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Autor(en): **Bollé, D. / Gesztesy, F.**

Objekttyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **56 (1983)**

Heft 5

PDF erstellt am: **04.06.2024**

Persistenter Link: https://doi.org/10.5169/seals-115434

Helvetica Physica Acta, Vol. **56** (1983) 1064–1069

0018–0238/83/051064–06$1.50 + 0.20/0

On averaged angular time delay for two-body scattering

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(19. IV. 1983; rev. 1. VI. 1983)

Abstract. In this note, we introduce and discuss the concept of averaged angular time delay, in analogy with averaged total cross-sections.

I. Introduction

Recently, there has been a renewed interest in the study of time delay in scattering theory. (See Ref. [1–6], and the references in [6] for earlier results). These papers discuss the notion of global time delay and its relation to the scattering matrix, using a time-dependent approach.

In this note, we rigorously study the angular time delay from a stationary point of view. Heuristic discussions in this spirit can be found in Ref. [7, 8] and the references cited therein.

In particular, we introduce and discuss averaged angular time delay in analogy with recent treatments of averaged total cross-sections [9–11]. We show that it is equal to the trace of the on-shell global time-delay operator. In establishing this relation, we first have to prove the differentiability of the scattering matrix such that we know that time delay exists as a bounded operator. Furthermore, we have to show that the time-delay operator is trace class. This is done in Theorem 3 for the class of potentials $(1+|\mathbf{x}|)V(\mathbf{x}) \in L^1 \cap R$. This condition roughly implies that $V(\mathbf{x}) = 0(|\mathbf{x}|^{-4-\varepsilon})$, $\varepsilon > 0$ as $|\mathbf{x}| \to \infty$. Note that the differentiability of the scattering matrix has also been proved in Ref. [1, 4] for a more general class of potentials, roughly allowing a $|\mathbf{x}|^{-1-\varepsilon}$ behavior at infinity. The proof we present here is extremely simple and, in addition, yields the trace class property of the time-delay operator. Finally, in Theorem 4, we establish the continuity of the averaged angular time delay (and averaged total cross-section) with respect to interactions.

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II. Some results on two-body scattering

Let $V:\mathbb{R}^3 \to \mathbb{R}$ be a real measurable function and assume $V \in R$, where R denotes the Rollnik class (i.e. $\|V\|_R^2 = \int d^3x\, d^3y\, |V(\mathbf{x})|\,|V(\mathbf{y})|\,|\mathbf{x}-\mathbf{y}|^{-2} < \infty$). If $H_0 = -\Delta$ denotes the usual self-adjoint realization of the kinetic energy operator, we define the Hamiltonian $H = H_0 \dotplus V$ through the method of forms [12]. Introducing

$$v(\mathbf{x}) = |V(\mathbf{x})|^{1/2}, \qquad u(\mathbf{x}) = v(\mathbf{x}) \operatorname{sign} V(\mathbf{x}), \tag{2.1}$$

the symmetrized resolvent operator $uG_k v$ defined as the norm limit

$$uG_{\pm k} v = n - \lim_{\varepsilon \to 0^+} u(H_0 - k^2 \mp i\varepsilon)^{-1} v, \qquad k \geq 0, \tag{2.2}$$

is Hilbert–Schmidt and satisfies

$$uG_{-k} v = (uG_k v)^*. \tag{2.3}$$

The scattering wave functions $\Phi^\pm$ obey the following inhomogeneous Lippmann–Schwinger equations

$$\Phi^\pm(k\boldsymbol{\omega}, \mathbf{x}) = \Phi_0^\pm(k\boldsymbol{\omega}, \mathbf{x}) - (uG_{\mp k} v \Phi^\pm)(k\boldsymbol{\omega}, \mathbf{x}), \qquad k^2 \notin \mathscr{E}, \tag{2.4a}$$

which can also be written in the form

$$\Phi^\pm(k\boldsymbol{\omega}, \mathbf{x}) = ((1 + uG_{\mp k} v)^{-1} \Phi_0^\pm)(k\boldsymbol{\omega}, \mathbf{x}), \qquad k^2 \notin \mathscr{E}, \tag{2.4b}$$

where the $\Phi_0^\pm$ are defined by

$$\Phi_0^-(k\boldsymbol{\omega}, \mathbf{x}) = u(\mathbf{x}) e^{ik\boldsymbol{\omega}\cdot\mathbf{x}}, \qquad \Phi_0^+(k\boldsymbol{\omega}, \mathbf{x}) = v(\mathbf{x}) e^{ik\boldsymbol{\omega}\cdot\mathbf{x}}, \tag{2.5}$$

and where $\boldsymbol{\omega} \in S^2$, the unit sphere in $\mathbb{R}^3$. The set $\mathscr{E}$ is defined as

$$\mathscr{E} = \{k^2 \geq 0 \mid uG_k v\psi = -\psi \text{ for some } \psi \in L^2(\mathbb{R}^3),\ k \geq 0\}. \tag{2.6}$$

