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On the definition of time delay in scattering theory

M. Sassoli de Bianchi and Ph. A. Martin
Institut de Physique Théorique, Ecole Polytechnique Fédérale de Lausanne
CH-1015 Lausanne, Switzerland

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Abstract. We show that the time delay of a scattering process, defined as the difference of interacting and free sojourn times for increasing spatial regions, can only exist for sequences of dilated balls. The transformation properties of the Eisenbud-Wigner formula under translations are discussed.

1. Introduction

The theory of time delay has been the subject of numerous studies in the past. A commonly adopted definition of time delay involves the concept of the average sojourn time of the particle in a finite spatial region Σ. Consider a potential scattering system with total hamiltonian $H = H_0 + v$ and free hamiltonian $H_0 = -\Delta/2m$, where Δ is the laplacian on $L^2(\mathbb{R}^n), n \leq 3$ (m is the mass of the particle and we have set $\hbar = 1$) and denote $V_t = \exp(-iHt)$, $U_t = \exp(-iH_0t)$ the corresponding evolution groups. We assume that the potential v is such that the wave operators $\Omega_\pm \equiv$ s–$\lim_{t\to\infty} V_{\pm t}^\dagger U_{\pm t}$ exist and are complete and the scattering operator $S \equiv \Omega_+^\dagger \Omega_-$ is unitary [1].

To each finite spatial region $\Sigma \subset \mathbb{R}^n$, one can associate the corresponding total and free sojourn times in Σ with incoming state φ

$$T_\Sigma(\varphi) \equiv \int_{-\infty}^{\infty} dt \,\| P_\Sigma V_t \Omega_- \varphi \|^2, \quad T_\Sigma^0(\varphi) \equiv \int_{-\infty}^{\infty} dt \,\| P_\Sigma U_t \varphi \|^2 \tag{1.1}$$

where P_Σ denotes the projection operator onto the subspace of states localized in the region Σ. Then, the time delay of a scattering event with incoming state φ is defined as the difference of the total and free sojourn times as the region Σ extends over the whole space (see the review article [2])

$$\tau(\varphi) \equiv \lim_{\Sigma\to\mathbb{R}^n} \tau_\Sigma(\varphi) \tag{1.2}$$

with

$$\tau_\Sigma(\varphi) \equiv T_\Sigma(\varphi) - T_\Sigma^0(\varphi) \tag{1.3}$$

A large litterature is devoted to the proof of the existence of the limit (1.2) and its identity to the Eisenbud-Wigner time delay formula [1] (see in particular [3]-[11])

$$\tau_{\text{E-W}}(\varphi) \equiv -i\left(\varphi, S^\dagger \frac{dS}{dH_0}\varphi\right) \tag{1.4}$$

Although they bring into play a variety of mathematical methods, all the above mentioned references use only sequences of balls centered at the origin in their proofs. Therefore the question arises: does the limit (1.2) exist with other approximating sequences of regions Σ, for a sufficiently large class of potentials and of incoming states?

The authors generally do not motivate the choice of balls centered at the origin. Sometimes they hint more or less explicitely that it is a matter of convenience and that the time delay should not depend on a particular choice of a sequence $\Sigma \to \mathbb{R}^n$ in the limit (1.2) [2]. The purpose of this note is to clarify this question by establishing the two following points. Let Σ_1 be a fixed spatial region containing the origin. We assume that Σ_1 is a convex subset of $\mathbb{R}^n$ with "smooth surface" i.e., the boundary $\partial\Sigma_1$ of Σ_1 is a $(n-1)$−dimensional differentiable manifold. Considering domains $\Sigma_r(0)$ that are dilation of Σ_1 from the origin and their translates $\Sigma_r(\mathbf{c}), \mathbf{c} \in \mathbb{R}^n$,

$$\Sigma_r(\mathbf{c}) = \left\{\mathbf{x} \in \mathbb{R}^n | \frac{\mathbf{x}-\mathbf{c}}{r} \in \Sigma_1, r > 0\right\} \tag{1.5}$$

we show that

(i) $\lim_{r\to\infty} \tau_{\Sigma_r(\mathbf{c})}(\varphi)$ can exist in general only if Σ_1 is a ball centered at the origin;

(ii) in the latter case, the limit agrees with the E-W formula (1.4) only if $\mathbf{c} = 0$.

