Global and Eisenbud–Wigner time delay in scattering theory

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Abstract. We present a new method for proving the existence of the global time delay (defined in terms of sojourn times) as well as its identity with the Eisenbud–Wigner time delay in non-relativistic quantum scattering theory. We show that this method is applicable to scattering by local potentials $V(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^3$, that decay faster than $|\mathbf{x}|^{-4}$ but need not be rotation invariant.

1. Introduction

This paper is concerned with the relation between two definitions of time delay in non-relativistic quantum scattering theory. For motivations and references regarding these definitions we refer to the review article [1].

Let $\delta(\lambda)$ denote the phase shift, at the kinetic energy λ, for scattering by a spherically symmetric potential V in a given partial wave subspace. A simple heuristic argument shows that the number $\tau(\lambda) \equiv 2 \, d\delta(\lambda)/d\lambda$ may be interpreted as the delay of the outgoing radial wave packet with respect to the corresponding free wave packet. If $S(\lambda) = \exp(2i\delta(\lambda))$ denotes the associated S-matrix, then $\tau(\lambda) = -iS(\lambda)^* \, dS(\lambda)/d\lambda$. The corresponding expression for a general (not necessarily spherically symmetric) interaction is the operator

$$\tau(\lambda) = -iS(\lambda)^* \frac{d}{d\lambda} S(\lambda) \qquad (1)$$

acting on functions of the angular variables $\boldsymbol{\omega} \equiv (\theta, \phi)$. $S(\lambda)$ is the S-matrix at energy λ (acting on functions of the angles θ and ϕ), and $\tau(\lambda)$ is called the *Eisenbud–Wigner time delay operator* at energy λ.

A physically somewhat more transparent definition of time delay uses the concept of sojourn times. If ψ_t denotes the (square-integrable) wave function at time t of a scattering state, then the real number

$$T_r(\psi) \equiv \int_{-\infty}^{\infty} dt \int_{|\mathbf{x}| \leq r} |\psi_t(\mathbf{x})|^2 \, d^3x \qquad (r > 0)$$

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may be interpreted as the total time spent by this state during its evolution inside the ball B_r of radius r centered at the origin (if ψ_0 is normalized to 1). The function ψ_t is a solution of the Schrödinger equation $i\, d\psi_t/dt = (\mathbf{P}^2 + V)\psi_t$ (we use units with $\hbar = 2m = 1$). If ϕ_t denotes a freely evolving wave packet, i.e. a solution of $i\, d\phi_t/dt = \mathbf{P}^2\phi_t$, which is asymptotic to ψ_t at $t = -\infty$, i.e. such that $\lim(\psi_t - \phi_t) = 0$ in the Hilbert space norm as $t \to -\infty$, then the difference

$$\tau_r(\phi) \equiv \int_{-\infty}^{\infty} dt \int_{|\mathbf{x}| \leq r} |\psi_t(\mathbf{x})|^2 \, d^3x - \int_{-\infty}^{\infty} dt \int_{|\mathbf{x}| \leq r} |\phi_t(\mathbf{x})|^2 \, d^3x \tag{2}$$

corresponds to the time delay for the ball B_r for scattering initiated in the state ϕ. (In terms of the Møller wave operator $\Omega_- \equiv \lim \exp[is(\mathbf{P}^2 + V)] \exp(-is\mathbf{P}^2)$ as $s \to -\infty$, ψ_t is given as $\psi_t = \Omega_-\phi_t$, hence the quantity $\tau_r(\phi)$ is entirely determined by $\phi \equiv \phi_{t=0}$). The *global time delay* for the initial state ϕ is defined as the limit of $\tau_r(\phi)$ as $r \to \infty$, if this limit exists, and will be denoted by $\tau_\infty(\phi)$.

The following mathematical problems then arise naturally: (i) Prove the existence of the limit of $\tau_r(\phi)$ as $r \to \infty$ for a suitable class of initial states ϕ, (ii) study under what conditions this limit is equal to the expectation value in the state ϕ of the family of operators $\{\tau(\lambda)\}$ defined by (1) (see Remark 2(b) further on for a precise mathematical definition of this expectation value).

For spherically symmetric potentials, these problems have been solved by restricting them to partial wave subspaces [2]–[4]. For non-spherically symmetric potentials there are interesting results for cases where the sojourn time $T_r(\phi)$ is replaced by some other quantity which may be interpreted as some approximate kind of sojourn time [5] [6]; the expression (2) for $\tau_r(\phi)$ was treated in [7] by a stationary method parts of which seem somewhat formal to us, and also in the earlier papers [8] [9] in which the problem of the limit of $\tau_r(\phi)$ was studied at fixed energy and required a suitable interpretation of the limiting procedure due to the appearance of oscillating terms. We refer to the review [1] and to [2]–[9] for additional references on time delay.

Our own approach is as follows. We use the observation made in [2] and [5] that in many circumstances the quantity $\tau_\infty(\phi)$ may be expressed as follows in terms of the scattering operator S: one defines

$$\sigma_r(\phi) = \int_0^{\infty} dt(\phi_t, (S^*F_rS - F_r)\phi_t), \tag{3}$$

where F_r denotes the projection operator onto the set of states localized in the ball B_r, and $(\cdot, \cdot)$ is the scalar product in the Hilbert space $L^2(\mathbb{R}^3)$, and has

$$\tau_\infty(\phi) \equiv \lim_{r \to \infty} \tau_r(\phi) = \lim_{r \to \infty} \sigma_r(\phi) \tag{4}$$

in the following sense: if one of the two limits exists, then so does the other one, and the two limits are equal. By writing $\phi_t = U_t^0\phi$, with $U_t^0 = \exp(-i\mathbf{P}^2 t)$, and by using the unitarity of S (i.e. $S^*S = I$) and the fact that S and U_t^0 commute, the

expression (3) for $\sigma_r(\phi)$ may be rewritten as

$$\sigma_r(\phi) = \left(\phi, S^*\left[\int_0^\infty U_t^{0*}F_rU_t^0\, dt, S\right]\phi\right). \tag{5}$$

The (bounded) first operator in the commutator will be shown to have the following asymptotic representation:

$$\int_0^\infty U_t^{0*}F_rU_t^0\, dt = \frac{r}{2}H_0^{-1/2} - i\, d/d\lambda + O\!\left(\frac{1}{r}\right), \tag{6}$$

where $d/d\lambda$ is the operator of differentiation with respect to the kinetic energy λ and $H_0 = \mathbf{P}^2$.

The first term on the r.h.s. of (6) commutes with S, the commutator of the second term with S leads to the Eisenbud–Wigner time delay upon insertion into (5), and the commutator of the last term with S converges to zero as $r \to \infty$. Some regularity conditions have to be imposed on the S-matrix or the scattering amplitude in order to control this last commutator. The S-matrix is not required to be derived from a local potential; the interaction may be of a more general type, and it need not be invariant under the rotation group.

In Section 2 we establish the asymptotic representation (6) and in Section 3 we apply this result to the time delay problem in two-body scattering theory by local short range interactions. More precisely we give sufficient conditions on the potential V for the validity of (4) and of the above-mentioned regularity conditions on the S-matrix. We think that these conditions are not optimal. Further applications will be presented elsewhere. We give the proofs in n dimensions, $n \geq 2$, since they are essentially independent of n. The physically interesting case is of course $n = 3$.

2. An asymptotic representation

We consider a non-relativistic (one-body) scattering system in n dimensions, where $n \geq 2$. We denote by $(\cdot\,,\cdot)$ and $\|\cdot\|$ the scalar product and the norm respectively, by $\mathbf{Q} = (Q_1, \ldots, Q_n)$ and $\mathbf{P} = (P_1, \ldots, P_n)$ the (self-adjoint) n-component position and momentum operator respectively in the (complex) Hilbert space $\mathscr{H} = L^2(\mathbb{R}^n)$, and we set $|\mathbf{Q}| \equiv (\mathbf{Q}^2)^{1/2} = (\sum_{j=1}^n Q_j^2)^{1/2}$ and $|\mathbf{P}| \equiv (\mathbf{P}^2)^{1/2} = (\sum_{j=1}^n P_j^2)^{1/2}$. The vectors in $\mathscr{H}$ (i.e. the wave functions) will be denoted from now on by f or g. The domain of definition of a linear operator T in $\mathscr{H}$ will be denoted by $D(T)$ and its norm by $\|T\|$.