$\mathscr{E}$ is a closed subset of $[0, \infty)$ with Lebesgue measure zero containing the singular continuous spectrum and positive eigenvalues of H [12]. Then we have (for a proof see [12, 13]).

Theorem 1. *Let $V \in L^1(\mathbb{R}^3) \cap R$, then the scattering operator S, associated with the pair (H, H_0) is unitary, commutes with H_0 and in the spectral representation of H_0, the corresponding on-shell operator $S(k)$ reads*

$$(S(k)\phi)(\boldsymbol{\omega}) = \phi(\boldsymbol{\omega}) - \frac{k}{2\pi i} \int_{S^2} d\omega' f(k, \boldsymbol{\omega}, \boldsymbol{\omega}')\phi(\boldsymbol{\omega}'), \qquad k^2 \notin \mathscr{E}, \qquad \phi \in L^2(S^2), \tag{2.7}$$

where $f(k, \boldsymbol{\omega}, \boldsymbol{\omega}')$ represents the on-shell scattering amplitude. For $k^2 \notin \mathscr{E}$, $S(k) - 1$ is a trace class-operator in $L^2(S^2)$, i.e. $[S(k) - 1] \in \mathscr{B}_1(L^2(S^2))$, $k^2 \notin \mathscr{E}$, and continuous in trace norm with respect to k. Furthermore, an explicit characterization of $f(k, \boldsymbol{\omega}, \boldsymbol{\omega}')$ is obtained from

$$\begin{aligned} f(k, \boldsymbol{\omega}, \boldsymbol{\omega}') &= -(4\pi)^{-1}(\Phi_0^+(k\boldsymbol{\omega}), \Phi^-(k\boldsymbol{\omega}')) \\ &= -(4\pi)^{-1}(\Phi^+(k\boldsymbol{\omega}), \Phi_0^-(k\boldsymbol{\omega}')), \qquad k^2 \notin \mathscr{E}. \end{aligned} \tag{2.8}$$

Finally, $f(k, \boldsymbol{\omega}, \boldsymbol{\omega}')$ is uniformly continuous in all variables if k^2 varies in compact intervals not intersecting $\mathscr{E}$.

Following [9–11], the averaged total cross-section $\bar{\sigma}(k)$ is defined as

$$\bar{\sigma}(k)=(4\pi)^{-1}\int_{S^2} d\omega \int_{S^2} d\omega' \, |f(k,\boldsymbol{\omega},\boldsymbol{\omega}')|^2$$
$$=\frac{\pi}{k^2}\|S(k)-1\|_2^2=-\frac{2\pi}{k}\operatorname{Re}(\operatorname{Tr}(S(k)-1)). \tag{2.9}$$

Theorem 1 then immediately leads to

Theorem 2. *Assume $V\in L^1(\mathbb{R}^3)\cap R$. Then for $k^2\notin\mathscr{E}$, $\bar{\sigma}(k)$ is finite and continuous in k. In addition, the optical theorem*

$$\sigma(k,\boldsymbol{\omega})=\int_{S^2} d\omega' \, |f(k,\boldsymbol{\omega},\boldsymbol{\omega}')|^2=\frac{4\pi}{k}\operatorname{Im} f(k,\boldsymbol{\omega},\boldsymbol{\omega}) \tag{2.10}$$

is valid.