Since the results (i) and (ii) are of geometrical origin, we first establish them in the context of the classical scattering theory in section 2. We treat the quantum mechanical case in section 3 and present some comments in section 4.

2. Classical scattering

We follow essentially the treatement presented in [11]. Let $\{\mathbf{x}(t), \mathbf{p}(t)\}$ be a classical scattering trajectory with asymptotic momenta $\mathbf{p}_\pm \equiv \lim_{t\to\pm\infty} \mathbf{p}(t)$ ($|\mathbf{p}_+| = |\mathbf{p}_-| \equiv |\mathbf{p}|$ because of energy conservation) and set $\tilde{\mathbf{x}}(t) \equiv \mathbf{x}(t) - \mathbf{p}(t)t/m$. Denoting by $-t_-$ and t_+ ($t_\pm > 0$) the times at which the particle enters and leaves the region $\Sigma_r(\mathbf{c})$ and assuming

[1] In this paper the general formula (1.4) is referred to as the Eisenbud-Wigner (E-W) formula. Sometimes, E-W formula designates the energy derivative of the phase shifts in the special case of spherical symmetry.

[2] For instance, in [3] it is noted that the result of proposition 2 of this reference is independent of the choice of Σ, but in fact its application to potential scattering requires the use of balls centered at the origin. See also the final discussion in [10].

for simplicity that the potential v has compact support (enclosed in $\Sigma_r(\mathbf{c})$ for r large enough), one has $\mathbf{p}(\pm t_\pm) = \mathbf{p}_\pm$ and

$$t_\pm = \mp \frac{m}{|\mathbf{p}|^2} \mathbf{p}_\pm \cdot (\tilde{\mathbf{x}}_\pm - \mathbf{x}_\pm) \tag{2.1}$$

with $\tilde{\mathbf{x}}_\pm \equiv \tilde{\mathbf{x}}(\pm t_\pm)$ and $\mathbf{x}_\pm \equiv \mathbf{x}(\pm t_\pm)$.