If w and θ are complex-valued functions defined on $\mathbb{R}^n$ and $[0, \infty)$ respectively, we denote by $w(\mathbf{Q})$ and $\theta(|\mathbf{Q}|)$ the operators of multiplication in $L^2(\mathbb{R}^n)$ by $w(\mathbf{x})$ and $\theta(|\mathbf{x}|)$ respectively, and by $\theta(|\mathbf{P}|)$ the operator of multiplication by $\theta(|\mathbf{k}|)$ in the momentum representation of the wave functions:

$$[\theta(|\mathbf{Q}|)f](\mathbf{x}) = \theta(|\mathbf{x}|)f(\mathbf{x}), \qquad [\mathscr{F}\theta(|\mathbf{P}|)f](\mathbf{k}) = \theta(|\mathbf{k}|)\tilde{f}(\mathbf{k}), \tag{7}$$

where $\tilde{g} \equiv \mathcal{F}g$ denotes the Fourier transform of $g \in L^2(\mathbb{R}^n)$. In particular, if $\theta = \chi_{[0,1]}$ is the characteristic function of the interval $[0, 1]$, defined by $\chi_{[0,1]}(u) = 1$ if $0 \le u \le 1$ and $\chi_{[0,1]}(u) = 0$ if $u > 1$, then $\chi_{[0,1]}(|\mathbf{Q}|/r)$ is nothing but the orthogonal projection F_r onto the subspace of states localized in the ball $B_r = \{\mathbf{x} \in \mathbb{R}^n \mid |\mathbf{x}| \le r\}$:

$$[\chi_{[0,1]}(|\mathbf{Q}|/r)f](\mathbf{x}) = (F_r f)(\mathbf{x}) = \begin{cases} f(\mathbf{x}) & \text{if } |\mathbf{x}| \le r \\ 0 & \text{if } |\mathbf{x}| > r. \end{cases} \tag{8}$$

We also define $\theta^\perp : [0, \infty) \to \mathbb{C}$ by $\theta^\perp(u) = 1 - \theta(u)$.

We denote by $H_0 = \mathbf{P}^2$ the free Hamiltonian and by $\{U_t^0\}_{t \in \mathbb{R}}$ the associated evolution group, i.e. $U_t^0 = \exp(-iH_0 t)$. For $t \in \mathbb{R}$ we set $W_t = \exp(i\mathbf{Q}^2 t)$ and let C_t be the following unitary operator (the classical approximation of U_t^0):

$$(C_t f)(\mathbf{x}) = (2it)^{-n/2} \exp\left(\frac{i\mathbf{x}^2}{4t}\right) \tilde{f}\left(\frac{\mathbf{x}}{2t}\right). \tag{9}$$

By expressing U_t^0 as an integral operator in configuration space, it is easy to show that (see e.g. [10] or [11], Lemma 3.16):

$$U_t^0 = C_t W_{1/(4t)}. \tag{10}$$

Since for any $f, g \in \mathcal{H}$:

$$(C_t f, \theta(|\mathbf{Q}|)C_t g) = \frac{1}{|2t|^n} \int d^n x\, \theta(|\mathbf{x}|) \overline{\tilde{f}\left(\frac{\mathbf{x}}{2t}\right)} \tilde{g}\left(\frac{\mathbf{x}}{2t}\right)$$

$$= \int d^n k\, \theta(|2t\mathbf{k}|) \overline{\tilde{f}(\mathbf{k})} \tilde{g}(\mathbf{k}),$$

we have the identity

$$C_t^* \theta(|\mathbf{Q}|)C_t = \theta(2\,|t|\,|\mathbf{P}|). \tag{11}$$

To obtain the asymptotic expansion (6), it suffices to use the expression (10) for U_t^0 and to develop the factor $W_{1/(4t)}$ into a power series, i.e. to write

$$U_t^0 = C_t \sum_{l=0}^{\infty} \frac{1}{l!} \left(\frac{i\mathbf{Q}^2}{4t}\right)^l. $$

For $\kappa \ge 0$, we denote by $\mathcal{D}_\kappa$ the set of all wave functions $f \in L^2(\mathbb{R}^n)$ such that (i) $f \in D(|\mathbf{Q}|^\kappa)$, (ii) $\tilde{f}$ has compact support in $\mathbb{R}^n \setminus \{0\}$ (i.e. there are numbers $0 < a < b < \infty$, depending on f, such that $\tilde{f}(\mathbf{k}) = 0$ for all $\mathbf{k} \in \mathbb{R}^n$ such that $|\mathbf{k}| \notin [a, b]$). We define A_0 to be the symmetric operator

$$A_0 = \frac{1}{2}\left(\frac{1}{|\mathbf{P}|^2}\mathbf{P} \cdot \mathbf{Q} + \mathbf{Q} \cdot \mathbf{P}\frac{1}{|\mathbf{P}|^2}\right) \tag{12}$$

with domain $D(A_0) = \mathcal{D}_1$, where $\mathbf{P} \cdot \mathbf{Q} \equiv \sum_{j=1}^n P_j Q_j$.

Theorem. *Let* $\theta : [0, \infty) \to [0, \infty)$ *be a bounded continuously differentiable function such that* $\theta(u) = 1$ *in a neighbourhood of* $u = 0$ *and* $\theta(u) = 0$ *in a*

neighbourhood of $u = \infty$, or let $\theta = \chi_{[0,1]}$. Then one has for all f, $g \in \mathcal{D}_2$:

$$\lim_{r \to \infty} \left[\int_0^\infty \left(f, U_t^{0*} \theta\left(\frac{|\mathbf{Q}|}{r}\right) U_t^0 g \right) dt - \frac{r}{2} \int_0^\infty \theta(u) \, du (f, H_0^{-1/2} g) \right]$$
$$= -\tfrac{1}{2}(f, A_0 g). \tag{13}$$

If θ is C^1, it suffices to assume that f, $g \in \mathcal{D}_{1+\epsilon}$ for some $\epsilon > 0$.

Remark 1. The term involving A_0 in (13) corresponds to the term denoted $-i \, d/d\lambda$ in (6). To see this, it suffices to express $(f, A_0 g)$ in the spectral representation of H_0 and to observe that $A_0 = 2i \, d/d\lambda$ in that representation (see [12], pp. 168–170). More precisely, we identify $L^2(\mathbb{R}^n)$ with $L^2([0, \infty)$, $L^2(S^{n-1}); d\lambda)$ in such a way that H_0 becomes multiplication by λ, and we write f_λ for the component of f at energy λ (f_λ is a function of the angles on the unit sphere S^{n-1}, obtained by expressing f in spherical polar coordinates in momentum space, see [12], p. 170). We then have for $f \in \mathcal{H}$ and $g \in \mathcal{D}_1$:

$$-\tfrac{1}{2}(f, A_0 g) = -\frac{1}{2} \int_0^\infty d\lambda \left(f_\lambda, 2i \frac{d}{d\lambda} g_\lambda \right)_0, \tag{14}$$

where $(\cdot, \cdot)_0$ denotes the scalar product in $L^2(S^{n-1})$ (the integral with respect to the angles; we shall also write $\|\cdot\|_0$ for the norm in $L^2(S^{n-1})$). In (14), $dg_\lambda/d\lambda$ denotes the distributional derivative of the vector-valued function $\lambda \mapsto g_\lambda$. If g satisfies the stronger condition $g \in \mathcal{D}_2$, then it belongs to $D(A_0^2)$, hence to the domain of the (maximal) differential operator $d^2/d\lambda^2$, so that the function $\lambda \mapsto g_\lambda$ is strongly continuously differentiable.

Remark 2. (a) In order to insert the asymptotic representation (13) into (5), one has to require that f and Sf belong to $\mathcal{D}_2$. In other words there should be a dense subset of $\mathcal{D}_2$ which is mapped into $\mathcal{D}_2$ by S. This is the regularity condition on S mentioned in the Introduction. In rough terms it means that the scattering amplitude should be twice differentiable with respect to all variables (energy and angles). See also Section 3.

(b) Since the scattering operator commutes with H_0, it is decomposable in the spectral representation of H_0, i.e. given by a family $\{S(\lambda)\}_{\lambda>0}$ of unitary operators acting in $L^2(S^{n-1})$ in such a way that $(Sf)_\lambda = S(\lambda)f_\lambda$. From (5) and (13), the unitarity of S and the fact that $S^* H_0^{-1/2} S = H_0^{-1/2}$ we obtain that, for each f satisfying $f \in \mathcal{D}_2$ and $Sf \in \mathcal{D}_2$:

$$\sigma_\infty(f) \equiv \lim_{r \to \infty} \sigma_r(f) = -\tfrac{1}{2}(f, S^*[A_0, S]f). \tag{15}$$

Formally, writing $A_0 = 2i \, d/d\lambda$, this implies that

$$\sigma_\infty(f) = -i \int_0^\infty d\lambda \left(f_\lambda, S(\lambda)^* \left\{ \frac{d}{d\lambda} S(\lambda) \right\} f_\lambda \right)_0 \equiv \int_0^\infty d\lambda (f_\lambda, \tau(\lambda)f_\lambda)_0. \tag{15'}$$

Without having recourse to distributional derivatives, one can justify the passage from (15) to (15') for example in the following situations. (i) If $S(\lambda)$ is

strongly continuously differentiable with respect to λ, so that $dS(\lambda)/d\lambda$ is a bounded operator in $L^2(S^{n-1})$. (ii) If $S(\lambda)$ is strongly continuous in λ; in fact one may then write:

$$\frac{S(\lambda + \varepsilon) - S(\lambda)}{\varepsilon} f_\lambda = \frac{1}{\varepsilon}[S(\lambda + \varepsilon)f_{\lambda+\varepsilon} - S(\lambda)f_\lambda] - S(\lambda + \varepsilon)\left[\frac{1}{\varepsilon}(f_{\lambda+\varepsilon} - f_\lambda)\right],$$

and since $\lambda \mapsto f_\lambda$ and $\lambda \mapsto S(\lambda)f_\lambda$ are continuously differentiable (see Remark 1) and $S(\lambda)$ is continuous, each term on the r.h.s. is strongly convergent as $\varepsilon \to 0$, so that $dS(\lambda)/d\lambda$ is well defined on f_λ. (iii) If the set $\{g \in \mathcal{H} \mid g \in \mathcal{D}_2 \text{ and } Sg \in \mathcal{D}_2\}$ contains all vectors of the form $g_\lambda = \eta(\lambda)h$ with $\eta \in C_0^\infty((0, \infty))$ and h belonging to some dense subset $\mathcal{M}$ of $L^2(S^{n-1})$. In this case, by choosing η such that $\eta(\lambda) = 1$ on some interval $[a, b] \subset (0, \infty)$, one obtains that $\lambda \mapsto S(\lambda)h$ is strongly continuously differentiable on (a, b), for each $h \in \mathcal{M}$. Hence $dS(\lambda)/d\lambda$ defines a (possibly unbounded) operator in $L^2(S^{n-1})$ with dense domain independent of λ.

