kind of time delay was considered in [25]. Here we apply the description of a beam that was used for the derivation of the scattering cross section in section 7-3 of [20].

Let $\mathcal{E}$ be the set of wavefunctions $g \in L^2(\mathbf{R}^n)$ satisfying (i) $\|g\| = 1$, (ii) the Fourier transform $\tilde{g}$ of g belongs to $L^\infty(\mathbf{R}^n)$ and (iii) there is $\omega_o \in S^{n-1}$ such that the support of $\tilde{g}$ is a compact subset of the open cone $\{k \in \mathbf{R}^n \mid k\cdot\omega_o > 0\}$. For fixed $g \in \mathcal{E}$, we denote by Π the $(n-1)$-dimensional hyperplane orthogonal to ω_o and consider an ensemble of states obtained by translating g by vectors $b \in \Pi$, with a uniform distribution over Π of the values of b. Thus the beam generated by g is the collection $\{U(b)g \mid b \in \Pi\}$, with $[U(b)g](x) = g(x-b), x \in \mathbf{R}^n$. We denote by $\Sigma(g)$ the support of g in the spectral representation of H_0, i.e. $\Sigma(g) = \{\lambda \in \mathbf{R}^+ \mid \sqrt{\lambda}\omega \in \operatorname{supp}\tilde{g} \text{ for some } \omega \in S^{n-1}\}$.

The basic result for determining physical quantities defined in terms of a beam is given in the following lemma for the proof of which we refer to the appendix.

Lemma 4. *Consider a Hilbert space $\mathcal{K} \equiv L^2(\mathcal{O}, m)$ over some measure space $(\mathcal{O}, m)$ and let g be a vector in $\mathcal{E}$. For $\lambda \in \mathbf{R}^+$, let $X_1(\lambda), X_2(\lambda) : \mathcal{K} \to L^2(S^{n-1})$ be Hilbert–Schmidt operators satisfying $\|X_j(\lambda)\|_2 \leqslant const < \infty$ for all $\lambda \in \Sigma(g)$, $(j = 1, 2)$. Set $Y(\lambda) = X_1(\lambda)X_2(\lambda)^*$ and let $Y = \{Y(\lambda)\}$ be the associated decomposable operator in $L^2(\mathbf{R}^n)$. Then*

$$\int_\Pi \mathrm{d}b\langle U(b)g, YU(b)g\rangle = (2\pi)^{n-1}\int_{\Sigma(g)} \lambda^{-(n-1)/2}\,\mathrm{d}\lambda \int_{S^{n-1}} Y(\lambda;\omega,\omega)[\omega\cdot\omega_o]^{-1}|g_\lambda(\omega)|^2\,\mathrm{d}\omega. \tag{38}$$

Here $Y(\lambda;\omega,\omega')$ is the integral kernel of the trace class operator $Y(\lambda)$, given as follows in terms of the kernels $X_j(\lambda;\omega,\xi)$ of the Hilbert–Schmidt operators $X_j(\lambda) (j = 1, 2)$:

$$Y(\lambda;\omega,\omega') = \int_\mathcal{O} X_1(\lambda;\omega,\xi)\overline{X_2(\lambda;\omega',\xi)}m(\mathrm{d}\xi). \tag{39}$$

To obtain physically relevant information from this lemma, one will choose the wavefunction g such that its momentum support is very small. Suppose that $(\lambda,\omega) \mapsto Y(\lambda,\omega,\omega)$ is continuous, and consider a sequence $\{g_\ell\}$ in $\mathcal{E}$ such that the support of $\tilde{g}_\ell$ (the Fourier transform of g_ℓ) shrinks to a single point $k_o = \sqrt{\lambda_o}\omega_o$ as $\ell \to \infty$. Then the expression on the rhs of (38) will converge to $(2\pi)^{n-1}\lambda_o^{-(n-1)/2}Y(\lambda_o,\omega_o,\omega_o)$. Upon averaging this quantity over all initial directions ω_o, one obtains (Θ_n denotes the surface area of S^{n-1} and Π the $(n-1)$-dimensional hyperplane orthogonal to ω_o)

$$\frac{1}{\Theta_n}\int_{S^{n-1}} \mathrm{d}\omega_o \lim_{\ell\to\infty}\int_\Pi \mathrm{d}b\langle U(b)g_\ell, YU(b)g_\ell\rangle = \frac{(2\pi)^{n-1}}{\lambda_o^{(n-1)/2}\Theta_n}\operatorname{Tr} Y(\lambda_o). \tag{40}$$

As an example, let us take $\mathcal{K} = L^2(\mathbf{R}^n)$, $X_j(\lambda) = T_j(\lambda)$ with $T_j(\lambda)$ as in (31). Then $Y(\lambda)$ is just the on-shell time delay operator. So, under the conditions of proposition 4, the time delay for a beam of energy λ, averaged over all initial directions, is given by the formula

$$\bar{\tau}(\lambda) = \frac{(2\pi)^{n-1}}{\lambda^{(n-1)/2}\Theta_n} \operatorname{Tr} T(\lambda) = \frac{(2\pi)^{n-1}}{\lambda^{(n+1)/2}\Theta_n i} \operatorname{Tr} \tilde{U}(K_{\lambda+i0} - (K_{\lambda-i0}). \tag{41}$$

Another example is obtained by taking $\mathcal{K} = L^2(S^{n-1})$, $X_1(\lambda) = X_2(\lambda) = R(\lambda)^*$, with $R(\lambda)$ as in (25). Then $\operatorname{Tr} Y(\lambda) = \operatorname{Tr} R(\lambda)^* R(\lambda) = \|R(\lambda)\|_2^2$. Since the probability for scattering of g into a cone $\mathcal{C}$ (not containing the forward direction ω_o) is given as $\int_{\Sigma(g)} \mathrm{d}\lambda \int_{\mathcal{C}\cap S^{n-1}} |[R(\lambda)g_\lambda](\omega)|^2\, \mathrm{d}\omega$ (see [26] or lemma 6.7 of [20]), the averaged total scattering cross section $\bar{\sigma}(\lambda)$ at energy λ, for scattering of a beam, is

$$\bar{\sigma}(\lambda) = \frac{(2\pi)^{n-1}}{\Theta_n} \lambda^{-(n-1)/2} \|R(\lambda)\|_2^2. \tag{42}$$

It will be useful to know expressions for $\bar{\sigma}(\lambda)$ similar to (26)–(28). By using the stationary formula (25) for $R(\lambda)$, the cyclicity of the trace and lemma 3, one finds that

$$\begin{aligned}
\frac{\Theta_n}{(2\pi)^{n+1}} \lambda^{(n-1)/2} \bar{\sigma}(\lambda) &= \frac{1}{(2\pi)^2} \operatorname{Tr}[R(\lambda)^* R(\lambda)] \\
&= \operatorname{Tr}[M_{AU}(\lambda)^* M_{AU}(\lambda) M_{(A\Omega_-)^*}(\lambda)^* M_{(A\Omega_-)^*}(\lambda)] \\
&= \frac{1}{2\pi \mathrm{i}} \operatorname{Tr}[M_{AU}(\lambda)^* M_{AU}(\lambda)(K_{\lambda+i0} - K_{\lambda-i0})] \qquad (43) \\
&= \operatorname{Tr}\big[M_{AU}(\lambda)\big(I + W^o_{\lambda+i0}\big)^{-1^*} M_A(\lambda)^* M_A(\lambda)\big(I + W^o_{\lambda+i0}\big)^{-1} M_{AU}(\lambda)^*\big]. \qquad (44)
\end{aligned}$$

5. Analyticity of time delay and scattering cross section

For the remainder of the paper we consider exponentially decaying potentials. More precisely, we assume that $V = UA^2$ is as follows :

(E_α) (i) $A(x) = \mathrm{e}^{-\alpha\langle x\rangle}$ with $\alpha > 0$;

(ii) $U = U_1 + U_2$ with real U_1 and U_2 satisfying $\langle x\rangle U_1 \in L^\infty(\mathbf{R}^n), x \cdot \nabla U_1 \in L^\infty(\mathbf{R}^n)$; $\langle x\rangle U_2 \in L^\infty(\mathbf{R}^n) + L^q(\mathbf{R}^n)$ for some q satisfying $q \geqslant 2$ and $q > n/2$.