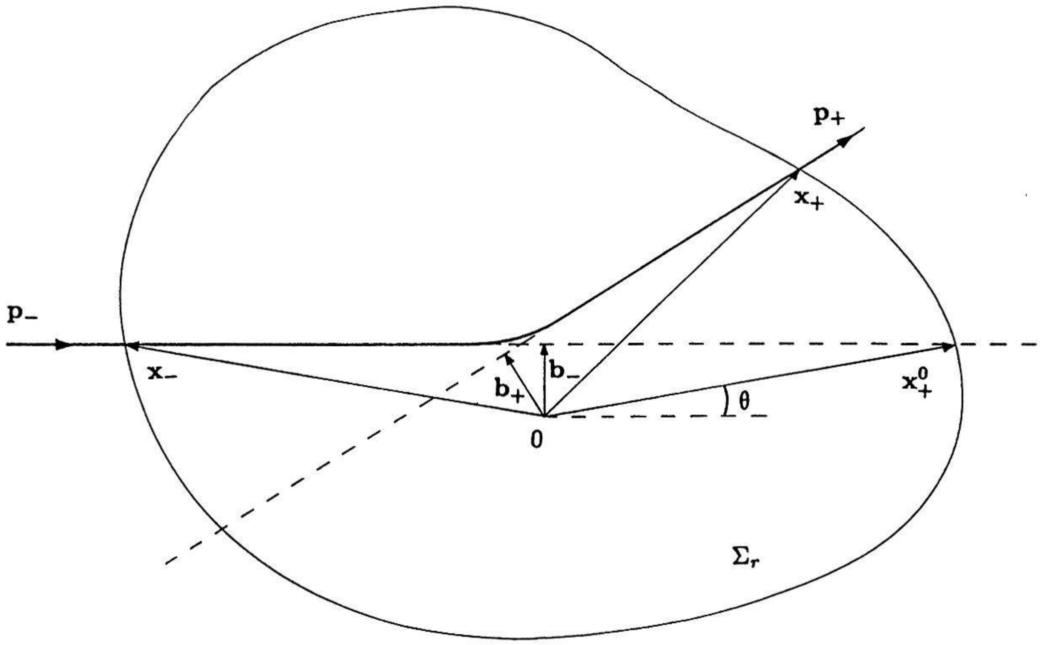

Fig. 1. *Dilated region $\Sigma_r \equiv \Sigma_r(0)$ from the origin.*

Then, the sojourn time of the particle in $\Sigma_r(\mathbf{c})$ is given by

$$T_{\Sigma_r(\mathbf{c})} = t_- + t_+ = \frac{m}{|\mathbf{p}|^2}(\mathbf{p}_- \cdot \tilde{\mathbf{x}}_- - \mathbf{p}_+ \cdot \tilde{\mathbf{x}}_+) - \frac{m}{|\mathbf{p}|^2}(\mathbf{p}_- \cdot \mathbf{x}_- - \mathbf{p}_+ \cdot \mathbf{x}_+) \tag{2.2}$$

The free sojourn time $T^0_{\Sigma_r(\mathbf{c})}$ corresponding to a free trajectory

$$\{\mathbf{x}^0(t) = \mathbf{x}_- + \mathbf{p}_-(t + t_-)/m, \mathbf{p}^0(t) = \mathbf{p}_-\} \tag{2.3}$$

with the same incoming momentum $\mathbf{p}_-$ and entering time $-t_-$ is

$$T^0_{\Sigma_r(\mathbf{c})} = -\frac{m}{|\mathbf{p}|^2}(\mathbf{p}_- \cdot \mathbf{x}_- - \mathbf{p}_- \cdot \mathbf{x}^0_+) \tag{2.4}$$

From (2.2),(2.4), we define the time delay $\tau_{\Sigma_r(\mathbf{c})}$ for the finite region $\Sigma_r(\mathbf{c})$ as in (1.3) by

$$\tau_{\Sigma_r(\mathbf{c})} = T_{\Sigma_r(\mathbf{c})} - T^0_{\Sigma_r(\mathbf{c})} = \tau^1_{\Sigma_r(\mathbf{c})} + \tau^2_{\Sigma_r(\mathbf{c})} \tag{2.5}$$

where

$$\tau^1_{\Sigma_r(\mathbf{c})} \equiv \frac{m}{|\mathbf{p}|^2}(\mathbf{p}_- \cdot \tilde{\mathbf{x}}_- - \mathbf{p}_+ \cdot \tilde{\mathbf{x}}_+) \tag{2.6}$$

$$\tau^2_{\Sigma_r(\mathbf{c})} \equiv \frac{m}{|\mathbf{p}|^2}(\mathbf{p}_+\cdot \mathbf{x}_+ - \mathbf{p}_-\cdot \mathbf{x}^0_+) \tag{2.7}$$

As $r \to \infty$ (i.e., $t_\pm \to \infty$), the first contribution (2.6) will be given by

$$\lim_{r\to\infty} \tau^1_{\Sigma_r(\mathbf{c})} = \frac{m}{|\mathbf{p}|^2}\left(\lim_{t\to-\infty} \mathbf{p}(t)\cdot \tilde{\mathbf{x}}(t) - \lim_{t\to\infty} \mathbf{p}(t)\cdot \tilde{\mathbf{x}}(t)\right) \equiv \tau^{\text{cl}} \tag{2.8}$$

This limit (which is trivial for a potential with compact support) has been shown to exist for a large class of potentials and to be equal to the usual classical time delay (τ^{cl} is the classical analogue of the E-W time delay (1.4)) [11].