Equation (15′) gives a precise meaning to the statement that the global time delay and the Eisenbud–Wigner time delay are identical (provided that the equality (4) holds).

Remark 3. (a) Below we shall give a simple proof of the theorem for the physically interesting case where $\theta = \chi_{[0,1]}$. We shall indicate the proof for the case where θ is C^1 in an appendix. We shall only show that the remainder term, denoted by $O(1/r)$ in (6), tends to zero as $r \to \infty$, i.e. that this term is $o(1)$; somewhat stronger conditions on f and Sf have to be imposed in order to estimate this term as $O(1/r)$.

(b) It suffices to prove (13) for $g = f$. The case $g \neq f$ can then be obtained by using the polarization identity for (f, Tg), where T is a linear operator in $\mathcal{H}$ ([13], Problem I.6.13).

Proof of the theorem (for $\theta = \chi_{[0,1]}$ and $n \geq 3$). (i) We use (10) and (11), then make the change of variables $t \mapsto s = r(2t)^{-1}$ and set $v = (2r)^{-1}$ to find that

$$\int_0^\infty \left(f, U_t^{0*}\theta\left(\frac{|\mathbf{Q}|}{r}\right)U_t^0 f\right) dt = \int_0^\infty \left(f, W_{1/(4t)}^*C_t^*\theta\left(\frac{|\mathbf{Q}|}{r}\right)C_t W_{1/(4t)}f\right) dt$$

$$= \int_0^\infty \left(f, W_{1/(4t)}^*\theta\left(\frac{2t}{r}|\mathbf{P}|\right)W_{1/(4t)}f\right) dt$$

$$= \frac{1}{4v}\int_0^\infty \left(f, W_{vs}^*\theta\left(\frac{|\mathbf{P}|}{s}\right)W_{vs}f\right) \frac{ds}{s^2}. \qquad (16)$$

Furthermore we have

$$\frac{1}{4v}\int_0^\infty \left(f, \theta\left(\frac{|\mathbf{P}|}{s}\right)f\right) \frac{ds}{s^2} = \frac{1}{4v}\int_0^\infty \frac{ds}{s^2}\int d^n k \,\theta\left(\frac{|\mathbf{k}|}{s}\right)|\tilde{f}(\mathbf{k})|^2$$

$$= \frac{1}{4v}\int_0^\infty du\int d^n k \frac{1}{|\mathbf{k}|}\theta(u)|\tilde{f}(\mathbf{k})|^2 = \frac{r}{2}\int_0^\infty \theta(u)\,du(f, H_0^{-1/2}f), \qquad (17)$$

where we have made the change of variables $s \mapsto u = |\mathbf{k}|/s$ (for fixed $\mathbf{k}$), and the interchange of the order of integration is justified since $\tilde{f}(\mathbf{k}) = 0$ in a neighbourhood of the origin.

The preceding two identities show that the l.h.s. of (13) (for $g = f$) is equal to

$$K_\infty(f) \equiv \lim_{\nu \to 0} \frac{1}{4} \int_0^\infty \frac{ds}{\nu s^2} \left[\left(f, W_{\nu s}^* \theta\left(\frac{|\mathbf{P}|}{s}\right) W_{\nu s} f \right) - \left(f, \theta\left(\frac{|\mathbf{P}|}{s}\right) f \right) \right]. \tag{18}$$

(ii) To prove the theorem, we shall show that one may interchange the limit and the integral in (18), by invoking the Lebesgue dominated convergence theorem. This will be done in (iii) below. We assume this result for the moment, take $f \in \mathcal{D}_2 \subset D(\mathbf{Q}^2)$ and $\theta = \chi_{[0,1]}$ and write χ for $\chi_{[0,1]}$ for the sake of shortness. We then have

$$\begin{aligned} K_\infty(f) &= \frac{1}{4} \int_0^\infty \frac{ds}{s^2} \frac{d}{d\nu} \left(f, W_{\nu s}^* \chi\left(\frac{|\mathbf{P}|}{s}\right) W_{\nu s} f \right) \Big|_{\nu=0} \\ &= \frac{i}{4} \int_0^\infty \frac{ds}{s} \left[\left(f, \chi\left(\frac{|\mathbf{P}|}{s}\right) \mathbf{Q}^2 f \right) - \left(\mathbf{Q}^2 f, \chi\left(\frac{|\mathbf{P}|}{s}\right) f \right) \right] \\ &= \frac{i}{4} \int_0^\infty \frac{ds}{s} \int_{|\mathbf{k}| \leq s} d^n k [\overline{\tilde{f}(\mathbf{k})}(\mathcal{F} \mathbf{Q}^2 f)(\mathbf{k}) - \overline{(\mathcal{F} \mathbf{Q}^2 f)(\mathbf{k})} \tilde{f}(\mathbf{k})]. \end{aligned} \tag{19}$$

The integral over $d^n k$ is zero for small s (since $\tilde{f}(\mathbf{k}) = 0$ near the origin) as well as for large s (since $\tilde{f}(\mathbf{k}) = 0$ near infinity and $\mathbf{Q}^2$ is symmetric, i.e. $(f, \mathbf{Q}^2 f) = (\mathbf{Q}^2 f, f)$). Hence an integration by parts gives (using spherical polar coordinates $\mathbf{k} = |\mathbf{k}| \, \omega \equiv k\omega$ with $\omega = \mathbf{k}/|\mathbf{k}| \in S^{n-1}$ and $d^n k = k^{n-1} \, dk \, d\omega$):

$$\begin{aligned} K_\infty(f) &= -\frac{i}{4} \int_0^\infty ds \log s \frac{d}{ds} \int_0^s dk k^{n-1} \int_{S^{n-1}} d\omega [\cdots] \\ &= -\frac{i}{4} \int_0^\infty s^{n-1} \, ds \log s \int_{S^{n-1}} d\omega [\overline{\tilde{f}(s\omega)}(\mathcal{F} \mathbf{Q}^2 f)(s\omega) - \overline{(\mathcal{F} \mathbf{Q}^2 f)(s\omega)} \tilde{f}(s\omega)] \\ &= -\frac{i}{4} [(\log |\mathbf{P}| f, \mathbf{Q}^2 f) - (\mathbf{Q}^2 f, \log |\mathbf{P}| f)]. \end{aligned} \tag{20}$$

Since $\mathbf{Q} = i\nabla$ in momentum space, we have

$$\begin{aligned} [\mathcal{F}(\log |\mathbf{P}| \, \mathbf{Q}^2 f - \mathbf{Q}^2 \log |\mathbf{P}| f)](\mathbf{k}) &= -\log |\mathbf{k}| \, (\Delta \tilde{f})(\mathbf{k}) + \Delta [\log |\mathbf{k}| \, \tilde{f}(\mathbf{k})] \\ &= 2(\nabla \log |\mathbf{k}|) \cdot \nabla \tilde{f}(\mathbf{k}) + (\Delta \log |\mathbf{k}|) \tilde{f}(\mathbf{k}) \\ &= 2 \frac{\mathbf{k}}{|\mathbf{k}|^2} \cdot \nabla \tilde{f}(\mathbf{k}) + \frac{n-2}{|\mathbf{k}|^2} \tilde{f}(\mathbf{k}), \end{aligned}$$

in other terms we have on $\mathcal{D}_2$:

$$(\log |\mathbf{P}|) \mathbf{Q}^2 - \mathbf{Q}^2 \log |\mathbf{P}| = \frac{1}{|\mathbf{P}|^2} (-2i\mathbf{P} \cdot \mathbf{Q} + n - 2) = -2iA_0$$

(see eq. (5.79) of [12] for the last identity). This shows that the limit on the l.h.s. of (13) (with $g = f$) exists and is equal to $(-\frac{1}{2})(f, A_0 f)$, as claimed.

(iii) It remains to prove the applicability of the Lebesgue dominated convergence theorem to (18). For this we rewrite (18) (with $\theta = \chi$) as

$$K_\infty(f) = \lim_{\nu \to +0} \frac{1}{4} \int_0^\infty \frac{ds}{s} \left[\left(\frac{W_{\nu s} - I}{\nu s} f, \chi\left(\frac{|\mathbf{P}|}{s}\right) W_{\nu s} f \right) + \left(\chi\left(\frac{|\mathbf{P}|}{s}\right) f, \frac{W_{\nu s} - I}{\nu s} f \right) \right], \quad (21)$$

where I denotes the identity operator in $\mathcal{H}$, and we shall repeatedly use the Schwarz inequality $|(g, h)| \le \|g\| \|h\|$.