3. Averaged angular time delay

In the following we discuss the necessary modifications of the above approach in order to study the concept of averaged angular time delay in a rigorous way. We start with

Lemma 1. *Let $(1+|\mathbf{x}|)V\in L^1(\mathbb{R}^3)\cap R$ and $k^2\notin\mathscr{E}$. Then $(1+|\mathbf{x}|)^{1/2}\,\Phi^{\pm}(k\boldsymbol{\omega},\mathbf{x})$ is strongly continuous in $L^2(\mathbb{R}^3)$ with respect to k for all $\boldsymbol{\omega}\in S^2$ and $f(k,\boldsymbol{\omega},\boldsymbol{\omega}')$ is continuously differentiable with respect to k for all $\boldsymbol{\omega},\boldsymbol{\omega}'\in S^2\times S^2$. In particular, $S(k)$ is continuously differentiable in trace norm, i.e. $S'(k)\in\mathscr{B}_1(L^2(S^2))$ and $(-k(2\pi i)^{-1}f(k,\boldsymbol{\omega},\boldsymbol{\omega}'))'$ is the kernel of $S'(k)$. (The $'$ denotes the derivative with respect to k).*

Proof. The strong continuity of $(1+|\mathbf{x}|)^{1/2}\Phi^{\pm}(k\boldsymbol{\omega},\mathbf{x})$ is clear from (2.4) and the condition on V. (cf. [12], Section IV.5). To prove the rest of the lemma, we first note that, using (2.4) and (2.8)

$$\begin{aligned}f'(k,\boldsymbol{\omega},\boldsymbol{\omega}')&=i(4\pi)^{-1}(|\boldsymbol{\omega}\cdot\mathbf{x}|^{1/2}\Phi_0^+(k\boldsymbol{\omega}),\operatorname{sign}(\boldsymbol{\omega}\cdot\mathbf{x})\,|\boldsymbol{\omega}\cdot\mathbf{x}|^{1/2}\Phi^-(k\boldsymbol{\omega}'))\\&\quad+(4\pi)^{-1}(\Phi^+(k\boldsymbol{\omega}),(uG_k'v\Phi^-)(k\boldsymbol{\omega}'))\\&\quad-i(4\pi)^{-1}(|\boldsymbol{\omega}'\cdot\mathbf{x}|^{1/2}\Phi^+(k\boldsymbol{\omega}),\operatorname{sign}(\boldsymbol{\omega}'\cdot\mathbf{x})\,|\boldsymbol{\omega}'\cdot\mathbf{x})|^{1/2}\Phi_0^-(k\boldsymbol{\omega}')),\\&\qquad k^2\notin\mathscr{E},\end{aligned} \tag{3.1}$$

where $uG_k'v$ denotes the Hilbert–Schmidt operator represented by the kernel

$$(uG_k'v)(\mathbf{x},\mathbf{y})=i(4\pi)^{-1}u(\mathbf{x})e^{ik|\mathbf{x}-\mathbf{y}|}v(\mathbf{y}). \tag{3.2}$$

Equation (3.1) proves the assertions for the on-shell scattering amplitude $f(k,\boldsymbol{\omega},\boldsymbol{\omega}')$. Next, following Ref. [13], we introduce the maps

$$A_V(k):\begin{cases}L^2(\mathbb{R}^3)\to L^2(S^2)\\ g(\mathbf{x})\to(A_V(k)g)(\boldsymbol{\omega})=\int_{\mathbb{R}^3}d^3x\,u(\mathbf{x})e^{-ik\boldsymbol{\omega}\cdot\mathbf{x}}g(\mathbf{x})\end{cases} \tag{3.3}$$

and

$$A_V(k)^*:\begin{cases} L^2(S^2)\to L^2(\mathbb{R}^3) \\ \phi(\boldsymbol{\omega})\to(A_V(k)^*\phi)(\mathbf{x})=\int_{S^2} d\omega u(\mathbf{x})e^{ik\boldsymbol{\omega}\cdot\mathbf{x}}\phi(\boldsymbol{\omega}). \end{cases} \tag{3.4}$$

Since $A_{|V|}(k)\in\mathcal{B}_2(L^2(\mathbb{R}^3), L^2(S^2))$ we have that

$$S(k)-1=\frac{-k}{2\pi i}A_{|V|}(k)(1+uG_kv)^{-1}A_V(k)^*\in\mathcal{B}_1(L^2(S^2)), \qquad k^2\notin\mathscr{E}. \tag{3.5}$$