It remains to examine the second contribution (2.7). Consider first domains $\Sigma_r \equiv \Sigma_r(0)$ that are dilated from the origin and let $d(\hat{\mathbf{u}})$ be the distance from the origin to the boundary $\partial\Sigma_1$ of the initial region Σ_1 in the direction $\hat{\mathbf{u}}$ ($|\hat{\mathbf{u}}| = 1$). As $r \to \infty$ we have

$$\mathbf{x}^0_+ = (rd(\hat{\mathbf{p}}_-) + B^0)\hat{\mathbf{p}}_- + \mathbf{b}_- + O(r^{-1}) \tag{2.9}$$

$$\mathbf{x}_+ = (rd(\hat{\mathbf{p}}_+) + B)\hat{\mathbf{p}}_+ + \mathbf{b}_+ + O(r^{-1}) \tag{2.10}$$

where B^0, B are finite quantities which vanish if Σ_1 is a ball centered at the origin, $\hat{\mathbf{p}}_\pm \equiv \mathbf{p}_\pm/|\mathbf{p}|$, and $\mathbf{b}_\mp$ are the incoming and outcoming impact parameters (see fig.1). To show (2.9), consider, as r varies, that $d(\hat{\mathbf{x}}^0_+) = d(\cos\theta\hat{\mathbf{p}}_- + \sin\theta\hat{\mathbf{b}}_-) \equiv f(\theta)$ is a function of the angle θ between $\hat{\mathbf{x}}^0_+ \equiv \mathbf{x}^0_+/|\mathbf{x}^0_+|$ and $\hat{\mathbf{p}}_-$, given by

$$\sin\theta = \frac{|\mathbf{b}_-|}{|\mathbf{x}^0_+|} = \frac{|\mathbf{b}_-|}{rd(\hat{\mathbf{x}}^0_+)} \tag{2.11}$$

Thus, one has

$$d(\hat{\mathbf{x}}^0_+) = d(\hat{\mathbf{p}}_-) + O(r^{-1}), \quad \theta = \frac{|\mathbf{b}_-|}{rd(\hat{\mathbf{p}}_-)} + O(r^{-2}) \tag{2.12}$$

and for r large, one obtains

$$\begin{aligned}\mathbf{x}^0_+ &= |\mathbf{x}^0_+|\hat{\mathbf{x}}^0_+ = rf(\theta)(\cos\theta\hat{\mathbf{p}}_- + \sin\theta\hat{\mathbf{b}}_-)\\ &= r\left(d(\hat{\mathbf{p}}_-) + \frac{|\mathbf{b}_-|}{rd(\hat{\mathbf{p}}_-)}f'(0)\right)\left(\hat{\mathbf{p}}_- + \frac{\mathbf{b}_-}{rd(\hat{\mathbf{p}}_-)}\right) + O(r^{-1})\end{aligned} \tag{2.13}$$

This gives (2.9) with $B^0 = |\mathbf{b}_-|f'(0)/d(\hat{\mathbf{p}}_-)$. Obviously, for a ball centered at the origin $f(\theta) = 1$ and $B^0 = 0$. One finds (2.10) in the same way. Thus,

$$\hat{\mathbf{p}}_-\cdot \mathbf{x}^0_+ = rd(\hat{\mathbf{p}}_-) + B^0 + O(r^{-1}) \tag{2.14}$$

$$\hat{\mathbf{p}}_+\cdot \mathbf{x}_+ = rd(\hat{\mathbf{p}}_+) + B + O(r^{-1}) \tag{2.15}$$

For the translated domains $\Sigma_r(\mathbf{c})$, $\mathbf{c} \neq 0$, the same formulae (2.14),(2.15) hold for $\hat{\mathbf{p}}_-\cdot (\mathbf{x}^0_+ - \mathbf{c})$ and $\hat{\mathbf{p}}_+\cdot (\mathbf{x}_+ - \mathbf{c})$. Hence, one finds in general

$$\tau^2_{\Sigma_r(\mathbf{c})} = \frac{m}{|\mathbf{p}|}\left(r\,(d(\hat{\mathbf{p}}_+) - d(\hat{\mathbf{p}}_-)) + \mathbf{c}\cdot (\hat{\mathbf{p}}_+ - \hat{\mathbf{p}}_-) + B - B^0\right) + O(r^{-1}) \tag{2.16}$$