Since $\tau^{-1}(W_\tau - I)f$ converges strongly to $i\mathbf{Q}^2 f$ as $\tau \to 0$, we may choose a number $\delta > 0$ such that $\|\tau^{-1}(W_\tau - I)f\| \le 2 \|\mathbf{Q}^2 f\|$ for all $\tau \in [-\delta, \delta]$. We then have

$$\left\| \frac{1}{\nu s} (W_{\nu s} - I)f \right\| \le \begin{cases} 2 \|\mathbf{Q}^2 f\| & \text{if } \nu s \le \delta \\ \dfrac{2}{\delta} \|f\| & \text{if } \nu s \ge \delta. \end{cases} \quad (22)$$

Since

$$\frac{|\mathbf{k}|}{s} \chi_{[0,1]}\left(\frac{|\mathbf{k}|}{s}\right) \le \chi_{[0,1]}\left(\frac{|\mathbf{k}|}{s}\right) \le 1 \quad \text{for all } \mathbf{k} \in \mathbb{R}^n, \quad (23)$$

one has the following estimates:

$$\frac{1}{s} \left\| \chi\left(\frac{|\mathbf{P}|}{s}\right) W_{\nu s} f \right\| = \left\| \frac{|\mathbf{P}|}{s} \chi\left(\frac{|\mathbf{P}|}{s}\right) \frac{1}{|\mathbf{P}|} W_{\nu s} f \right\| \le \left\| \frac{1}{|\mathbf{P}|} W_{\nu s} f \right\|$$

$$= \left\| \frac{1}{|\mathbf{P}|} (I + \mathbf{Q}^2)^{-1} W_{\nu s} (I + \mathbf{Q}^2) f \right\|$$

$$\le \left\| \frac{1}{|\mathbf{P}|} (I + \mathbf{Q}^2)^{-1} \right\| \|(I + \mathbf{Q}^2)f\|. \quad (24)$$

It is well known that the norm of the operator $|\mathbf{P}|^{-1}(I + \mathbf{Q}^2)^{-1}$ in $L^2(\mathbb{R}^n)$ is finite if $n \ge 3$ (this is nothing but the fact, written after exchanging the role of $\mathbf{P}$ and $\mathbf{Q}$, that the Coulomb potential is bounded relative to $H_0 \equiv \mathbf{P}^2$, see e.g. [11], Example 8.9). Hence (22) and (24) imply that the integrand in (21) is bounded by a constant independent of ν and s, which is sufficient for applying the Lebesgue dominated convergence theorem on any finite interval $[0, s_0]$.

For $s \to \infty$ one needs a different estimate. For this we observe that, except for a change of its sign, the integrand in (18) (and hence also that in (21)) remains the same if θ is replaced by $\theta^\perp \equiv 1 - \theta$ (and hence χ by $\chi^\perp \equiv 1 - \chi$ in (21)). Thus it suffices to show for example that

$$\xi_{\nu,s}(f) \equiv \frac{1}{s} \left| \left(\frac{W_{\nu s} - I}{\nu s} f, \chi^\perp\left(\frac{|\mathbf{P}|}{s}\right) W_t f \right) \right| \le \frac{M}{s^2} \quad (25)$$

for some constant M (depending on f), all $v > 0$, all $s > 0$ and $t = 0$, vs.

To prove (25), we observe that, similarly to (23):

$$\frac{s}{|\mathbf{k}|} \chi_{[0,1]}^{\perp}\left(\frac{|\mathbf{k}|}{s}\right) \leq \chi_{[0,1]}^{\perp}\left(\frac{|\mathbf{k}|}{s}\right) \leq 1. \tag{26}$$

Hence, as in (24):

$$s\left\| \chi^{\perp}\left(\frac{|\mathbf{P}|}{s}\right) W_t f \right\| \leq \left\| \chi^{\perp}\left(\frac{|\mathbf{P}|}{s}\right) |\mathbf{P}| \, W_t f \right\| \leq \| \, |\mathbf{P}| \, W_t f \|$$

$$= \left(\sum_{j=1}^{n} \| P_j W_t f \|^2 \right)^{1/2} \leq \sum_{j=1}^{n} \| P_j W_t f \| \tag{27}$$

(see Lemma 5 in the Appendix for an explanation of the equality used in (27)). Since $P_j = -i \, \partial/\partial x_j$, we have $[P_j, W_t] = 2t W_t Q_j$, so that the last term in (27) is majorized by the expression

$$\sum_{j=1}^{n} \| W_t(P_j f + 2t Q_j f) \| \leq \sum_{j=1}^{n} \left(\| P_j f \| + 2 |t| \, \| Q_j f \| \right)$$

$$\leq n(\| \, |\mathbf{P}| f \| + 2vs \, \| \, |\mathbf{Q}| f \|), \tag{28}$$

since $|t| \leq vs$. Together with (22), this leads to the following upper bound for the l.h.s. of (25): (α) if $vs \leq \delta$:

$$\xi_{v,s}(f) \leq \frac{1}{s^2} 2 \, \| \mathbf{Q}^2 f \| \, [n \, \| \, |\mathbf{P}| f \| + 2n\delta \, \| \, |\mathbf{Q}| f \|],$$

(β) if $vs \geq \delta$:

$$\xi_{v,s}(f) \leq \frac{1}{s^2} \| (W_{vs} - I) f \| \left[n \frac{\| \, |\mathbf{P}| f \|}{vs} + 2n \, \| \, |\mathbf{Q}| f \| \right]$$

$$\leq \frac{2n}{s^2} \| f \| \left[\frac{\| \, |\mathbf{P}| f \|}{\delta} + 2 \, \| \, |\mathbf{Q}| f \| \right].$$

This implies (25) and thus completes the proof. ∎

3. Time delay

The result of our theorem, combined with the remarks already made, has the following implication for the time delay:

Proposition 1. *Consider a (one-body) scattering system in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$, $n \geq 2$, with free Hamiltonian $H_0 = \mathbf{P}^2$ and total Hamiltonian H. Assume the existence of the wave operators $\Omega_{\pm} = s - \lim \exp(iHt) \exp(-iH_0 t)$ as $t \to \pm\infty$ respectively, let $S = \Omega_+^* \Omega_-$ be the associated scattering operator and*

assume that $S^*S = I$. For $g \in \mathcal{H}$ and $r > 0$, define

$$\tau_r(g) = \int_{-\infty}^{\infty} dt[\|F_r e^{-iHt}\Omega_- g\|^2 - \|F_r e^{-iH_0 t} g\|^2].$$ (29)

Let $f \in L^2(\mathbb{R}^n)$ be such that (i) $f \in \mathcal{D}_2$, (ii) $Sf \in \mathcal{D}_2$, (iii)

$$\lim_{r \to \infty} [\tau_r(f) - \sigma_r(f)] = 0,$$ (30)

where $\sigma_r(f)$ is defined by (5).[2]) Then $\tau_r(f)$ converges to a finite limit as $r \to \infty$, and this limit is given in terms of the Eisenbud–Wigner time delay in the sense specified in Remark 2(b).

As an application of Proposition 1 we verify the existence of the time delay in potential scattering, i.e. for $H = H_0 + V$, where V is the operator of multiplication by a real-valued function $v(\mathbf{x})$ which, for $n = 3$, is essentially required to decay faster than $|\mathbf{x}|^{-4}$. We denote by $\sigma_p^+(H)$ the set of all positive eigenvalues of the Hamiltonian H and by Δ_S the spherical Laplacian, i.e. the restriction of the Laplace operator Δ to the unit sphere S^{n-1} in $\mathbb{R}^n$. We denote also by Δ_S the self-adjoint realization of the spherical Laplacian in $L^2(S^{n-1})$; it is well known that this operator has purely discrete spectrum (its eigenvalues are $\{l(l + n - 2) \mid l = 0, 1, 2, \ldots\}$, the degeneracy of each eigenvalue is finite, and the eigenfunctions are the surface spherical harmonics [14]).

Proposition 2. *In $\mathcal{H} = L^2(\mathbb{R}^n)$, $n \geq 2$, let $H_0 = \mathbf{P}^2$ and $H = \mathbf{P}^2 + v(\mathbf{Q})$, where $v : \mathbb{R}^n \to \mathbb{R}$ has the form*

$$v(\mathbf{x}) = (1 + |\mathbf{x}|)^{-\alpha}[v_\infty(x) + v_q(x)],$$ (31)

where $\alpha > \max\{4, (n + 5)/2\}$, $v_\infty \in L^\infty(\mathbb{R}^n)$ and $v_q \in L^q(\mathbb{R}^n)$ for some q satisfying $q \geq 2$ and $q > n/2$. Let $\mathcal{E}$ be the set of all functions $g \in L^2(\mathbb{R}^n)$ that have the following form in the spectral representation of H_0 (see Remark 1):

$$g_\lambda = \rho(\lambda)h,$$ (32)

where $\rho : (0, \infty) \to [0, \infty)$ is three times continuously differentiable and has compact support in $(0, \infty) \backslash \sigma_p^+(H)$, and h is a (λ-independent) vector in $L^2(S^{n-1})$ belonging to the domain of definition of the spherical Laplacian Δ_S. Denote by $\mathcal{D}$ the set of all finite linear combinations of functions in $\mathcal{E}$. Then, for each $f \in \mathcal{D}$, the generalized sequence $\{\tau_r(f)\}_{r>0}$ converges to a finite limit as $r \to \infty$, and this limit is given by the expression (15') ($\lambda \mapsto S(\lambda)$ is continuously differentiable).