For $k_0^2\notin\mathscr{E}$ and $|k-k_0|$ small enough such that also $k^2\notin\mathscr{E}$, we consider, using equations (2.4), (2.7) and (2.8),

$$\begin{aligned}[S(k)-S(k_0)]/(k-k_0)=-\frac{1}{2\pi i}\Bigg\{&A_{|V|}(k)(1+uG_kv)^{-1}A_V(k)^* \\ &+\left[\frac{k_0}{k-k_0}(A_{|V|}(k)-A_{|V|}(k_0))(1+|\mathbf{x}|)^{-1/2}\right] \\ &\cdot[(1+|\mathbf{x}|)^{1/2}(1+uG_kv)^{-1}A_V(k)^*] \\ &+k_0A_{|V|}(k_0)\frac{1}{k-k_0}[(1+uG_kv)^{-1}-(1+uG_{k_0}v)^{-1}]A_V(k)^* \\ &+[k_0A_{|V|}(k_0)(1+uG_{k_0}v)^{-1}(1+|\mathbf{x}|)^{1/2}] \\ &\cdot\left[\frac{1}{k-k_0}(1+|\mathbf{x}|)^{-1/2}(A_V(k)^*-A_V(k_0)^*)\right]\Bigg\}\end{aligned} \tag{3.6}$$

Looking e.g. at the kernel of the operator $(1+|\mathbf{x}|)^{1/2}(1+uG_kv)^{-1}A_V(k)^*$, we infer from Lemma 1 that this operator is in $\mathcal{B}_2(L^2(S^2), L^2(\mathbb{R}^3))$ and continuous with respect to k in Hilbert–Schmidt norm. Similarly $[k_0/(k-k_0)][A_{|V|}(k)-A_{|V|}(k_0)]$ $(1+|\mathbf{x}|)^{-1/2}$ converges in Hilbert–Schmidt norm to a $\mathcal{B}_2(L^2(\mathbb{R}^3), L^2(S^2))$-valued operator with kernel $-ik_0(\boldsymbol{\omega}\cdot\mathbf{x})(1+|\mathbf{x}|)^{-1/2}u(\mathbf{x})\exp(-ik_0\boldsymbol{\omega}\cdot\mathbf{x})$. Thus recalling also (3.5) we have that $S'(k_0)\in\mathcal{B}_1(L^2(S^2))$ with kernel $(-k_0(2\pi i)^{-1}f(k_0,\boldsymbol{\omega},\boldsymbol{\omega}'))'$. ■

In analogy with eq. (2.9) we now introduce the averaged angular time delay $\bar{\tau}(k)$ by the following definition

$$\bar{\tau}(k)=\int_{S^2} d\omega\tau_a(k,\boldsymbol{\omega}), \qquad k>0, \qquad k^2\notin\mathscr{E}, \tag{3.7}$$

where the angular time delay τ_a is given by [7, 8]

$$\begin{aligned}\tau_a(k,\boldsymbol{\omega})=&\frac{1}{4\pi k}\frac{\partial}{\partial k}(\operatorname{Re} kf(k,\boldsymbol{\omega},\boldsymbol{\omega})) \\ &+\frac{k}{8\pi^2}\int_{S^2} d\omega'\,|f(k,\boldsymbol{\omega},\boldsymbol{\omega}')|^2\frac{\partial}{\partial k}(\arg f(k,\boldsymbol{\omega},\boldsymbol{\omega}')), \qquad k>0, \qquad k^2\notin\mathscr{E}.\end{aligned} \tag{3.8}$$

We then have

Theorem 3. *Let $(1+|\mathbf{x}|)V\in L^1(\mathbb{R}^3)\cap R$. Then, for $k>0$ and $k^2\notin\mathscr{E}$, the averaged angular time delay $\bar{\tau}(k)$ is finite and continuous in k. Furthermore*

$$\bar{\tau}(k)=\operatorname{Tr}(\tau(k)), \qquad k>0, \qquad k^2\notin\mathscr{E}, \tag{3.9}$$

where $\tau(k)$ is the on-shell time delay operator defined by

$$\tau(k) = -\frac{i}{2k} S^*(k)S'(k), \qquad k>0, \qquad k^2 \notin \mathscr{E}. \tag{3.10}$$

Proof. the continuity of $\bar{\tau}(k)$ and the fact that $\tau(k) \in \mathscr{B}_1(L^2(S^2))$ follow from Lemma 1. Equation (3.9) is directly obtained from equations (2.7), (3.7)–(3.8) and unitarity of S which allows (3.10) to be written in the form

$$\tau(k) = \frac{1}{2}\left[-\frac{i}{2k} S^*(k)S'(k) + \frac{i}{2k} S^{*\prime}(k)S(k)\right], \qquad k>0, \qquad k^2 \notin \mathscr{E}. \quad \blacksquare \tag{3.11}$$

Remark 1. a) If V is spherically symmetric, then
$\bar{\tau}(k) = \sum_l (2l+1) \frac{1}{k} \frac{\partial}{\partial k} \delta_l(k),$

where $\delta_l(k)$ is the partial wave phase shift.

b) For a connection between $\bar{\tau}(k)$ and two-body Levinson's theorem in a generalised form we refer to [14–16] and [6].

c) Definition (3.7) and Theorem 3 easily extend to relative time delay (as discussed e.g. in [3]).