We say that V satisfies condition $(E_{\alpha,n})$ if $q > n$ in (ii).

Since $[(\partial_j A)/A](x) = -\alpha x_j/\langle x\rangle$, the operator $\tilde{U}$ from equation (4) here takes the following form:

$$\tilde{U} = \tilde{U}_1 + \tilde{U}_2 + \frac{\mathrm{i}}{2} P \cdot Q U_2 - \frac{\mathrm{i}}{2} U_2 Q \cdot P \tag{45}$$

with

$$\tilde{U}_1 = U_1 - \alpha\langle Q\rangle^{-1} Q^2 U_1 + \frac{1}{2} Q \cdot \nabla U_1 \quad \text{and} \quad \tilde{U}_2 = \left(1 - \frac{n}{2}\right) U_2 - \alpha\langle Q\rangle^{-1} Q^2 U_2. \tag{46}$$

We note that $\tilde{U}_1 \in L^\infty(\mathbf{R}^n)$ and $\tilde{U}_2 \in L^\infty(\mathbf{R}^n) + L^q(\mathbf{R}^n)$ with q as in (E_α).

We shall consider integral operators $M^\pm_{A\theta}(z) : L^2(\mathbf{R}^n) \to L^2(S^{n-1})$ defined by kernels $2^{-1/2}(2\pi)^{-n/2} z^{(n-2)/4}\, \mathrm{e}^{-\alpha\langle x\rangle}\theta(x)\, \mathrm{e}^{\pm \mathrm{i}\sqrt{z}\omega\cdot x}$, where $\theta : R^n \to \mathbf{C}$ and $z \in \mathbf{C}\backslash(-\infty, 0]$. Particular operators of this form are $M^\pm_A(z)$ $(\theta \equiv 1)$ and $M^\pm_{AU}(z)$ $(\theta = U)$. Here and in what follows the principal branch of the occurring roots is chosen (i.e. the branch cut is along $(-\infty, 0]$). For $z \in \mathbf{C}$, we write $z = \xi + \mathrm{i}\eta$ $(\xi, \eta \in \mathbf{R})$ and define a complex domain Λ by $\Lambda = \{z \in \mathbf{C}\backslash(-\infty, 0] \mid |\Im m\sqrt{z}| < \alpha\} = \{z \in \mathbf{C}\backslash(-\infty, 0] \mid \eta^2 < 4\alpha^2(\xi + \alpha^2)\}$. We note that

Λ is symmetric with respect to the real axis; apart from the cut on $(-\alpha^2, 0]$, it coincides with the interior of the parabola given by $\eta^2 = 4\alpha^2(\xi + \alpha^2)$.

Lemma 5. *Let $\theta \in L^\infty(\mathbf{R}^n) + L^q(\mathbf{R}^n)$ with $q \geqslant 2$ and $q > n/2$. Then we have the following.*

(a) $M^\pm_{A\theta}(z)$ are Hilbert–Schmidt operators for each $z \in \Lambda$.
(b) The functions $z \mapsto M^\pm_{A\theta}(z)$ are holomorphic in Hilbert–Schmidt norm in the domain Λ.
(c) The functions $z \mapsto M^\pm_{A\theta}(\bar{z})^* M^\pm_{A\theta}(z)$ are holomorphic in trace norm in the domain Λ.

Proof. The result of (a) is a consequence of the following bound for the Hilbert–Schmidt norm of $M^\pm_{A\theta}(z)$,

$$\left\| M^\pm_{A\theta}(z) \right\|_2^2 \leqslant \frac{\Theta_n}{2(2\pi)^n} |z|^{(n-2)/2} \int_{\mathbf{R}^n} |\theta(x)|^2 \, \mathrm{e}^{-2\alpha\langle x\rangle} \, \mathrm{e}^{2|\Im m\sqrt{z}||x|} \, \mathrm{d}x \tag{47}$$

by observing that the integral is finite for each $z \in \Lambda$ (using the Hölder inequality). For (b), it is enough to show that, as functions of $z \in \Lambda\backslash(-\infty, 0]$, the mappings $(x, \omega) \mapsto \mathrm{e}^{-\alpha\langle x\rangle} \mathrm{e}^{\pm \mathrm{i}\sqrt{z}\omega\cdot x}\theta(x)$ are differentiable in $L^2(\mathbf{R}^n \times S^{n-1})$. This is easily obtained by using the Lebesgue dominated convergence theorem, taking into account the bound

$$\begin{aligned} |\mathrm{e}^{\pm \mathrm{i}\zeta\omega\cdot x} - \mathrm{e}^{\pm \mathrm{i}\zeta'\omega\cdot x}| &= |\, \mathrm{e}^{\pm \mathrm{i}\zeta\omega\cdot x}\{1 - \mathrm{e}^{\pm \mathrm{i}(\zeta'-\zeta)\omega\cdot x}\}| \\ &\leqslant |\omega \cdot x||\zeta - \zeta'|\mathrm{e}^{|\Im m\sqrt{z}||x|} \max\{1, |\mathrm{e}^{\pm \mathrm{i}(\zeta'-\zeta)\omega\cdot x}|\}. \end{aligned}$$

Finally (c) is a simple consequence of (b) (using $\|YZ\|_1 \leqslant \|Y\|_2\|Z\|_2$). □

We introduce the notation $\{K^{o+}_z\}$ for the restriction of the family $\{K^o_z\}$ to the upper half complex plane $\mathbf{C}^+ = \{z \in \mathbf{C} \mid \Im m\, z > 0\}$. Similarly, for $z \in \mathbf{C}^+$, we shall write W^{o+}_z, K^+_z and W^+_z for the operator W^o_z, K_z and W_z, respectively. We are interested in finding analytic extensions of these families of operators across $\mathbf{R}^+$ into the lower half complex plane. These extensions will be denoted by $\hat{K}^{o+}_z$, $\hat{W}^{o+}_z$ etc. So for example there will be an analytic $\mathcal{B}(\mathcal{H})$-valued function $z \mapsto \hat{K}^{o+}_z$ on $\mathbf{C}^+ \cup \Lambda$ such that $\hat{K}^{o+}_z = K^{o+}_z = K^o_z$ for $z \in \mathbf{C}^+$. For z in the lower half complex plane $\mathbf{C}^-$ we shall denote the operators K^o_z, W^o_z etc by $\hat{K}^{o-}_z$, $\hat{W}^{o-}_z$ etc and their analytic extensions into the upper half plane by $\hat{K}^{o-}_z$, $\hat{W}^{o-}_z$ etc.

Lemma 6. *Assume that V satisfies (E_α). Then we have the following.*

(a) The functions $z \mapsto K^{o+}_z$ and $z \mapsto W^{o+}_z$ have holomorphic continuations in norm, denoted by $\hat{K}^{o+}_z$ and $\hat{W}^{o+}_z$ respectively, to $\mathbf{C}^+ \cup \Lambda$. The functions $z \mapsto K^{o-}_z$ and $z \mapsto W^{o-}_z$ have holomorphic continuations in norm, denoted $\hat{K}^{o-}_z$ and $\hat{W}^{o-}_z$ respectively, to $\mathbf{C}^- \cup \Lambda$.
(b) The operators $\hat{K}^{o\pm}_z$ and $\hat{W}^{o\pm}_z$ are compact for each $z \in \Lambda$.
(c) For $z \in \Lambda$ one has $[\hat{K}^{o-}_z]^* = \hat{K}^{o+}_{\bar{z}}$.
(d) For $z \in \Lambda$ one has $\mathcal{R}(\hat{K}^{o\pm}_z) \subset \mathcal{D}(U)$ and $U\hat{K}^{o\pm}_z = \hat{W}^{o\pm}_z$.
(e) The functions $\Lambda \ni z \mapsto (I + \hat{W}^{o\pm}_z)^{-1}$ are meromorphic in norm. The poles of $(I + \hat{W}^{o+}_z)^{-1}$ (if any) lie in the lower half plane (i.e. in $\Lambda \cap \mathbf{C}^-$), those of $(I + \hat{W}^{o-}_z)^{-1}$ in the upper half plane, and the residues at these poles are finite rank operators.
(f) The functions $z \mapsto K^\pm_z$ have meromorphic extensions, as compact operator-valued functions, to the domains $\mathbf{C}^\pm \cup \Lambda$.