Remarks. (i) The condition (32) on g means that the Fourier transform $\tilde{g}(\mathbf{k})$ of g factorizes into a function $\rho(\mathbf{k}^2)$ of the square of the wave vector $\mathbf{k}$ times a function $h(\boldsymbol{\omega})$ of the angular variables $\boldsymbol{\omega} = \mathbf{k}/|\mathbf{k}|$, with $h \in D(\Delta_S)$. The function ρ

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[2]) Notice that $|\sigma_r(f)| < \infty$ for each $f \in \mathcal{H}$ and each $r < \infty$, since the operator F_r is H_0-smooth (see e.g. [1]).

is required to be zero in a neighbourhood of each positive eigenvalue of H ($\sigma_p^+(H)$ is formed of at most a discrete set of points [15]). (ii) By using the result (*J*2) given in the proof below, one can see that the dense set $\mathcal{D}$ is a domain of essential self-adjointness for the Eisenbud–Wigner time delay operator.

Proof. (i) The existence of the wave operators $\Omega_\pm$, their strong asymptotic completeness and hence the unitarity of S are well known for the class of potentials considered here (see e.g. [12]). To deduce Proposition 2 from Proposition 1, it suffices to show that

(A) if $f \in \mathcal{E}$, then $f \in \mathcal{D}_2$ and $Sf \in \mathcal{D}_2$,

(B) the equation (30) is valid for each $f \in \mathcal{D}$.

The validity of (B) and of part of (A) follows from results proved by Jensen in [5]. We shall use two results from [5] which we cite as (*J*1) and (*J*2) and which are special cases of Lemma 4.6 and Theorem 3.5 of [5] respectively, applied to the class of potentials considered here (it suffices to assume $\alpha > 4$ for this). We denote by A the infinitesimal generator of the dilation group in $L^2(\mathbb{R}^n)$, i.e.

$$A = \tfrac{1}{2}(\mathbf{P} \cdot \mathbf{Q} + \mathbf{Q} \cdot \mathbf{P}), \tag{33}$$

and we set $U_t = \exp(-iHt)$ and $U_t^0 = \exp(-iH_0t)$.

(*J*1) If $g \in L^2(\mathbb{R}^n)$ satisfies $g \in D(A^3)$ and $\phi(H_0)g = g$ for some $\phi \in C_0^\infty((0, \infty))$, then

$$\int_0^\infty \|(U_t\Omega_+ - U_t^0)g\| \, dt < \infty \tag{34}$$

and

$$\int_{-\infty}^0 \|(U_t\Omega_- - U_t^0)g\| \, dt < \infty. \tag{35}$$

(*J*2) The S-matrix $S(\lambda)$ is three times continuously differentiable in λ on $(0, \infty)\backslash\sigma_p^+(H)$, where the derivatives are with respect to the operator norm.

(ii) To prove (B), we follow [1]. We notice that, in the spectral representation of H_0, the operator (33) has the form

$$(Af)_\lambda = 2i\lambda \, df_\lambda/d\lambda + if_\lambda. \tag{36}$$

Consequently, since the function ρ in the definition (32) of $\mathcal{E}$ is assumed to be three times differentiable, $f \in \mathcal{D}$ implies $f \in D(A^3)$. By using also (*J*2), we see that $f \in \mathcal{D}$ also implies $Sf \in D(A^3)$. Since ρ has compact support in $(0, \infty)$, it follows that, if $f \in \mathcal{D}$, the inequalities (34) and (35) are true for $g = f$ and $g = Sf$.

Now, since $\Omega_- f = \Omega_- S^*Sf = \Omega_+ Sf$, we have

$$\tau_r(f) - \sigma_r(f) = \int_{-\infty}^0 dt[\|F_r U_t \Omega_- f\|^2 - \|F_r U_t^0 f\|^2]$$

$$+ \int_0^\infty dt[\|F_r U_t \Omega_+ Sf\|^2 - \|F_r U_t^0 Sf\|^2].$$

Both integrands converge to zero for each t as $r \to \infty$, and their absolute values can be majorized uniformly in r by

$$(\|F_r U_t \Omega_- f\| + \|F_r U_t^0 f\|) \, |\, \|F_r U_t \Omega_- f\| - \|F_r U_t^0 f\|\,|$$
$$\leq 2 \|f\| \, \|F_r U_t \Omega_- f - F_r U_t^0 f\| \leq 2 \|f\| \, \|(U_t \Omega_- - U_t^0) f\|$$

and

$$(\|F_r U_t \Omega_+ Sf\| + \|F_r U_t^0 Sf\|) \, |\, \|F_r U_t \Omega_+ Sf\| - \|F_r U_t^0 Sf\|\,|$$
$$\leq 2 \|f\| \, \|(U_t \Omega_+ - U_t^0) Sf\|$$

respectively. We saw above that for $f \in \mathcal{D}$ these bounds belong to $L^1((-\infty, 0); dt)$ and $L^1((0, \infty); dt)$ respectively. Hence $\tau_r(f) - \sigma_r(f) \to 0$ as $r \to \infty$ by the Lebesgue dominated convergence theorem.

(iii) To prove (A), it suffices to verify that $f \in \mathcal{E}$ implies $f \in D(\mathbf{Q}^2)$ and $Rf \in D(\mathbf{Q}^2)$, where $R \equiv S - I$. Now in momentum space the operator $\mathbf{Q}^2$ is just the negative Laplacian:

$$(\mathcal{F}\mathbf{Q}^2 g)(\mathbf{k}) = -\Delta \tilde{g}(\mathbf{k}) = \left(-\frac{\partial^2}{\partial |\mathbf{k}|^2} - \frac{n-1}{|\mathbf{k}|} \frac{\partial}{\partial |\mathbf{k}|} - \frac{\Delta_S}{|\mathbf{k}|^2} \right) \tilde{g}(\mathbf{k}), \tag{37}$$

at least if $\tilde{g}$ is a smooth function. When rewritten in the spectral representation of H_0, (37) becomes

$$(\mathbf{Q}^2 g)_\lambda = \left[-4\lambda \frac{d^2}{d\lambda^2} - 4\frac{d}{d\lambda} + \frac{(n-2)^2}{4\lambda} - \frac{\Delta_S}{\lambda} \right] g_\lambda. \tag{38}$$

If g has the form (32), with ρ and h satisfying the assumptions specified below (32), then clearly each term on the r.h.s of (38) belongs to $L^2((0, \infty), L^2(S^{n-1}); d\lambda)$, hence their sum defines a vector $\hat{g}$ in $\mathcal{H}$. Since $\mathbf{Q}^2$ is given by (38) on smooth functions, one then has (use partial integration for the terms involving $d/d\lambda$ and the self-adjointness of Δ_S):

$$(\mathbf{Q}^2 f, g) = (f, \hat{g}) \qquad \forall f \in \mathcal{S}(\mathbb{R}^n),$$

where $\mathcal{S}(\mathbb{R}^n)$ denotes the Schwartz space of infinitely differentiable functions of rapid decrease. Thus, if $g \in \mathcal{E}$, then g belongs to the domain of the adjoint of $\mathbf{Q}^2|_{\mathcal{S}(\mathbb{R}^n)}$. Since $\mathbf{Q}^2$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^n)$, this means that $g \in \mathcal{E}$ implies $g \in D(\mathbf{Q}^2)$. This proves the first part of (A).

For the second part, assume again that $g \in \mathcal{E}$. Since $S(\lambda)$ is three times differentiable on $(0, \infty) \backslash \sigma_p^+(H)$ and ρ has compact support in $(0, \infty) \backslash \sigma_p^+(H)$, we see that Sg (and hence also Rg) is in the domain of the first three operators in the square bracket in (38) (viewed as operators in $L^2((0, \infty), L^2(S^{n-1}); d\lambda)$.) To show that $Rg \in D(\mathbf{Q}^2)$, it thus remains to prove that $\{-\lambda^{-1} \Delta_S (Rg)_\lambda\}_{\lambda > 0}$ determines a vector in $L^2((0, \infty), L^2(S^{n-1}); d\lambda)$. This will be done in Lemmas 1–3 below by applying a method based on Hilbert–Schmidt estimates introduced in [16]. ∎

For the remaining estimate, we set $Z(\lambda) = -\Delta_S/\lambda$ and define Z to be the associated operator in $\mathcal{H} = L^2(\mathbb{R}^n)$. In the spectral representation of H_0, Z is

given as $(Zf)_\lambda = -\lambda^{-1}\Delta_S f_\lambda$. From (38) and the relation $A_0 = 2i\, d/d\lambda$, we see that, formally:

$$\mathbf{Q}^2 = A_0 H_0 A_0 + \gamma_n H_0^{-1} + Z, \qquad \gamma_n = \tfrac{1}{4}(n-2)^2. \tag{39}$$

We denote by $\mathcal{B}(\mathcal{H})$ the set of all bounded, everywhere defined operators in the Hilbert space $\mathcal{H}$, by $\mathcal{B}_2(\mathcal{H})$ the set of all Hilbert–Schmidt operators in $\mathcal{H}$ and by $\|B\|_2$ the Hilbert–Schmidt norm of the operator B.