Remark 2. Under appropriate additional assumptions on V, the singular continuous spectrum of H is empty (cf. [13] and references therein). In that case $\mathscr{E}$ consists of the positive point spectrum of H. It has been shown in [15] that under suitable conditions on V, the positive eigenvalues of H decouple from the scattering phenomena in the sense that the scattering amplitude remains continuous at these points. However, the threshold point $k=0$ needs a separate discussion. If $0 \in \mathscr{E}$, one has to distinguish whether it is a bound state of H, or a resonance, or both. (cf. e.g. Ref. [17]). Only if $0 \notin \mathscr{E}$ or if 0 is a bound state of H, the averaged total cross-section $\bar{\sigma}(0_+)$ remains finite. On the contrary, the limit of the averaged time delay, $\lim_{k\to 0_+} \bar{\tau}(k)$, never exists, irrespective whether $0 \in \mathscr{E}$ or not.

Finally, we state a continuity result for the averaged angular time delay and the averaged total cross-section with respect to the interactions. Assume $V, V_n \in L^1(\mathbb{R}^3) \cap R$ to be real valued, $n=1,2,\ldots$ and denote by $\mathscr{E}_n$ the exceptional sets corresponding to $H_n = H_0 + V_n$ (cf. equation (2.6)). Furthermore, let $\bar{\sigma}_n(k)$ and $\bar{\tau}_n(k)$ be the averaged total cross-section respectively the averaged angular time delay for the interaction V_n. Then we have

Theorem 4. a) *Suppose* $V, V_n \in L^1(\mathbb{R}^3) \cap R$, $n=1,2,\ldots$ *and*
$\lim_{n\to\infty} \|V_n - V\|_1 = 0, \qquad \lim_{n\to\infty} \|V_n - V\|_R = 0.$ *Then*

$$\lim_{n\to\infty} \bar{\sigma}_n(k) = \bar{\sigma}(k), \qquad k^2 \notin \mathscr{E}. \tag{3.12}$$

b) *Assume* $(1+|\mathbf{x}|)V$, $(1+|\mathbf{x}|)V_n \in L^1(\mathbb{R}^3) \cap R$, $n=1,2,\ldots$ *and*
$\lim_{n\to\infty} \|(1+|\mathbf{x}|)(V_n - V)\|_1 = 0, \qquad \lim_{n\to\infty} \|(1+|\mathbf{x}|)(V_n - V)\|_R = 0.$ *Then*

$$\lim_{n\to\infty} \bar{\tau}_n(k) = \bar{\tau}(k), \qquad k^2 \notin \mathscr{E}. \tag{3.13}$$

Proof. Continuity of the scattering amplitude $f_n(k, \boldsymbol{\omega}, \boldsymbol{\omega}')$ and the scattering matrix $S_n(k)$ associated with the pair of Hamiltonians (H_n, H_0) under the hypothesis a) has been proved in Ref. [18]. By exactly the same methods, assumption b) implies continuity of $f'_n(k, \boldsymbol{\omega}, \boldsymbol{\omega}')$ and $S'_n(k)$, completing the proof. (We remark that by the joint continuity of uG_kv in k and V, $k^2 \in \mathscr{E}$ implies $k^2 \notin \mathscr{E}_n$ for n large enough). ∎

Of course, the concept of time delay is not restricted to the simple case of two-body potential scattering. In the literature, one finds discussion of time delay for multiparticle systems ([7], [19] and [6]). Also nonlocal [20], dissipative [6, 21] and Couloumb interactions [3] were investigated. Finally, we also mention a recent treatment of the Lax–Philips scattering theory [5]. It is clear that our approach presented above could be extended to all these situations.

Acknowledgments

The authors would like to thank the Institute for Theoretical Physics of the University of Graz, respectively the University of Leuven for their hospitality and financial support.

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