Proof. (a), (b) Let $z \in \mathbf{C}^+$. For $b > 1$, denote by E_b the spectral projection of H_0 for the interval $(1/b, b)$ and set $E_b^\perp = I - E_b$. By taking into account (12) and then using Cauchy's theorem, we get

$$K_z^{o+} = AR_z^o E_b A + AR_z^o E_b^\perp A = \int_{1/b}^{b} \frac{1}{\lambda - z} M_A(\lambda)^* M_A(\lambda)\, \mathrm{d}\lambda + AR_z^o E_b^\perp A$$
$$= \int_\gamma \frac{1}{\lambda - z} M_A(\bar{\zeta})^* M_A(\zeta)\, \mathrm{d}\zeta + AR_z^o E_b^\perp A, \tag{48}$$

where γ is any smooth curve in $\Lambda \cap \mathbf{C}^-$ leading from the point $1/b$ to the point b. Equation (48) implies that K_z^{o+} admits a holomorphic extension to the domain $\Lambda\backslash\{(0, 1/b] \cup [b, \infty)\}$, hence to Λ since b is arbitrary. Equation (48) also shows that the thus defined operators $\hat{K}_z^{o+}$ ($z \in \Lambda$) are compact. The other assertions in (a) and (b) are obtained similarly.
(c) This follows from the relation $K_z^{o*} = K_{\bar{z}}^o$ by analytic continuation.
(d) If $z \in \mathbf{C}^+, h \in \mathcal{D}(U)$ and $g \in \mathcal{H}$, we have $\langle Uh, K_z^{o+} g\rangle = \langle h, W_z^{o+} g\rangle$. By analytic continuation we get that $\langle Uh, \hat{K}_z^{o+} g\rangle = \langle h, \hat{W}_z^{o+} g\rangle$. This shows that $\hat{K}_z^{o+} g \in \mathcal{D}(U)$ and $U\hat{K}_z^{o+} g = \hat{W}_z^{o+} g$. See also lemma 2(c).
(e) As explained after equation (16), the operator $I + W_z^{o+}$ (resp. $I + W_z^{o-}$) is invertible for each $z \in \mathbf{C}^+ \cup \mathbf{R}^+$ (resp. $z \in \mathbf{C}^- \cup \mathbf{R}^+$), with inverse in $\mathcal{B}(\mathcal{H})$. Therefore the statements of (e) are consequences of the analytic Fredholm theorem (see, e.g., [23]).
(f) This follows from (a),(b) and (e) by taking into account equation (16). □

Proposition 5. *Assume that V satisfies (E_α). Then we have the following.*
(a) For $z \in \Lambda$, the operators $\hat{K}_z^{o+} - \hat{K}_z^{o-}$ and $\hat{W}_z^{o+} - \hat{W}_z^{o-}$ are trace class and given as follows:

$$\hat{K}_z^{o+} - \hat{K}_z^{o-} = 2\pi \mathrm{i} M_A(\bar{z})^* M_A(z) \tag{49}$$

and

$$\hat{W}_z^{o+} - \hat{W}_z^{o-} = 2\pi \mathrm{i} M_{AU}(\bar{z})^* M_A(z). \tag{50}$$

(b) The functions $z \mapsto \hat{K}_z^{o+} - \hat{K}_z^{o-}$ and $z \mapsto \hat{W}_z^{o+} - \hat{W}_z^{o-}$ are holomorphic in trace norm in the domain Λ.
(c) The function $\Lambda \ni z \mapsto \hat{K}_z^{+} - \hat{K}_z^{-}$ is meromorphic in trace norm.

Proof. Equations (49) and (50) hold for real z, hence for all $z \in \Lambda$ by analytic continuation. The holomorphy of these functions in trace norm then follows from lemma 5(c). The fact that the meromorphy of the difference $\hat{K}_z^{+} - \hat{K}_z^{-}$ holds in trace norm is obtained from (21) by taking into account the result of (b) and lemma 6. □

Proposition 5 implies that the trace of the time delay $\tau(\lambda)$, defined on $\mathbf{R}^+$ and given by (26), has a meromorphic continuation to the domain Λ, namely

$$\tau(z) = \frac{-\mathrm{i}}{z} \mathrm{Tr}\big\{\tilde{U}\big[\hat{K}_z^{+} - \hat{K}_z^{-}\big]\big\}. \tag{51}$$

The possible poles of this function in the lower half plane lie in the set $\Xi^- := \{z \in \Lambda \cap \mathbf{C}^- \mid (I + \hat{W}_z^{o+})$ is not invertible$\}$. The points in Ξ^- are often referred to as *resonance poles*, because the poles of the meromorphically continued S-matrix $S(z) = I - 2\pi \mathrm{i} M_A(z)\big(I + \hat{W}_z^{o+}\big)^{-1} M_{AU}(\bar{z})^*$ (see, e.g., proposition 10.12 of [20]) must belong to Ξ^-. In many situations each point in Ξ^- is in fact a pole of $S(z)$ (we refer to [27, 28] for more detailed investigations of this question). In our context it is important to realize that poles of the time delay in $\mathbf{C}^-$ will coincide with resonance poles. Also one may expect that a resonance pole will often be a pole of both the S-matrix and the time delay. This corroborates the idea mentioned in the introduction that a physical resonance should involve a large scattering cross section and a large (though positive) time delay. Section 6 below contains some details on this.

The poles in $\mathbf{C}^-$ of the meromorphic continuations of the physical quantities $\bar\tau(\lambda)$ and $\bar\sigma(\lambda)$ determined by the theory of scattering of a beam (equations (41) and (43)) will also belong to the set Ξ^- of resonance poles; indeed we have $\bar\tau(z) = (2\pi)^{n-1}z^{-(n-1)/2}\tau(z)/\Theta_n$ and

$$\bar\sigma(z) = \frac{(2\pi)^n}{\Theta_n i} z^{-(n-1)/2}\,\mathrm{Tr}\big[M_{AU}(\bar z)^* M_{AU}(z)\big(\hat K_z^+ - \hat K_z^-\big)\big]. \tag{52}$$

However, equations (51) and (52) show that these quantities may also have poles in the upper half plane $\mathbf{C}^+$, namely in the set $\Xi^+ := \{z \in \Lambda \cap \mathbf{C}^+ | (I + \hat W_z^{o-}) \text{ is not invertible}\}$. When approximating the time delay or the scattering cross section at real values of z by pole contributions, the poles in Ξ^+ will have to be taken into account along with the resonance poles in the lower half plane (see section 6).

In the preceding context it is interesting and useful to know that poles in the upper half plane and poles in the lower half plane appear in pairs in the sense that $z \in \Xi^+$ if and only if $\bar z \in \Xi^-$. Indeed, proposition 6(a) below shows for example that if the null space $\mathcal{N}(I + \hat W_z^{o-})$ of the operator $I + \hat W_z^{o-}$ is non-trivial (i.e. of dimension at least 1), then so is the null space of $(I + \hat W_{\bar z}^{o+})^*$, which implies that $\mathcal{N}(I + \hat W_{\bar z}^{o+}) \neq \{0\}$ (because $\mathcal{N}(I + K)$ and $\mathcal{N}(I + K^*)$ have the same dimension if K is compact; see, e.g., theorem 6.8 in [29]).