To each pair $\{\eta_1, \eta_2\}$ of functions from $(0, \infty)$ to $\mathbb{C}$ satisfying $\|\eta_k\|_+^2 \equiv \int_0^\infty |\eta_k(\lambda)|^2\, d\lambda < \infty$ $(k = 1, 2)$, we associate an operator $P(\eta_1, \eta_2)$ in $\mathcal{B}(L^2(\mathbb{R}^n))$ defined as follows in the spectral representation of H_0:

$$[P(\eta_1, \eta_2)f]_\lambda = \eta_1(\lambda)\int_0^\infty \overline{\eta_2(\mu)}f_\mu\, d\mu, \tag{40}$$

where the integral is a vector-valued integral in $L^2(S^{n-1})$ and $\bar{z}$ denotes the complex conjugate number to z in $\mathbb{C}$. We set $P(\eta) \equiv P(\eta, \eta)$ and observe that $\|\eta\|_+^{-2}P(\eta)$ is the orthogonal projection onto the subspace

$$\mathcal{H}(\eta) \equiv \{f \in L^2(\mathbb{R}^n) \mid f_\lambda = \eta(\lambda)h \text{ for some } h \in L^2(S^{n-1})\} \tag{41}$$

(see Proposition 6.9 of [12]).

Lemma 1. *Let V and H be as in Proposition 2. Let $\eta : (0, \infty) \to \mathbb{C}$ be three times continuously differentiable and of compact support in $(0, \infty)$, and let $\phi \in C_0^\infty((0, \infty))$ be such that $\phi(\lambda) = 1$ for all λ in the support of η. Then, for each $t \in \mathbb{R}$, the closure of the densely defined operator $\phi(H)VU_t^0 ZP(\eta)$ belongs to $\mathcal{B}_2(\mathcal{H})$, and*

$$\int_{-\infty}^\infty \|\phi(H)VU_t^0 ZP(\eta)\|_2\, dt < \infty. \tag{42}$$

Proof. (i) It follows from Lemma 2.31 of [12] that $V(I + \delta\mathbf{Q}^2)\phi(H_0)$ and the closure of $\phi(H)[v_\infty(\mathbf{Q}) + v_q(\mathbf{Q})]$ belong to $\mathcal{B}(\mathcal{H})$ for each $\delta \geq 0$. Since $\phi(H_0)$ commutes with U_t^0 and Z, we have

$$\phi(H)VU_t^0 ZP(\eta) = \phi(H)V\phi(H_0)U_t^0 ZP(\eta),$$

which is well defined on the dense set

$$\mathcal{M}(\eta) \equiv \{f \in L^2(\mathbb{R}^n) \mid f_\lambda = \eta(\lambda)h + g_\lambda \text{ with}$$
$$h \in D(\Delta_S) \subset L^2(S^{n-1}) \text{ and } g \in \mathcal{H}(\eta)^\perp\}. \tag{43}$$

Next we notice that

$$(A_0 H_0 A_0 + \gamma_n H_0^{-1})U_t^0 P(\eta) = \sum_{l=0}^2 t^l U_t^0 P(\eta_l, \eta), \tag{44}$$

with

$$\eta_0(\lambda) = \frac{\gamma_n}{\lambda} \eta(\lambda) - 4\eta'(\lambda) - 4\lambda\eta''(\lambda),$$

$$\eta_1(\lambda) = 4i\eta(\lambda) + 8i\lambda\eta'(\lambda), \qquad \eta_2(\lambda) = 4\lambda\eta(\lambda).$$

It follows in particular that the operator

$$\phi(H)V(A_0H_0A_0 + \gamma_nH_0^{-1})U_t^0P(\eta) \equiv \phi(H)V\phi(H_0)(A_0H_0A_0 + \gamma_nH_0^{-1})U_t^0P(\eta)$$

is defined everywhere in $\mathcal{H}$ and bounded, for each $t \in \mathbb{R}$. Since $U_t^0Z = ZU_t^0$, we then obtain from (39) that, for $f \in \mathcal{M}(\eta)$:

$$\begin{aligned}
\phi(H)VU_t^0ZP(\eta)f &= \phi(H)V\mathbf{Q}^2U_t^0P(\eta)f \\
&\quad - \phi(H)V(A_0H_0A_0 + \gamma_nH_0^{-1})U_t^0P(\eta)f \\
&= \phi(H)V\mathbf{Q}^2\phi(H_0)U_t^0P(\eta)f \\
&\quad - \phi(H)V\phi(H_0)(A_0H_0A_0 + \gamma_nH_0^{-1})U_t^0P(\eta)f. \tag{45}
\end{aligned}$$

Now the operator (44) is in $\mathcal{B}(\mathcal{H})$, $(\xi + \delta\mathbf{Q}^2)(I + |\mathbf{Q}|)^{-\alpha}\phi(H_0)$ is a Hilbert–Schmidt operator if $\alpha > (n + 4)/2$ and $\xi, \delta \geq 0$ (see e.g. [12], Proposition 3.6), and the closure of $\phi(H)[v_\infty(\mathbf{Q}) + v_q(\mathbf{Q})]$ is in $\mathcal{B}(\mathcal{H})$. Hence (45) implies that $\phi(H)VU_t^0ZP(\eta)$ has an extension belonging to $\mathcal{B}_2(\mathcal{H})$.

(ii) We now prove (42). By using the results of (i) above, one sees that it suffices to show that, for $\alpha > (n + 5)/2$:

$$J_l \equiv \int_{-\infty}^\infty t^l \,\|(I + \delta_l\mathbf{Q}^2)(I + |\mathbf{Q}|)^{-\alpha}U_t^0P(\rho_l, \eta)\|_2 \, dt < \infty, \tag{46}$$

where $l = 0, 1, 2$, $\delta_0 = 1$, $\delta_1 = \delta_2 = 0$ and $\rho_l : (0, \infty) \to \mathbb{C}$ has compact support in $(0, \infty)$ and is $(l + 1)$ times continuously differentiable, i.e. $\rho_l \in C_0^{l+1}((0, \infty))$.

To prove (46), we notice that, if $w(\mathbf{Q})$ is a function of the position operator $\mathbf{Q}$, one can exactly calculate integrals of the form

$$G_k \equiv \int_{-\infty}^\infty t^{2k} \,\|(I + |\mathbf{Q}|)^{-k}w(\mathbf{Q})U_t^0P(\psi, \eta)\|_2^2 \, dt. \tag{47}$$

More precisely, these integrals can be expressed in terms of norms of the type $\|\,|\mathbf{x}|^\nu(1 + |\mathbf{x}|)^{-k}w(\mathbf{x})\|_{L^2(\mathbb{R}^n)}^2$ $(0 \leq \nu \leq k)$, $\|\eta\|_+^2$ and $\|\lambda^\gamma\psi^{(m)}(\lambda)\|_+^2$ with $\gamma \in \mathbb{R}$ (see Lemma 6.11 of [12] for $k = 0$ and $k = 1$; the cases $k = 2$ and $k = 3$ which are also needed below are similar to the case $k = 1$ but involve additional partial integrations in (6.50) of [12]). For our purposes here, it is not necessary to know exact expressions for the integrals (47), it suffices to observe that one obtains the following bounds for these quantities:

$$G_k \leq c_k \,\|w\|_{L^2(\mathbb{R}^n)}^2 \,\|\eta\|_+^2 \sum_{m=0}^k \|\lambda^{\gamma_{km}}\psi^{(m)}\|_+^2, \tag{48}$$

where c_k and γ_{km} are finite constants (depending on n) and $\psi^{(m)}(\lambda) = d^m\psi(\lambda)/d\lambda^m$. In particular, let us take $\psi = \rho_l$ and $k = 0, 1, \ldots, l + 1$ and use the assumption that $\rho_l \in C_0^{l+1}((0, \infty))$. It follows that there are finite constants $C_{l\kappa}$

$(l = 0, 1, 2; \kappa = 0, 1, \ldots, l + 1)$, depending on n, ρ_l and η, such that for each $\zeta \geq \kappa$:

$$\int_{-\infty}^{\infty} t^{2\kappa} \|(I + |\mathbf{Q}|)^{-\zeta} w(\mathbf{Q}) U_t^0 P(\rho_l, \eta)\|_2^2 \, dt \leq C_{l\kappa} \|w\|_{L^2(\mathbb{R}^n)}^2. \tag{49}$$