If the limit of $\tau^2_{\Sigma_r(\mathbf{c})}$, as $r \to \infty$, has to exist for all possible scattering events, then $d(\hat{\mathbf{p}}_+) = d(\hat{\mathbf{p}}_-)$ for all $\hat{\mathbf{p}}_+$, implying that Σ_1 must be a ball centered at the origin. This establishes (i). In this case one has $B = B^0 = 0$ and (2.5),(2.8),(2.16) give

$$\lim_{r\to\infty} \tau_{\Sigma_r(\mathbf{c})} = \tau^{\mathrm{cl}} + \mathbf{c}\cdot \frac{m}{|\mathbf{p}|}(\hat{\mathbf{p}}_+ - \hat{\mathbf{p}}_-) \tag{2.17}$$

Therefore, it follows from (2.17) that $\lim_{r\to\infty} \tau_{\Sigma_r(\mathbf{c})} = \tau^{\mathrm{cl}}$ only if $\mathbf{c} = 0$, showing (ii).

3. Quantum mechanical scattering

Here we follow the method of [6], assuming the conditions of the proposition 2 of this reference. Let $\tau_{\Sigma_r}(\varphi)$ be the time delay for a dilated region Σ_r with characteristic function

$$\chi_{\Sigma_r}(\mathbf{x}) = \chi_{\Sigma_1}(\mathbf{x}/r) = \begin{cases} 1 & \text{if } \mathbf{x}/r \in \Sigma_1 \\ 0 & \text{otherwise} \end{cases} \tag{3.1}$$

Then the following facts are true

(a)
$$\lim_{r\to\infty} (\tau_{\Sigma_r}(\varphi) - \sigma_{\Sigma_r}(\varphi)) = 0 \tag{3.2}$$

where

$$\sigma_{\Sigma_r}(\varphi) \equiv \int_0^\infty dt\, \Big((S\varphi, U_t^\dagger \chi_{\Sigma_r}(\mathbf{q}) U_t S\varphi) - (\varphi, U_t^\dagger \chi_{\Sigma_r}(\mathbf{q}) U_t \varphi)\Big) \tag{3.3}$$

(b) The difference

$$K_r(\varphi) \equiv \int_0^\infty dt\, (\varphi, U_t^\dagger \chi_{\Sigma_r}(\mathbf{q}) U_t \varphi) - r\int_0^\infty du\, (\varphi, \frac{m}{|\mathbf{p}|}\chi_{\Sigma_1}(u\hat{\mathbf{p}})\varphi) \tag{3.4}$$

remains bounded as $r \to \infty$ and the same is true for $K_r(S\varphi)$.

The point (a) is a general fact which does not depend on the choice of the region Σ_1 (see the case (B) in the proposition 2 of ref. [6]). The result (b) is obtained by the same arguments as in (iii) p.488-489 of ref. [6][3]. The combination of (a) and (b) shows that $\tau_{\Sigma_r}(\varphi)$ can have a limit only if

$$r\int_0^\infty du\, \Big((S\varphi, \frac{m}{|\mathbf{p}|}\chi_{\Sigma_1}(u\hat{\mathbf{p}})S\varphi) - (\varphi, \frac{m}{|\mathbf{p}|}\chi_{\Sigma_1}(u\hat{\mathbf{p}})\varphi)\Big) \tag{3.5}$$

has a limit as $r \to \infty$. Noting that $\int_0^\infty du\chi_{\Sigma_1}(u\hat{\mathbf{k}}) = d(\hat{\mathbf{k}})$, (3.5) can be written in the alternative forms (using $[S, H_0] = 0$)

$$r\left(\varphi, \frac{m}{|\mathbf{p}|}(S^\dagger d(\hat{\mathbf{p}})S - d(\hat{\mathbf{p}}))\varphi\right) = r\int d^n k\, \frac{m}{|\mathbf{k}|} d(\hat{\mathbf{k}})\left(|(\widetilde{S\varphi})(\mathbf{k})|^2 - |\tilde{\varphi}(\mathbf{k})|^2\right) \tag{3.6}$$

[3] Note that, except for the use of the more general region Σ_r, $K_r(\varphi)$ is identical to the definition (18) of ref. [6] (for finite r and taking (16),(17) of this reference into account). In ref. [6] the mass m is set equal to $1/2$.