Proposition 6. *(a) Let V satisfy (E_α), $z \in \Lambda$ and $f \in \mathcal{N}(I + \hat W_z^{o-})$. Then $\hat K_z^{o-} f \in \mathcal{N}((I + \hat W_{\bar z}^{o+})^*)$, and $\hat K_z^{o-} f \neq 0$ if $f \neq 0$.*
(b) Assume that V satisfies condition $(E_{\alpha,n})$. If $z \in \Lambda$ and $g \in \mathcal{N}((I + \hat W_z^{o+})^*)$, then $Ug \in \mathcal{N}(I + \hat W_{\bar z}^{o-})$, and $Ug \neq 0$ if $g \neq 0$.
(c) Under the assumption of (b) one has for all $z \in \Lambda$:

$$\dim \mathcal{N}(I + \hat W_z^{o-}) = \dim \mathcal{N}((I + \hat W_{\bar z}^{o+})^*) = \dim \mathcal{N}(I + \hat W_{\bar z}^{o+}).$$

Proof. We shall use the relation $[\hat K_z^{o+}]^* = \hat K_{\bar z}^{o-}$ from lemma 6.
(a) Let $f \in \mathcal{N}(I + \hat W_z^{o-})$. Then $f = -\hat W_z^{o-} f = Uh$ with $h = -\hat K_z^{o-} f \in \mathcal{D}(U)$ (lemma 6(d)). So $(I + \hat W_{\bar z}^{o+})^* h = (I + \hat K_z^{o-} U)h = h + \hat K_z^{o-} f = h - h = 0$. If $f \neq 0$, we must have $h \neq 0$ (since $f = Uh$).
(b) Let $g \in \mathcal{N}((I + \hat W_z^{o+})^*)$. Then $g = -\hat W_z^{o+^*} g$. By lemma 9(b) given in the appendix, we then have $g \in \mathcal{D}(U)$ and $Ug = -\hat W_{\bar z}^{o-} Ug$. So $Ug \in \mathcal{N}(I + \hat W_{\bar z}^{o-})$. Also, since $g = -\hat K_z^{o+^*} Ug$, we must have $Ug \neq 0$ if $g \neq 0$.
(c) By the results of (a) and (b) there is a one-to-one correspondence between $\mathcal{N}(I + \hat W_z^{o-})$ and $\mathcal{N}((I + \hat W_{\bar z}^{o+})^*)$. The second equality follows from theorem 6.8 of [29] mentioned above. □

We add two results which are related to proposition 6 and which will be of interest in the next section. We write $(\hat K_\zeta^{o\pm})'$ for $[\mathrm{d}/\mathrm{d}z \hat K_z^{o\pm}]|_{z=\zeta}$.

Lemma 7. *(a) Let V satisfy (E_α) and let $f \in \mathcal{N}(I + \hat W_z^{o+})$, with $z = \lambda - \mathrm{i}\Gamma \in \Lambda$ for some $\lambda > 0$ and $\Gamma > 0$. Then*

$$\langle f, M_A(\bar z)^* M_A(z) f\rangle = \frac{\Gamma}{2\pi}\int_{-1}^{1} \big\langle f, \big(\hat K_{\lambda+\mathrm{i}s\Gamma}^{o-}\big)' f\big\rangle\,\mathrm{d}s. \tag{53}$$

(b) Let V satisfy $(E_{\alpha,n})$ and let $g \in \mathcal{N}((I + \hat W_z^{o+})^*)$, with z as in (a). Then

$$\langle g, M_{AU}(\bar z)^* M_{AU}(z) g\rangle = \frac{\Gamma}{2\pi}\int_{-1}^{1} \big\langle Ug, \big(\hat K_{\lambda+\mathrm{i}s\Gamma}^{o+}\big)' Ug\big\rangle\,\mathrm{d}s. \tag{54}$$

Proof. (a) Let $f \in \mathcal{N}\big(I + \hat{W}_z^{o+}\big)$. Then, as in the proof of proposition 6, we have $f = Uh$ with $h = -\hat{K}_z^{o+} f$ satisfying $\big(I + \hat{W}_{\bar{z}}^{o-}\big)^* h = 0$. Thus we have

$$\big\langle h, \big(I + \hat{W}_{\bar{z}}^{o-}\big) f\big\rangle = 0. \tag{55}$$

Also, by taking into account (49) and lemma 6(d) we obtain

$$2\pi \mathrm{i}\langle f, M_A(\bar{z})^* M_A(z) f\rangle = \big\langle h, \big(\hat{W}_z^{o+} - \hat{W}_z^{o-}\big) f\big\rangle = -\big\langle h, \big(I + \hat{W}_z^{o-}\big) f\big\rangle. \tag{56}$$

Addition of (55) and (56) leads to

$$2\pi \mathrm{i}\langle f, M_A(\bar{z})^* M_A(z) f\rangle = \big\langle h, \big(\hat{W}_{\bar{z}}^{o-} - \hat{W}_z^{o-}\big) f\big\rangle = \big\langle f, \big(\hat{K}_{\bar{z}}^{o-} - \hat{K}_z^{o-}\big) f\big\rangle. \tag{57}$$

(53) follows from (57) by virtue of the mean value theorem.
(b) By proposition 6(b) we have $Ug \in \mathcal{N}\big(I + \hat{W}_{\bar{z}}^{o-}\big)$. A simple adjustment of the arguments used in (a) above then leads to

$$\begin{aligned} 2\pi \mathrm{i}\langle g, M_{AU}(\bar{z})^* M_{AU}(z) g\rangle &= 2\pi \mathrm{i}\langle Ug, M_A(\bar{z})^* M_A(z) Ug\rangle \\ &= \big\langle Ug, \big(\hat{K}_{\bar{z}}^{o+} - \hat{K}_z^{o+}\big) Ug\big\rangle, \end{aligned}$$

from which (54) follows with the mean value theorem. □

6. A Breit–Wigner type approximation

It is interesting to consider the situation where a scattering pole (and hence also its conjugate pole) lies very close to the real axis. So let us assume that $z_o = \lambda_o - \mathrm{i}\Gamma$ ($0 < \Gamma \ll \lambda_o$) is a resonance pole, with $\bar{z}_o = \lambda_o + \mathrm{i}\Gamma$ its conjugate pole. Assume, furthermore, that there is a number m not less than 3 such that the disc $\{|z - \lambda_o| < m\Gamma\}$ of radius $m\Gamma$ centred at λ_o is contained in Λ and contains no resonance poles other than z_o. One can then expect to obtain a reasonable approximation for the time delay (given by equation (28)) and the scattering cross section (equation (44)) at energies λ near λ_o by evaluating $\big(I + W_{\lambda+\mathrm{i}0}^o\big)^{-1}$ in terms of the Laurent series at z_o of $\big(I + \hat{W}_z^{o+}\big)^{-1}$ and by omitting terms in $(\lambda - z_o)^k$ with $k \geqslant 0$.

Following [30] we write the power series for $I + \hat{W}_z^{o+}$ at z_o as

$$I + \hat{W}_z^{o+} = \sum_{k=0}^{\infty} A_k (z - z_o)^k, \qquad A_k \in \mathcal{B}(\mathcal{H}), \tag{58}$$

so that $A_0 = I + \hat{W}_{z_o}^{o+}$ and $A_1 = \big(\hat{W}_{z_o}^{o+}\big)' := \big[\mathrm{d}/\mathrm{d}z \hat{W}_z^{o+}\big]\big|_{z=z_o}$. Since $z \mapsto \hat{W}_z^{o+}$ is a holomorphic operator-valued function, the number -1 is an eigenvalue of $\hat{W}_z^{o+}$ for each z in some neighbourhood of z_o. The associated projection is

$$\mathcal{P}(z) = \frac{1}{2\pi \mathrm{i}} \int_\gamma \big(\zeta + \hat{W}_z^{o+}\big)^{-1} \mathrm{d}\zeta, \tag{59}$$

where $\gamma = \{\zeta \in \mathbf{C} \,|\, |\zeta - 1| = \varepsilon\}$ for ε sufficiently small [24, 30]. We set $\mathcal{P}_o = \mathcal{P}(z_o)$. Let us make the additional hypothesis that the eigenvalue -1 of $\hat{W}_{z_o}^{o+}$ has algebraic multiplicity 1. Then $\mathcal{P}_o$ is an idempotent operator of rank 1. In particular, the null space of $I + \hat{W}_{z_o}^{o+}$ is one-dimensional. We fix a normalized vector χ in this null space: $\hat{W}_{z_o}^{o+}\chi = -\chi$, $\|\chi\| = 1$ and $\mathcal{P}_o\chi = \chi$. Then $\mathcal{P}_o$ has the form $\mathcal{P}_o = |\chi\rangle\langle\eta|$ for some $\eta \in \mathcal{H}$, with $\langle\eta, \chi\rangle = 1$. It follows that $\mathcal{P}_o^*\eta = \eta$, so that $\eta \in \mathcal{N}\big(\big(I + \hat{W}_{z_o}^{o+}\big)^*\big)$ since $\mathcal{P}_o^*$ is the projection associated with the eigenvalue -1 of the adjoint $\hat{W}_{z_o}^{o+*}$ of $\hat{W}_{z_o}^{o+}$. We observe that $\|\eta\| \geqslant 1$ (since $\langle\eta, \chi\rangle = 1$), with strict inequality in general (equality can hold only if $\mathcal{P}_o^* = \mathcal{P}_o$, i.e. if $\mathcal{P}_o$ is an orthogonal projection).