To deduce (46) from (49), we choose $\epsilon > 0$ such that $\epsilon < \min \{\tfrac{1}{2}, \alpha - (n + 5)/2\}$ and define $N_{t,l}(\mathbf{x}, \mathbf{y})$ to be the integral kernel in $L^2(\mathbb{R}^n)$ of the Hilbert–Schmidt operator $B_{t,l} \equiv (I + |\mathbf{Q}|)^{l+(1/2)+\epsilon}(I + \delta_l \mathbf{Q}^2)(I + |\mathbf{Q}|)^{-\alpha} U_t^0 P(\rho_l, \eta)$. We set

$$\kappa_{l\epsilon} \equiv \int_{-\infty}^{\infty} s^{2l}(1 + s^2)^{-l-\epsilon-1/2} \, ds$$

and use the Schwarz inequality in $L^2(\mathbb{R}; dt)$ to obtain that

$$\begin{aligned}
J_l^2 &\leq \kappa_{l\epsilon} \int_{-\infty}^{\infty} dt (1 + t^2)^{l+\epsilon+1/2} \|(I + |\mathbf{Q}|)^{-l-\epsilon-1/2} B_{t,l}\|_2^2 \\
&= \kappa_{l\epsilon} \int_{-\infty}^{\infty} dt \iint d^n x \, d^n y \left(\frac{1 + t^2}{(1 + |\mathbf{x}|)^2}\right)^{l+\epsilon+1/2} |N_{t,l}(\mathbf{x}, \mathbf{y})|^2 \\
&= \kappa_{l\epsilon} \int_{-\infty}^{\infty} dt \iint d^n x \, d^n y \left[\left(\frac{1 + t^2}{(1 + |\mathbf{x}|)^2}\right)^{l+1} |N_{t,l}(\mathbf{x}, \mathbf{y})|^2\right]^{\epsilon+1/2} \\
&\quad \cdot \left[\left(\frac{1 + t^2}{(1 + |\mathbf{x}|)^2}\right)^{l} |N_{t,l}(\mathbf{x}, \mathbf{y})|^2\right]^{-\epsilon+1/2}.
\end{aligned}$$

By applying the Hölder inequality with $p = (\tfrac{1}{2} + \epsilon)^{-1}$, $q = (\tfrac{1}{2} - \epsilon)^{-1}$ and $p^{-1} + q^{-1} = 1$ in $L^1(\mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n; dt \, d^n x \, d^n y)$, one finds that

$$\begin{aligned}
J_l^2 &\leq \kappa_{l\epsilon} \left[\int_{-\infty}^{\infty} dt (1 + t^2)^{l+1} \|(I + |\mathbf{Q}|)^{-(l+1)} B_{t,l}\|_2^2\right]^{1/2+\epsilon} \\
&\quad \cdot \left[\int_{-\infty}^{\infty} dt (1 + t^2)^{l} \|(I + |\mathbf{Q}|)^{-l} B_{t,l}\|_2^2\right]^{1/2-\epsilon}. \tag{50}
\end{aligned}$$

Each of the square brackets on the r.h.s. of (50) is a sum of terms having the form of the l.h.s. of (49), with $w(\mathbf{x}) = (1 + \delta_l \mathbf{x}^2)(1 + |\mathbf{x}|)^{-\alpha+l+(1/2)+\epsilon}$, and the finiteness of the r.h.s. of (50) follows from (49). ∎

Lemma 2. *Let V, H and η be as in Lemma 1. Then the closure of $R^* Z P(\eta)$ belongs to $\mathcal{B}_2(\mathcal{H})$.*

Proof. Let ϕ be as in Lemma 1 and $f \in \mathcal{M}(\eta)$ (see (43)). Then $f \in D(R^* Z P(\eta))$, and

$$\begin{aligned}
R^* Z P(\eta) f &= \Omega_-^* (\Omega_+ - \Omega_-) Z P(\eta) f = \Omega_-^* \phi(H)(\Omega_+ - \Omega_-)\phi(H_0) Z P(\eta) f \\
&= \Omega_-^* \phi(H) \int_{-\infty}^{\infty} dt \frac{d}{dt} U_t^* U_t^0 \phi(H_0) Z P(\eta) f \\
&= i \Omega_-^* \left[\int_{-\infty}^{\infty} dt \, U_t^* \phi(H) V U_t^0 Z P(\eta)\right] f.
\end{aligned}$$

By Lemma 1, the integral in the square bracket defines a Hilbert–Schmidt operator (use for instance Proposition 1.22 (b) of [12] in the Hilbert space $\mathcal{B}_2(\mathcal{H})$). Hence the densely defined operator $R^*ZP(\eta)$ is closable, and its closure is in $\mathcal{B}_2(L^2(\mathbb{R}^n))$. ∎

Lemma 3. *Let V, H and $\mathcal{E}$ be as in Proposition 2, and let $g \in \mathcal{E}$. Then $Rg \in D(Z)$.*

Proof. (i) Let $\{e_k\}$ be an orthonormal basis of $L^2(S^{n-1})$ formed of eigenvectors of Δ_S, and let f_k be defined by $(f_k)_\lambda = \eta(\lambda)e_k$, where η is a function satisfying the hypotheses of Lemmas 1 and 2. Then, since $\{f_k/\|\eta\|_+\}$ is an orthonormal basis of the range $\mathcal{H}(\eta)$ of $P(\eta)$, the Hilbert–Schmidt norm of the closure of $R^*ZP(\eta)$ is given by

$$\|R^*ZP(\eta)\|_2^2 = \frac{1}{\|\eta\|_+^2} \sum_{k=1}^{\infty} \|R^*ZP(\eta)f_k\|^2$$

$$= \|\eta\|_+^2 \int_0^{\infty} d\lambda\, |\eta(\lambda)|^2 \sum_{k=1}^{\infty} \|R(\lambda)^*Z(\lambda)e_k\|_0^2 < \infty. \tag{51}$$

Hence $\sum_{k=1}^{\infty} \|R(\lambda)^*Z(\lambda)e_k\|_0^2 < \infty$ for almost all $\lambda \in \Gamma(\eta) \equiv \{\mu > 0 \mid \eta(\mu) \neq 0\}$. By varying η one finds that the preceding inequality holds for a.a. $\lambda > 0$. This implies that the operator $R(\lambda)^*Z(\lambda)$, defined on the dense set $\mathcal{N}$ of all finite linear combinations of $e_1, e_2, \ldots$, has an extension $X(\lambda)$ belonging to $\mathcal{B}_2(L^2(S^{n-1}))$ (set $\beta_{jk} = (e_j, R(\lambda)^*Z(\lambda)e_k)_0$ and notice that $\sum_{jk} |\beta_{jk}|^2 < \infty$; hence the operator whose matrix elements in the basis $\{e_k\}$ are β_{jk} is in $\mathcal{B}_2(L^2(S^{n-1}))$, see e.g. Proposition 3.4 of [12]). (51) implies that

$$\|R^*ZP(\eta)\|_2^2 = \|\eta\|_+^2 \int_0^{\infty} d\lambda\, |\eta(\lambda)|^2 \|X(\lambda)\|_2^2$$

$$= \|\eta\|_+^2 \int_0^{\infty} d\lambda\, |\eta(\lambda)|^2 \|X(\lambda)^*\|_2^2 < \infty. \tag{52}$$

(ii) Next let $h \in L^2(S^{n-1})$. Then, for each $e \in \mathcal{N}$:

$$(R(\lambda)h, Z(\lambda)e)_0 = (h, X(\lambda)e)_0 = (X(\lambda)^*h, e)_0.$$

This shows that $R(\lambda)h$ is in the domain of the adjoint of $Z(\lambda)|_{\mathcal{N}}$. But $[Z(\lambda)|_{\mathcal{N}}]^* = Z(\lambda)$, because Δ_S is essentially self-adjoint on $\mathcal{N}$ (since $\mathcal{N}$ contains a basis of $L^2(S^{n-1})$ formed of eigenvectors of Δ_S). Hence $R(\lambda)h \in D(Z(\lambda))$ and $Z(\lambda)R(\lambda)h = X(\lambda)^*h$ for almost all $\lambda > 0$.

(iii) Now let $g \in \mathcal{E}$, i.e. $g_\lambda = \rho(\lambda)h$ as in (32). Observe that, by the result of (ii):

$$(ZRg)_\lambda = \rho(\lambda)Z(\lambda)R(\lambda)h = \rho(\lambda)X(\lambda)^*h \quad \text{a.e.} \tag{53}$$

Thus

$$\int_0^\infty d\lambda \, \|(ZRg)_\lambda\|_0^2 = \int_0^\infty d\lambda \, |\rho(\lambda)|^2 \, \|X(\lambda)^* h\|_0^2$$

$$\le \int_0^\infty d\lambda \, |\rho(\lambda)|^2 \, \|X(\lambda)^*\|_2^2 \, \|h\|_0^2.$$

The last expression is finite by (52), hence (53) defines a vector in $L^2((0, \infty)$, $L^2(S^{n-1}); d\lambda)$. ■

Appendix

We indicate here a proof of the Theorem of Section 2 for the case where θ is a C^1-function. We shall use the following simple facts.