This is clearly the quantum analogue of the classical term $r(m/|\mathbf{p}|)(d(\hat{\mathbf{p}}_+)-d(\hat{\mathbf{p}}_-))$ occuring in (2.16). Because of the unitarity of S on the energy shell, it vanishes if Σ_1 is a ball centered at the origin ($d(\hat{\mathbf{k}}) = 1$). If Σ_1 is not spherical, the factor of r in (3.6) will certainly not vanish for some scattering system and some choice of the incoming state φ: thus τ_{Σ_r} diverges as $r \to \infty$. For the case of translated regions $\Sigma_r(\mathbf{c})$, it suffices to replace $\chi_{\Sigma_r}(\mathbf{q})$ by $\chi_{\Sigma_r}(\mathbf{q}-\mathbf{c})$ in (3.4) or equivalently $K_r(\varphi)$ by $K_r^{\mathbf{c}}(\varphi) \equiv K_r(e^{i\mathbf{p}\cdot\mathbf{c}}\varphi)$. Thus $K_r^{\mathbf{c}}(\varphi)$ and $K_r^{\mathbf{c}}(S\varphi)$ are bounded as $r \to \infty$ and the conclusion is the same. This shows (i) in the quantum case.

When Σ_1 is a ball centered at the origin and $\mathbf{c} = 0$, it is shown in [6] that

$$\lim_{r\to\infty} \tau_{\Sigma_r}(\varphi) = (\varphi, S^\dagger[S, A_0]\varphi) = \tau_{\text{E-W}}(\varphi) \tag{3.7}$$

with

$$A_0 \equiv \frac{m}{2}\left(\frac{1}{|\mathbf{p}|^2}\mathbf{p}\cdot\mathbf{q} + \mathbf{q}\cdot\mathbf{p}\frac{1}{|\mathbf{p}|^2})\right)$$

If $\mathbf{c} \neq 0$, A_0 is replaced by its translate $e^{-i\mathbf{c}\cdot\mathbf{p}}A_0e^{i\mathbf{c}\cdot\mathbf{p}} = A_0 - \mathbf{c}\cdot m\mathbf{p}/|\mathbf{p}|^2$ giving in this case

$$\lim_{r\to\infty} \tau_{\Sigma_r(\mathbf{c})}(\varphi) = \tau_{\text{E-W}}(\varphi) + \mathbf{c}\cdot\left(\varphi, \frac{m}{|\mathbf{p}|}(S^\dagger\hat{\mathbf{p}}S - \hat{\mathbf{p}})\varphi\right) \tag{3.8}$$

which is the quantum analogue of (2.17). Hence (ii) follows.

4. Concluding remarks

The present analysis shows that the definition (1.2)-(1.3) of the time delay with incoming state φ makes sense only for balls. Classically this follows from the purely geometrical fact that the difference between the interacting and free trajectory lengths remains finite, in general, only for balls. Thus (2.17) or (3.8) are the most general formulae for the time delay defined as a difference of sojourn times for sequences of increasing spatial regions.

Let us investigate the transformation properties of (3.8) under translations[4]. If the origin of the spatial coordinate system is translated to a point $\mathbf{a}$, one has

$$S \longrightarrow S_{\mathbf{a}} \equiv e^{i\mathbf{p}\cdot\mathbf{a}}Se^{-i\mathbf{p}\cdot\mathbf{a}} \tag{4.1a}$$

$$\varphi \longrightarrow \varphi_{\mathbf{a}} \equiv e^{i\mathbf{p}\cdot\mathbf{a}}\varphi \tag{4.1b}$$

$$\mathbf{c} \longrightarrow \mathbf{c} - \mathbf{a} \tag{4.1c}$$

We observe that the complete formula (3.8) is invariant under the transformation (4.1), whereas the E-W formula (1.4) is not[5]. Indeed, if $\tau_{\text{E-W}}^{\mathbf{a}}(\varphi)$ is the E-W formula for

[4] The same discussion and the same conclusions apply to the classical formula (2.17).