Lemma 8. *Assume as above that $\mathcal{P}_o$ is an operator of rank* 1, $\mathcal{P}_o = |\chi\rangle\langle\eta|$. *Also assume that* $a := \langle \eta, (\hat{W}^{o+}_{z_o})'\chi\rangle \neq 0$. *Then the pole at z_o of $(I + \hat{W}^{o+}_z)^{-1}$ is of order 1 (i.e. it is a simple pole) and the associated Laurent series implies that*

$$\left(I + \hat{W}^{o+}_z\right)^{-1} = \frac{\mathcal{P}_o}{a(z - z_o)} + \phi(z), \tag{60}$$

where ϕ is holomorphic in the domain $\{|z - \lambda_o| < m\Gamma\}$.

Proof. By the analytic Fredholm theorem [23] there is $N < \infty$ such that the Laurent series of $(I + \hat{W}^{o+}_z)^{-1}$ at z_o has the form

$$\left(I + \hat{W}^{o+}_z\right)^{-1} = \sum_{k=-N}^{\infty} B_k (z - z_o)^k, \qquad B_k \in \mathcal{B}(\mathcal{H}). \tag{61}$$

Under the hypotheses of the lemma, we must have $N = 1$ (i.e. $B_k = 0$ for $k < -1$) and $B_{-1} = B_{-1}\mathcal{P}_o = \mathcal{P}_o B_{-1} = \mathcal{P}_o B_{-1}\mathcal{P}_o$. This follows from theorem 2 of [30] the hypotheses of which are easily seen to be satisfied: hypothesis (ii) is just the condition that $a \neq 0$, and hypothesis (i), namely $A_0^2 f = 0 \Rightarrow A_0 f = 0$, is not difficult to check: if f is such that $A_0^2 f = 0$, then $A_0 f = c\chi$ for some constant c (because $\mathcal{N}(A_0)$ is one-dimensional in our situation), and then $c = \langle \eta, c\chi\rangle = \langle \eta, A_0 f\rangle = \langle A_0^* \eta, f\rangle = 0$ because $A_0^*\eta = 0$.

The equation $\sum_{k=-1}^{\infty} B_k (z - z_o)^k \times \sum_{j=0}^{\infty} A_j (z - z_o)^j = I$ now shows that $I = B_{-1}A_1 + B_0 A_0$. Since $A_0\chi = 0$ this implies that $\chi = B_{-1}A_1\chi = B_{-1}\mathcal{P}_o A_1 \chi = a B_{-1}\chi$. So $B_{-1} = B_{-1}\mathcal{P}_o = |B_{-1}\chi\rangle\langle\eta| = (1/a)|\chi\rangle\langle\eta| = (1/a)\mathcal{P}_o$, which proves (60). □

By inserting in (28) and (44) the approximate expressions $[a(\lambda - z_o)]^{-1}\mathcal{P}_o$ and $[\bar{a}(\lambda - \bar{z}_o)]^{-1}\mathcal{P}_o^*$ for $(I + W^o_{\lambda+\mathrm{i}0})^{-1}$ and $(I + W^o_{\lambda+\mathrm{i}0})^{-1*}$ respectively, we get that in this approximation (designated by the symbol $\simeq$)

$$\begin{aligned}
\bar{\tau}(\lambda) &\simeq \frac{(2\pi)^n}{\Theta_n} \frac{\lambda^{-(n+1)/2}}{|a|^2[(\lambda - \lambda_o)^2 + \Gamma^2]} \mathrm{Tr}[M_A(\lambda)\mathcal{P}_o \tilde{U} \mathcal{P}_o^* M_A(\lambda)^*] \\
&= \frac{(2\pi)^n}{\Theta_n} \frac{\lambda^{-(n+1)/2}}{|a|^2[(\lambda - \lambda_o)^2 + \Gamma^2]} \mathrm{Tr}[M_A(\lambda)|\chi\rangle\langle\eta, \tilde{U}\eta\rangle\langle\chi| M_A(\lambda)^*] \\
&= \frac{(2\pi)^n}{\Theta_n} \frac{\lambda^{-(n+1)/2}}{|a|^2[(\lambda - \lambda_o)^2 + \Gamma^2]} \langle\eta, \tilde{U}\eta\rangle \|M_A(\lambda)\chi\|^2
\end{aligned} \tag{62}$$

and

$$\begin{aligned}
\bar{\sigma}(\lambda) &\simeq \frac{(2\pi)^{n+1}}{\Theta_n} \frac{\lambda^{-(n-1)/2}}{|a|^2[(\lambda - \lambda_o)^2 + \Gamma^2]} \mathrm{Tr}[M_{AU}(\lambda)\mathcal{P}_o^* M_A(\lambda)^* M_A(\lambda)\mathcal{P}_o M_{AU}(\lambda)^*] \\
&= \frac{(2\pi)^{n+1}}{\Theta_n} \frac{\lambda^{-(n-1)/2}}{|a|^2[(\lambda - \lambda_o)^2 + \Gamma^2]} \|M_{AU}(\lambda)\eta\|^2 \|M_A(\lambda)\chi\|^2.
\end{aligned} \tag{63}$$

Let us mention some interesting features of these expressions. As in the Breit–Wigner formula, both (62) and (63) have a factor $(\lambda - \lambda_o)^2 + \Gamma^2$ in the denominator, and both contain a factor $\|M_A(\lambda)\chi\|^2$ in the numerator. By the mean value theorem, replacement of $\|M_A(\lambda)\chi\|^2$ by $\langle\chi, M_A(\bar{z}_o)^* M_A(z_o)\chi\rangle$ will introduce an error proportional to Γ, and $\langle\chi, M_A(\bar{z}_o)^* M_A(z_o)\chi\rangle = c\Gamma$ for some constant c (depending on V and z_o; see lemma 7(a)). In this sense the approximate time delay $\bar{\tau}(\lambda)$, equation (62), contains a factor $\Gamma/[(\lambda - \lambda_o)^2 + \Gamma^2]$, and its sign is determined by the quantity $\langle\eta, \tilde{U}\eta\rangle$. The fact that it is the virial $\tilde{V}$ rather than the potential itself that is important in determining the sign of the time delay has also been stressed in earlier publications (e.g. [11, 31]).

The averaged total scattering cross section $\bar{\sigma}(\lambda)$, equation (63), contains, apart from $\|M_A(\lambda)\chi\|^2$, also a factor $\|M_{AU}(\lambda)\eta\|^2$. As above, its replacement by the quantity $\langle\eta, M_{AU}(\bar{z_o})^* M_{AU}(z_o)\eta\rangle$ amounts to an error proportional to Γ, and again $\langle\eta, M_{AU}(\bar{z_o})^* M_{AU}(z_o)\eta\rangle = c'\Gamma$ for some constant c' by lemma 7(b). So, in such an approximation, $\bar{\sigma}(\lambda)$ will contain a factor $\Gamma^2/[(\lambda-\lambda_o)^2+\Gamma^2]$, i.e., it will be of the usual Breit–Wigner type.

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Appendix. Time delay for potentials with local singularities

In section 3 we have limited the proofs of different properties of time delay to potentials having some degree of regularity, in particular no local singularities (i.e. potentials with $U_2 = 0$). In general, the operator $\tilde{U}$ of equation (4) will have the following form:

$$\tilde{U} = \tilde{U}_1 + \tilde{U}_2 + \frac{\mathrm{i}}{2} P\cdot QU_2 - \frac{\mathrm{i}}{2} U_2 Q\cdot P, \tag{A.1}$$

with $\tilde{U}_1$ and $\tilde{U}_2$ given by (46). Each term in (A.1) gives a contribution to the time delay operator, as shown for example by (2). We shall discuss here the contributions from $\tilde{U}_2$ and $P\cdot QU_2$. We recall that the functions $\tilde{U}_2$ and $\langle\cdot\rangle U_2$ belong to $L^\infty(\mathbf{R}^n) + L^q(\mathbf{R}^n)$, where q satisfies $q \geqslant 2$ and $q > n/2$ (even $q > n$ in propositions 3 and 4, also in section 6).