Lemma 4 ([11], *equations* (3.34) *and* (3.63)). *Let* $\tau, z \in \mathbb{R}$ *and* $\gamma \in [0, 1]$. *Then*

$$|e^{iz} - 1| \le 2^{1-\gamma} |z|^\gamma, \tag{54}$$

$$\left| \frac{1}{\tau} (e^{iz\tau} - 1) - iz \right| \le 2 |z|. \tag{55}$$

Lemma 5. *One has* $D(|\mathbf{Q}|) = \bigcap_{j=1}^n D(Q_j)$, *and for* $f, g \in D(|\mathbf{Q}|)$:

$$(|\mathbf{Q}| f, |\mathbf{Q}| g) = \sum_{j=1}^n (Q_j f, Q_j g), \tag{56}$$

$$\lim_{\tau \to 0} \frac{1}{\tau} (f, (W_{t+\tau} - W_t)g) = i \sum_{j=1}^n (Q_j f, Q_j W_t g). \tag{57}$$

Proof. For $h \in D(|\mathbf{Q}|)$, set $h_r = F_r h$, where F_r is defined by (8), and notice that $h_r \in D(\mathbf{Q}^2)$ and that $|\mathbf{Q}| \, h_r \to |\mathbf{Q}| \, h$ and $Q_j h_r \to Q_j h$ in the Hilbert space norm as $r \to \infty$. The first two assertions now follow from the following set of identities:

$$(|\mathbf{Q}| f, |\mathbf{Q}| g) = \lim_{r \to \infty} (|\mathbf{Q}| f_r, |\mathbf{Q}| g_r) = \lim_{r \to \infty} (f_r, \mathbf{Q}^2 g_r)$$

$$= \lim_{r \to \infty} \sum_{j=1}^n (f_r, Q_j^2 g_r) = \sum_{j=1}^n \lim_{r \to \infty} (Q_j f_r, Q_j g_r)$$

$$= \sum_{j=1}^n (Q_j f, Q_j g).$$

Equation (57) can be checked by writing the scalar products as integrals in $L^2(\mathbb{R}^n)$ and by applying Lemma 4 and the Lebesgue dominated convergence theorem. ■

Assume now that the function θ in the theorem is C^1 and let $f \in \mathcal{D}_{1+\epsilon} \subset \mathcal{D}_1$ for some $\epsilon \in (0, 1)$. The proof of (13) in this situation is similar to the proof given in Section 2; a few steps will be done only formally, a rigorous justification is not difficult. Part (i) of the proof remains unchanged. For part (ii), we use (18) and (57) to obtain that

$$
\begin{aligned}
K_\infty(f) &= \frac{1}{4} \int_0^\infty \frac{ds}{s^2} \frac{d}{dv} \left(f, W_{vs}^* \theta\left(\frac{|\mathbf{P}|}{s}\right) W_{vs} f \right)\Big|_{v=0} \\
&= -\frac{i}{4} \int_0^\infty \frac{ds}{s} \sum_{j=1}^n \left[\left(Q_j f, Q_j \theta\left(\frac{|\mathbf{P}|}{s}\right) f \right) - \left(Q_j \theta\left(\frac{|\mathbf{P}|}{s}\right) f, Q_j f \right) \right] \\
&= \frac{1}{4} \int_0^\infty \frac{ds}{s} \sum_{j=1}^n \left[\left(Q_j f, \theta_{,j}\left(\frac{|\mathbf{P}|}{s}\right) f \right) + \left(\theta_{,j}\left(\frac{|\mathbf{P}|}{s}\right) f, Q_j f \right) \right],
\end{aligned}
$$

where $\theta_{,j}(|\mathbf{P}|/s)$ denotes the multiplication operator in momentum space by the function $\partial \theta(|\mathbf{k}|/s)/\partial k_j$. Now

$$
\frac{\partial \theta(|\mathbf{k}|/s)}{\partial k_j} = \frac{k_j}{|\mathbf{k}| s} \theta'\left(\frac{|\mathbf{k}|}{s}\right) = -\frac{k_j s}{|\mathbf{k}|^2} \frac{d\theta(|\mathbf{k}|/s)}{ds}. \tag{58}
$$

By using (58) and the assumption that $\theta(0) = 1$, $\theta(\infty) = 0$, one finds that

$$
\begin{aligned}
K_\infty(f) &= -\frac{1}{4} \int_0^\infty ds \frac{d}{ds} \left[\left(\frac{1}{\mathbf{P}^2} \mathbf{P} \cdot \mathbf{Q} f, \theta\left(\frac{|\mathbf{P}|}{s}\right) f \right) + \left(\theta\left(\frac{|\mathbf{P}|}{s}\right) f, \frac{1}{\mathbf{P}^2} \mathbf{P} \cdot \mathbf{Q} f \right) \right] \\
&= -\frac{1}{4} \left[\left(f, \mathbf{Q} \cdot \mathbf{P} \frac{1}{\mathbf{P}^2} f \right) + \left(f, \frac{1}{\mathbf{P}^2} \mathbf{P} \cdot \mathbf{Q} f \right) \right] = -\tfrac{1}{2}(f, A_0 f).
\end{aligned}
$$

The preceding identity completes part (ii) of the proof. For part (iii), we set $\tau = vs$ and rewrite the integrand in (18) as follows:

$$
\frac{1}{\tau s} \left((W_\tau - I)f, \theta\left(\frac{|\mathbf{P}|}{s}\right)f \right) + \frac{1}{\tau s} \left(\theta\left(\frac{|\mathbf{P}|}{s}\right)f, (W_\tau - I)f \right)
$$

$$
+ \frac{1}{\tau s} \left((W_\tau - I)f, \theta\left(\frac{|\mathbf{P}|}{s}\right)(W_\tau - I)f \right). \tag{59}
$$

The first and the second term are zero for $s \in (0, s_0]$, for some $s_0 > 0$ depending on the support of $\tilde{f}$, and the absolute value of each of them is majorized, for $0 < \tau \le \tau_0$, by

$$
\frac{2}{s} \sum_{j=1}^n \|Q_j f\| \left\| Q_j \theta\left(\frac{|\mathbf{P}|}{s}\right)f \right\|
$$

$$
\le \frac{2}{s} \sum_{j=1}^n \|Q_j f\| \left[\|\theta\|_{L^\infty} \|Q_j f\| + \frac{1}{s} \|\theta'\|_{L^\infty} \left\| \frac{P_j}{|\mathbf{P}|} f \right\| \right]. \tag{60}
$$

Hence the Lebesgue dominated convergence theorem applies to these two terms on $(0, s_1]$ for any $s_1 < \infty$. For the third term in (59) one has the following bound:

$$
\frac{1}{s^{1-\epsilon}} \left\| \left(\frac{|\mathbf{P}|}{s}\right)^{\epsilon/2} \left[\theta\left(\frac{|\mathbf{P}|}{s}\right) \right]^{1/2} \right\|^2 \left\| \frac{1}{|\mathbf{P}|^{\epsilon/2}} (I + |\mathbf{Q}|)^{-\epsilon} \right\|^2 \left\| \frac{W_\tau - I}{\tau^{1/2}} (I + |\mathbf{Q}|)^\epsilon f \right\|^2.
$$

The first norm is bounded by $c \, \|\theta\|_{L^\infty}^{1/2}$ for some finite constant c depending on ϵ and the support of θ; the second norm is finite since the operator $|\mathbf{P}|^{-\epsilon/2}(I + |\mathbf{Q}|)^{-\epsilon}$ is in $\mathscr{B}(\mathscr{H})$ (apply Lemma 3.13 of [12]), and the third norm is majorized by $2 \, \| \, |\mathbf{Q}| \, (I + |\mathbf{Q}|)^\epsilon f\|$ (use (54) with $\gamma = \frac{1}{2}$). Consequently the Lebesgue dominated convergence theorem applies also to the third term in (59) on $(0, s_1]$, for any $s_1 < \infty$.

For large s, we use instead of (59) the same expression with θ replaced by $\theta^\perp$ (which, except for an overall sign, is equal to the expression (59)). The first two terms are then zero for $s \geq s_2$, for some $s_2 < \infty$ depending on the support of $\tilde{f}$, and admit a bound similar to (60) for $s \leq s_2$.

For the third term we obtain the following bounds, by using the argument that led from (27) to (28):

(α) if $\tau \leq 1$:

$$\frac{1}{\tau s} \left| \left((W_\tau - I)f, \, \theta^\perp\left(\frac{|\mathbf{P}|}{s}\right)(W_\tau - I)f \right) \right|$$

$$\leq \frac{1}{s^3} \left\| \left(\frac{s}{|\mathbf{P}|}\right)^2 \theta^\perp\left(\frac{|\mathbf{P}|}{s}\right) \right\| \left\| |\mathbf{P}| \frac{W_\tau - I}{\tau^{1/2}} f \right\|^2$$

$$\leq \frac{1}{s^3} c \, \|\theta^\perp\|_{L^\infty} \left[\sum_{j=1}^n \left\| \frac{W_\tau - I}{\tau^{1/2}} P_j f \right\| + 2 \|Q_j f\| \right]^2,$$

(β) if $\tau \geq 1$:

$$\frac{1}{\tau s} \left| \left((W_\tau - I)f, \, \theta^\perp\left(\frac{|\mathbf{P}|}{s}\right)(W_\tau - I)f \right) \right|$$

$$\leq \frac{1}{s^2} \left\| \frac{s}{|\mathbf{P}|} \theta^\perp\left(\frac{|\mathbf{P}|}{s}\right) \right\| \|(W_\tau - I)f\| \left[\sum_{j=1}^n \left\| P_j \frac{W_\tau - I}{\tau} f \right\|^2 \right]^{1/2}$$

$$\leq \frac{1}{s^2} c \, \|\theta^\perp\|_{L^\infty} \cdot 2 \|f\| \left[\sum_{j=1}^n 2 \|P_j f\| + 2 \|Q_j f\| \right].$$

It now suffices to observe that, by (54) with $\gamma = \frac{1}{2}$:

$$\frac{1}{\tau^{1/2}} \|(W_\tau - I)P_j f\| \leq 2 \, \| \, |\mathbf{Q}| \, P_j f\| = 2 \left[\sum_{k=1}^n \|Q_k P_j f\|^2 \right]^{1/2},$$

which is finite because $f \in \mathscr{D}_1$ implies $f \in D(Q_k P_j)$ ($\mathscr{F} Q_k f$ has the same support as $\tilde{f}$). ∎

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