[5] The latter fact has been noted in [11]. In ref. [12], the one-dimensional analogue of (3.8) has been obtained by dilation of intervals centered on an arbitrary point c.

the translated system, one obtains easily (using $d|\mathbf{p}|/dH_0 = m/|\mathbf{p}|$)

$$\begin{aligned}\tau^{\mathbf{a}}_{\text{E-W}}(\varphi) &= -i\left(\varphi_{\mathbf{a}}, S^\dagger_{\mathbf{a}}\frac{dS_{\mathbf{a}}}{dH_0}\varphi_{\mathbf{a}}\right)\\ &= \tau_{\text{E-W}}(\varphi) + \mathbf{a}\cdot\left(\varphi, \frac{m}{|\mathbf{p}|}(S^\dagger\hat{\mathbf{p}}S - \hat{\mathbf{p}})\varphi\right)\end{aligned} \tag{4.2}$$

On the other hand, the formula (3.8) remains clearly invariant under the transformation (4.1), as it should by its very definition.

Therefore, the E-W formula (1.4) (obtained by setting $\mathbf{c} = 0$ in (3.8)) must be interpreted as follows: it refers to the S-operator and the incoming state φ in a frame having its origin located at the dilation center of the balls. Dilations around different points will distinguish among different translated systems according to (4.1a),(4.1b)[6].

We note that the situation is simpler when we consider cross-sections. A translation of the origin of the coordinate system will result in phase factors in the scattering amplitude and thus lead to the same cross-section. In other words, cross-section measurements give intrinsic informations on the scattering potential, independently of the choice of the reference frame. Is it possible to obtain also such informations from the time delay? In the case where the potential is spherically symmetric, the answer is obvious: choose as dilation center the center of the potential itself. This is the choice made in most of the papers without further comment. In this situation the E-W formula (1.4) agrees with the energy derivatives of the conventional phase-shifts; thus time delay and cross section yield in principle the same information. If the potential has no specific symmetry, there is no privileged center and the time delay depends on a conventional choice of the origin of the reference frame.

There exists however in all cases a more global intrinsic quantity, namely the trace $\mathrm{Tr}_E\tau_E$ of the energy shell time delay $\tau_E = -iS^\dagger_E dS_E/dE$. It is proven in [15,2] that this quantity is independent of the choice of the sequence $\Sigma \to \mathbb{R}^n$, i.e. it is the same for sequences of dilated regions of any shape around any center. This result is compatible with the discussion of the present paper. Indeed, under suitable conditions, one establishes in [15] that $S_E - I$ is a trace-class operator, implying that the trace on the energy shell of the term (3.6) is well defined

$$\mathrm{Tr}_E\left(S^\dagger_E d(\hat{\mathbf{p}})S_E - d(\hat{\mathbf{p}})\right) = \mathrm{Tr}_E\left((S_E - I)d(\hat{\mathbf{p}})S^\dagger_E\right) + \mathrm{Tr}_E\left(d(\hat{\mathbf{p}})(S^\dagger_E - I)\right) = 0 \tag{4.3}$$

It vanishes because of the cyclicity of the trace and the unitarity of S_E. The same is true for the second term in the right hand side of (3.8) and (4.2). Hence, for any sufficiently short ranged potential, spherically symmetric or not, $\mathrm{Tr}_E\tau_E$ is also independent of a specification of the reference frame. A similar result holds in the classical case [16].

[6] The Larmor clock is a concievable way of measuring directly the sojourn times by means of the precession of a spin in a weak magnetic field [13,14].

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