A first way of avoiding the occurrence of unbounded operators in the expression for $T(\lambda)$ is to fix a real number $m < \inf\sigma(H)$ and to define the operator $Z = \langle Q\rangle^\kappa (H+m)^{-1}\tilde{V}(H+m)^{-1}\langle Q\rangle^\kappa$, which belongs to $\mathcal{B}(\mathcal{H})$ and in terms of which one obtains from (2) the following formula for $T(\lambda)$:

$$T(\lambda) = \frac{2\pi(\lambda+m)^2}{\lambda} M_{(\langle Q\rangle^{-\kappa}\Omega_-)^*}(\lambda) Z M_{(\langle Q\rangle^{-\kappa}\Omega_-)^*}(\lambda)^*. \tag{A.2}$$

One then has $\tau(\lambda) = -\mathrm{i}\lambda^{-1}(\lambda+m)^2 \operatorname{Tr}[Z\langle Q\rangle^{-\kappa}(R_{\lambda+\mathrm{i}0} - R_{\lambda-\mathrm{i}0})\langle Q\rangle^{-\kappa}]$ for all potentials satisfying (C_κ) with $\kappa > n/2$. By evaluating commutators, one can transform this expression, for exponentially decaying potentials V (satisfying (E_α)), into the form

$$\tau(\lambda) = \frac{-\mathrm{i}}{\lambda} \operatorname{Tr}\{[\tilde{U}_1 + \mathcal{L}(\lambda)][K_{\lambda+\mathrm{i}0} - K_{\lambda-\mathrm{i}0}]\}, \tag{A.3}$$

where $\mathcal{L} : \mathbf{R}^+ \to \mathcal{B}(\mathcal{H})$ is a polynomial function of degree 2 given in terms of $U_2, (H+m)^{-1}, P_j, A$ and its derivatives. Equation (A.3) leads to the properties of the meromorphic continuation $\tau(z)$ of $\tau(\lambda)$ already discussed in section 5. The continuity properties of the kernel $T(\lambda;\omega,\omega')$ of $T(\lambda)$, proposition 4, can be obtained as in the proof of that proposition by taking for example $T_1(\lambda) = 2\pi\lambda^{-1}(\lambda+m)^2 M_{(\langle Q\rangle^{-\kappa}\Omega_-)^*}(\lambda)Z$ and $T_2(\lambda) = M_{(\langle Q\rangle^{-\kappa}\Omega_-)^*}(\lambda) = M_{\langle Q\rangle^{-\kappa}}(\lambda) \times \langle Q\rangle^\kappa \psi(H_0)\Omega_-^*\langle Q\rangle^{-\kappa}$ (as stated in example 4 one has $\langle Q\rangle^\kappa\psi(H_0)\Omega_-^*\langle Q\rangle^{-\kappa} \in \mathcal{B}(\mathcal{H})$ [21]).

An alternative approach consists in including the unbounded terms of $\tilde{U}$ in the operators $M_{(A\Omega_-)^*}(\lambda)$ occurring in (23). For example, the contribution of $\tilde{U}_2$ to the result of proposition 2 may be interpreted as $2\pi\lambda^{-1}M_{(A\Omega_-)^*\tilde{U}_2}(\lambda)M_{(A\Omega_-)^*}(\lambda)^*$, that of $(\mathrm{i}/2)P\cdot QU_2$ as $\mathrm{i}\pi\lambda^{-1}\sum_{j=1}^n M_{(A\Omega_-)^*P_j}(\lambda)M_{(A\Omega_-)^*Q_jU_2}(\lambda)^*$. The operators $M_C(\lambda)$ occurring in these expressions are well defined: three of them are of the form $M_{(A\Omega_-)^*\theta}(\lambda)$ discussed in examples 4 and 5, and $M_{(A\Omega_-)^*P_j}(\lambda)$ is treated by an argument similar to that in example 5 by observing that $P_jA\Omega_-E_0(J) = AP_j\psi(H)\langle Q\rangle^\kappa \times \langle Q\rangle^{-\kappa}\Omega_-E_0(J) - \mathrm{i}(\partial_jA)\Omega_-E_0(J)$, which shows that

$P_j A\Omega_-$ is locally H_0-smooth on $\mathbf{R}^+$. If $\kappa > n/2$, each of the above four operators $M_C(\lambda)$ is Hilbert–Schmidt.

If V satisfies $(C_{\kappa,n})$, then $X_j := Q_j U_2$ belongs to $L^\infty(\mathbf{R}^n) + L^q(\mathbf{R}^n)$ with $q > n$, so that $X_j P_j (H+m)^{-1} = X_j (H_0+m)^{-1/2} \times P_j (H_0+m)^{1/2}(H+m)^{-1} \in \mathcal{B}(\mathcal{H})$. Hence

$$X_j P_j A(H+m)^{-1}\langle Q\rangle^\kappa = X_j P_j (H+m)^{-1}[A\langle Q\rangle^\kappa - (\Delta A)(H+m)^{-1}\langle Q\rangle^\kappa - 2\mathrm{i}(\nabla A)\cdot P(H+m)^{-1}\langle Q\rangle^\kappa] \in \mathcal{B}(\mathcal{H})$$

(take into account lemma 1). This allows one to define $M_{(A\Omega_-)^* P_j Q_j U_2}(\lambda)$ as $M_{(A\Omega_-)^* P_j Q_j U_2}(\lambda) = (\lambda+m) M_{(H_0+m)^{-1}(A\Omega_-)^* P_j Q_j U_2}(\lambda) = (\lambda+m) M_{(\langle Q\rangle^{-\kappa}\Omega_-)^*} \times [X_j P_j A(H+m)^{-1}\langle Q\rangle^\kappa]^*$.

If V satisfies (C_κ) with $\kappa > n/2$, then the contributions from $\tilde U_2$ and $(\mathrm{i}/2)P\cdot QU_2/2$ to $\tau(\lambda)$, equation (26), may also be written as $-\mathrm{i}\lambda^{-1}\,\mathrm{Tr}[\tilde U_2 A(R_{\lambda+\mathrm{i}0} - R_{\lambda-\mathrm{i}0})A]$ and $(2\lambda)^{-1}\sum_{j=1}^n \mathrm{Tr}[Q_j U_2 A(R_{\lambda+\mathrm{i}0} - R_{\lambda-\mathrm{i}0})AP_j]$, respectively, where the operators like $Q_j U_2 A R_{\lambda\pm\mathrm{i}0} A P_j$ are well defined in $\mathcal{B}(\mathcal{H})$; see lemma 9 below for details. If V decays exponentially (condition $(E_{\alpha,n})$), one may then obtain a Breit–Wigner type approximation, as in section 6, by evaluating the traces in an orthonormal basis $\{e_k\}$ consisting of functions belonging to the Schwartz space $\mathcal{S}(\mathbf{R}^n)$. For example, with the assumptions and notations of section 6, one finds that

$$\begin{aligned}
\mathrm{Tr}[Q_j U_2 A(R_{\lambda+\mathrm{i}0} - R_{\lambda-\mathrm{i}0})AP_j] &= \sum_k \langle Q_j U_2 e_k, (K_{\lambda+\mathrm{i}0} - K_{\lambda-\mathrm{i}0})P_j e_k\rangle \\
&= 2\pi\mathrm{i}\sum_k \big\langle Q_j U_2 e_k, \big(I + W^o_{\lambda+\mathrm{i}0}\big)^{-1*} M_A(\lambda)^* M_A(\lambda)\big(I + W^o_{\lambda+\mathrm{i}0}\big)^{-1} P_j e_k\big\rangle \\
&\simeq \frac{2\pi\mathrm{i}}{|a|^2[(\lambda-\lambda_o)^2 + \Gamma^2]} \sum_k \langle Q_j U_2 e_k|\eta\rangle\langle\chi|M_A(\lambda)^* M_A(\lambda)|\chi\rangle\langle\eta|P_j e_k\rangle \\
&= \frac{2\pi\mathrm{i}}{|a|^2[(\lambda-\lambda_o)^2 + \Gamma^2]} \|M_A(\lambda)\chi\|^2 \mathrm{Tr}\{|Q_j U_2\eta\rangle\langle P_j\eta|\} \\
&= \frac{2\pi\mathrm{i}}{|a|^2[(\lambda-\lambda_o)^2 + \Gamma^2]} \|M_A(\lambda)\chi\|^2 \langle P_j\eta, Q_j U_2\eta\rangle.
\end{aligned}$$

Here we used the fact that $\eta \in \mathcal{D}(Q_j U_2) \cap \mathcal{D}(P_j)$ (see lemma 9). By treating in this way each contribution from (A.1) to $\tilde U$, one sees that the approximation (62) is valid for all potentials satisfying condition $(E_{\alpha,n})$, provided that $\langle\eta, \tilde U\eta\rangle$ is interpreted as $\langle\eta\tilde U_1\eta\rangle + \langle\eta, \tilde U_2\eta\rangle + (\mathrm{i}/2)\sum_{j=1}^n[\langle P_j\eta, Q_j U_2\eta\rangle - \langle Q_j U_2\eta, P_j\eta\rangle]$.

To present the details mentioned above, we introduce the following set $\mathcal{A}$ of closed operators: $\mathcal{A} = \{P_j, \theta\}$, where θ varies over the class multiplication operators by functions $\theta \in L^\infty(\mathbf{R}^n) + L^q(\mathbf{R}^n)$ with $q > n$. In the applications mentioned above, θ is one of the operators $I, \tilde U_2$ and $Q_j U_2$ $(j = 1, \ldots, n)$. If F is an operator from $\mathcal{A}$, then $F(H_0+m)^{-1/2}$ and $FA(H_0+m)^{-1/2}$ belong to $\mathcal{B}(\mathcal{H})$ (take into account lemma 3.13 of [22]). It follows that $F(H+m)^{-1/2}$ and $FA(H+m)^{-1/2}$ belong to $\mathcal{B}(\mathcal{H})$ (because $(H_0+m)^{1/2}(H+m)^{-1/2}$ is bounded; see proposition 9 in the appendix to IX.4 of [32]). It follows in particular that, if F_1 and F_2 are operators from $\mathcal{A}$, then $F_1 A R^o_z A F_2$ and $F_1 A R_z A F_2$ are well defined, bounded operators for each $z \in \mathbf{C}\backslash\sigma(H)$. Also, as seen before, $FA\Omega_-$ is locally H_0-smooth on $\mathbf{R}^+$ for $F \in \mathcal{A}$, so that the operators $M_{(A\Omega_-)^* F}(\lambda)$ are well defined. They belong to the Hilbert–Schmidt class if $\kappa > n/2$.

Lemma 9. *(a) Let V satisfy condition $(C_{\kappa,n})$ with $\kappa > n/2$, and let F_1 and F_2 be operators from $\mathcal{A}$. Then, for $\lambda > 0$, the limits $\lim_{\varepsilon\to+0} F_1 A R^o_{\lambda\pm\mathrm{i}\varepsilon} A F_2$ and $F_1 A R_{\lambda\pm\mathrm{i}\varepsilon} A F_2$ exist in* *norm and define bounded operators denoted $F_1 A R^o_{\lambda\pm i0} A F_2$ and $F_1 A R_{\lambda\pm i0} A F_2$, respectively. Furthermore*

$$M_{(A\Omega_-)^* F_1}(\lambda)^* M_{(A\Omega_-)^* F_2}(\lambda) = \frac{1}{2\pi i}[F_1 A R_{\lambda+i0} A F_2 - F_1 A R_{\lambda-i0} A F_2] \in \mathcal{B}_1(\mathcal{H}). \tag{A.4}$$

Also $\mathcal{R}(K_{\lambda\pm i0}) \subseteq \mathcal{D}(F_1)$, $F_1 K_{\lambda\pm i0} \in \mathcal{B}(\mathcal{H})$ and $F_1 A R_{\lambda\pm i0} A F_2$ is equal to the closure of $F_1 K_{\lambda\pm i0} F_2$.

(b) Let V satisfy condition $(E_{\alpha,n})$. Let $z \in \Lambda$ and $g \in \mathcal{R}(\hat{W}^{o+*}_z)$. Then $g \in \mathcal{D}(F)$ for each $F \in \mathcal{A}$, in particular $g \in \mathcal{D}(P_j) \cap \mathcal{D}(U) \cap \mathcal{D}(Q_j U)$. Furthermore, $\hat{W}^{o+*}_z g = \hat{K}^{o+*}_z U g$ and $U \hat{W}^{o+*}_z g = \hat{W}^{o-}_{\bar z} U g$.

Proof. (a) The operators $\langle Q\rangle^{-\kappa} R_{\lambda\pm i\varepsilon} \langle Q\rangle^{-\kappa}$ have limits in norm as $\varepsilon \to +0$. Taking in (17) $N = \langle Q\rangle^{-\kappa}$ and $C = FA$, with $F \in \mathcal{A}$, one finds that $FAR_{\lambda\pm i\varepsilon}\langle Q\rangle^{-\kappa}$ have limits in norm. In particular, $\lim_{\varepsilon\to+0} F_1 A R_{\lambda\pm i\varepsilon} A$ and $\lim_{\varepsilon\to+0}\langle Q\rangle^{-\kappa} R_{\lambda\pm i\varepsilon} A F_2$ exist in norm. Next, taking $N = AF_2$ and $C = F_1 A$ in (17), one arrives at the existence in norm of $\lim_{\varepsilon\to+0} F_1 A R_{\lambda\pm i\varepsilon} A F_2$. Since F_1 is closed and defined on the range of $A R_{\lambda\pm i\varepsilon} A$, the limit of $F_1 A R_{\lambda\pm i\varepsilon} A$ is equal to $F_1 K_{\lambda\pm i0}$, with $\mathcal{R}(K_{\lambda\pm i0}) \subseteq \mathcal{D}(F_1)$. The limit of $F_1 A R_{\lambda\pm i\varepsilon} A F_2$ is just the closure of $F_1 K_{\lambda\pm i0} F_2$.

To verify (A.4), one follows the arguments of part (i) of the proof of lemma 3; it suffices to write

$$F_1 A[R_{\lambda+i\varepsilon} - R_{\lambda-i\varepsilon}]E_p(H) A F_2 = F_1 A (H+m)^{-1/2} \times [(m+\lambda)(R_{\lambda+i\varepsilon} - R_{\lambda-i\varepsilon})E_p(H) + i\varepsilon(R_{\lambda+i\varepsilon} + R_{\lambda-i\varepsilon})E_p(H)] \times (H+m)^{-1/2} A F_2$$

and to observe that each term on the rhs converges to zero in norm as $\varepsilon \to 0$.

(b) For $F \in \mathcal{A}$ consider the holomorphic $\mathcal{B}(\mathcal{H})$-valued function $G_z := W^o_z F = U A R^o_z A F$ on $\mathbf{C}^+$. As in the proof of lemma 6(a) one finds that it has a holomorphic extension in norm, denoted $\hat{G}_z$, to $\mathbf{C}^+ \cup \Lambda$; the operator $M_{AF}(\lambda)$ that will occur in the equation corresponding to (47) has been studied in lemma 5 if $F = \theta$, and for $F = P_j$ we just have $M_{AP_j}(\lambda) = M_{P_j A}(\lambda) - i M_{(\partial_j A)}(\lambda)$, with $[M_{P_j A}(\lambda) f](\omega) = \sqrt{\lambda}\omega_j [M_A(\lambda) f](\omega)$.

Now let $g \in \mathcal{R}(\hat{W}^{o+*}_z)$, $g = \hat{W}^{o+*}_z h$ for some $h \in \mathcal{H}$. For $f \in \mathcal{D}(F)$ and $\zeta \in \mathbf{C}^+$, we have $\langle h, W^o_\zeta F f\rangle = \langle h, G_\zeta f\rangle$. By analytic continuation this implies that $\langle h, \hat{W}^{o+}_z F f\rangle = \langle h, \hat{G}_z f\rangle$, so that $\langle g, F f\rangle = \langle \hat{W}^{o+*}_z h, F f\rangle = \langle \hat{G}^*_z h, f\rangle$. This shows that $g \in \mathcal{D}(F)$. From lemma 6(d) we have, for each $f \in \mathcal{H}$,

$$\langle f, \hat{W}^{o+*}_z g\rangle = \langle U \hat{K}^{o+}_z f, g\rangle = \langle f, \hat{K}^{o+*}_z U g\rangle,$$

which shows that $\hat{W}^{o+*}_z g = \hat{K}^{o+*}_z U g = \hat{K}^{o-}_{\bar z} U g$. It follows that $U \hat{W}^{o+*}_z g = U \hat{K}^{o-}_{\bar z} U g = \hat{W}^{o-}_{\bar z} U g$. □

Proof of lemma 4.

(i) We have

$$\int_\Pi db \langle U(b)g, YU(b)g\rangle = \int_\Pi db \int_{\Sigma(g)} d\lambda \langle X_1(\lambda)^*[U(b)g]_\lambda, X_2(\lambda)^*[U(b)g]_\lambda\rangle_{\mathcal{K}}$$
$$= \int_\Pi db \int_{\Sigma(g)} d\lambda \int_{\mathcal{O}} m(d\xi) \overline{\{X_1(\lambda)^*[U(b)g]_\lambda\}(\xi)} \{X_2(\lambda)^*[U(b)g]_\lambda\}(\xi). \tag{A.5}$$

Let us denote the integrand on the rhs of (A.5) by $J(b, \lambda, \xi)$. Then

$$\int_\Pi db \int_{\Sigma(g)} d\lambda \int_{\mathcal{O}} m(d\xi) |J(b,\lambda,\xi)|$$
$$= \langle |\{X_1(\lambda)^*[U(b)g]_\lambda\}(\xi)|, |\{X_2(\lambda)^*[U(b)g]_\lambda\}(\xi)|\rangle_{L^2(\Pi\times\Sigma(g)\times\mathcal{O})}$$
$$\leqslant \|\{X_1(\lambda)^*[U(b)g]_\lambda\}(\xi)\|_{L^2(\Pi\times\Sigma(g)\times\mathcal{O})} \|\{X_2(\lambda)^*[U(b)g]_\lambda\}(\xi)\|_{L^2(\Pi\times\Sigma(g)\times\mathcal{O})}. \tag{A.6}$$

(ii) For $j = 1, 2$, we denote the integral kernel of $X_j(\lambda)^*$ by $\mathcal{X}_j(\lambda; \xi, \omega)$. Let us show that the functions

$$(b, \lambda, \xi) \mapsto \mathcal{G}_j(b, \lambda, \xi) := \{X_j(\lambda)^*[U(b)g]_\lambda\}(\xi) = \int_{S^{n-1}} \mathrm{e}^{-\mathrm{i}\sqrt{\lambda}\omega\cdot b}\mathcal{X}_j(\lambda; \xi, \omega) g_\lambda(\omega)\,\mathrm{d}\omega \tag{A.7}$$

belong to $L^2(\Pi \times \Sigma(g) \times \mathcal{O})$. For this we introduce in (A.7) a new integration variable u, namely, the orthogonal projection of ω onto the hyperplane Π. This change of variables is possible by the assumption on the support of $\tilde{g}$, and it is given by $u = \omega - (\omega \cdot \omega_o)\omega_o$ (hence $\omega(u) = u + \sqrt{1-u^2}\omega_o$, with u in the unit ball of Π). Observing that $\mathrm{d}\omega = [\omega \cdot \omega_o]^{-1}\,\mathrm{d}u$, we then have

$$\begin{aligned}\mathcal{G}_j(b, \lambda, \xi) &= \int_\Pi \mathrm{d}u\, \mathrm{e}^{-\mathrm{i}\sqrt{\lambda}u\cdot b}[\omega(u)\cdot\omega_o]^{-1}\mathcal{X}_j(\lambda; \xi, \omega(u)) g_\lambda(\omega(u)) \\ &= (2\pi)^{(n-1)/2}\big(\mathcal{F}_\Pi\big[(\omega(u)\cdot\omega_o)^{-1}\mathcal{X}_j(\lambda; \xi, \omega(u)) g_\lambda(\omega(u))\big]\big)(\sqrt{\lambda}b)\end{aligned} \tag{A.8}$$

where $\mathcal{F}_\Pi$ denotes $(n-1)$-dimensional Fourier transformation in Π. By using the Parseval identity for $\mathcal{F}_\Pi$, one obtains that

$$\begin{aligned}\int_{\Sigma(g)} \mathrm{d}\lambda \int_{\mathcal{O}} m(\mathrm{d}\xi) \int_\Pi \mathrm{d}b|\mathcal{G}_j(b, \lambda, \xi)|^2 &= (2\pi)^{n-1}\int_{\Sigma(g)} \lambda^{-(n-1)/2}\,\mathrm{d}\lambda \int_{\mathcal{O}} m(\mathrm{d}\xi) \\ &\quad\times \int_\Pi \mathrm{d}u|[\omega(u)\cdot\omega_o]^{-1}\mathcal{X}_j(\lambda; \xi, \omega(u)) g_\lambda(\omega(u))|^2 \\ &= (2\pi)^{n-1}\int_{\Sigma(g)} \lambda^{-(n-1)/2}\,\mathrm{d}\lambda \int_{\mathcal{O}} m(\mathrm{d}\xi)\int_{S^{n-1}} \mathrm{d}\omega|[\omega\cdot\omega_o]^{-1}|\mathcal{X}_j(\lambda; \xi, \omega) g_\lambda(\omega)|^2 \\ &\leqslant c(g)\int_{\Sigma(g)} \mathrm{d}\lambda \|X_j(\lambda)\|_2^2 < \infty,\end{aligned}$$

where $c(g)$ is a finite constant depending on the support of g and on $\|\tilde{g}\|_{L^\infty}$.
(iii) From (A.6) and the result of (ii) we see that $J(b, \lambda, \xi)$ is absolutely integrable. Thus we may interchange order of integration in (A.5). Integrating first over $\mathrm{d}b$, we get the integral

$$\int_\Pi \mathrm{d}b\overline{\{X_1(\lambda)^*[U(b)g]_\lambda\}(\xi)}\{X_2(\lambda)^*[U(b)g]_\lambda\}(\xi) = \int_\Pi \mathrm{d}b\,\overline{\mathcal{G}_1(b, \lambda, \xi)}\mathcal{G}_2(b, \lambda, \xi).$$

For almost all λ and ξ, the integrand belongs to $L^1(\Pi)$ and, as a function of b, is equal to the scalar product in $L^2(\Pi)$ of two functions each of which is a Fourier transform, by (A.8). Hence by the Parseval identity

$$\begin{aligned}\int_\Pi \mathrm{d}b\,\overline{\mathcal{G}_1(b, \lambda, \xi)}\mathcal{G}_2(b, \lambda, \xi) &= \frac{(2\pi)^{n-1}}{\lambda^{(n-1)/2}}\int_\Pi \mathrm{d}u[\omega(u)\cdot\omega_o]^{-2}\overline{\mathcal{X}_1(\lambda; \xi, \omega(u)) g_\lambda(\omega(u))}\mathcal{X}_2(\lambda; \xi, \omega(u)) g_\lambda(\omega(u)) \\ &= \frac{(2\pi)^{n-1}}{\lambda^{(n-1)/2}}\int_{S^{n-1}} \mathrm{d}\omega[\omega\cdot\omega_o]^{-1}\overline{\mathcal{X}_1(\lambda; \xi, \omega) g_\lambda(\omega)}\mathcal{X}_2(\lambda; \xi, \omega) g_\lambda(\omega).\end{aligned}$$

Upon applying $\int_{\Sigma(g)} \mathrm{d}\lambda \int_{\mathcal{O}} m(\mathrm{d}\xi)$ to this expression and observing that $X_j(\lambda; \omega, \xi) = \overline{\mathcal{X}_j(\lambda; \xi, \omega)}$ (see (39)), one obtains the result of the lemma. It is easy to check, as in (ii) above, that the integrand belongs to $L^1(\Sigma(g) \times \mathcal{O} \times S^{n-1})$, permitting the interchange of the order of integration). □

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