On the Hilbert-space approach to classical time delay

1981 J. Phys. A: Math. Gen. 14 1663

(http://iopscience.iop.org/0305-4470/14/7/022)

J. Phys. A: Math. Gen. 14 (1981) 1663–1674. Printed in Great Britain

On the Hilbert-space approach to classical time delay

D Bollé† and J D'Hondt

Instituut voor Theoretische Fysica, Universiteit Leuven, B-3030 Leuven, Belgium

Received 19 November 1980, in final form 21 January 1981

Abstract. Within the context of the Hilbert-space approach to classical mechanics, a definition of time delay for classical scattering systems is given. Its relation with the S-matrix is discussed by close analogy with the quantum case.

1. Introduction

Time delay has been discussed quite extensively in quantum mechanics for two- and N-particle scattering via short-range interactions (Bollé and Osborn 1979 and references cited therein). From these studies it is clear that this concept of time delay is of general importance. First of all, from the point of view of general scattering theory, this time-delay approach provides us with a method of extending the concept of the phase shift. Secondly, it plays a practical role in the study of the collision process in statistical mechanics (Bollé 1979a, b, Osborn 1977 and references cited therein).

For these reasons, an intriguing question is whether a similar set of results would be valid in classical N-particle scattering. Furthermore, we know that the long-range effects of Coulomb-type interactions which up to now have not been included in the quantum discussions are mostly classical in nature. Therefore, a classical time-delay picture may provide us with some useful ideas on how to include these long-range interactions in the quantum treatment.

A study of classical time delay can be carried out directly in phase space or by taking L^2 of phase space and using the Hilbert-space techniques developed for quantum scattering. This work reports a first set of results in the Hilbert-space approach, namely the definition of time delay and its connection with the S-matrix for classical two-particle scattering via short-range interactions. In close analogy with the corresponding quantum result, we find that the classical reduced time-delay operator is equal to the logarithmic derivative of the classical reduced S-operator. The methods we use to obtain this result can be extended to more complicated scattering systems. So, one can argue that for classical scattering also, time delay can be considered as a phase-shift-like function that is a characteristic of the scattering process.

This paper is organised into five sections. In § 2 we present the elements of classical Hilbert-space scattering (Hunziker 1968a, 1974) needed in our analysis. Section 3 defines classical time delay in this approach and writes it in a form in which the exact states of the interacting system are replaced by their asymptotic forms. Section 4

† Onderzoeksleider NFWO, Belgium

0305-4470/81/071663+12$01.50

studies the connection of this form with the classical S-matrix. In § 5 we briefly discuss our results. Finally, the Appendix includes the Fourier transform properties of the projection operator required by our derivation.

2. The Hilbert-space approach to classical scattering

In this section, we present the known features of classical Hilbert-space scattering (Hunziker 1968a, 1974) which we employ in this analysis.

We consider a classical two-particle system characterised by the Hamiltonian

$$H(\boldsymbol{r},\boldsymbol{p}) = p^2/2\mu + V(\boldsymbol{r}), \tag{2.1}$$

where $\boldsymbol{r}$ is the interparticle separation in the centre-of-mass system, $\boldsymbol{p}$ the relative momentum, $V(\boldsymbol{r})$ the potential and μ the reduced mass. The set $\Gamma = \{z \equiv (\boldsymbol{r},\boldsymbol{p}) : H(z) < \infty\}$ is the phase space of the system.

In the following we assume that the potential satisfies

(a) $V(\boldsymbol{r})$ is bounded from below by $V_- > -\infty$. For any $M < \infty$, $V(\boldsymbol{r})$ is continuous with bounded derivatives up to order two on $\{\boldsymbol{r}: V(\boldsymbol{r}) < M\}$

(b) $|\nabla_r V(\boldsymbol{r})| < \text{const.}\, r^{-2-\delta}, \quad \delta > 0.$

In this case, Newton's equation of motion

$$\dot{z} = (\dot{\boldsymbol{r}}, \dot{\boldsymbol{p}}) = (\boldsymbol{p}/\mu, -\nabla_r V(\boldsymbol{r})) \tag{2.2}$$

has unique solutions for any initial value $z_0 \in \Gamma$ and the maps

$$S_t : z_0 \to z_t, \qquad -\infty < t < +\infty \tag{2.3}$$

form a one-parameter group of canonical transformations of Γ onto Γ.

In the Hilbert-space approach, the states Ψ of the scattering system are taken to be elements of the Hilbert space $L^2(\Gamma)$. The dynamics is described by a strongly continuous unitary one-parameter group on $L^2(\Gamma)$ induced by the map S_t defined in equation (2.3), namely

$$U_t = \mathrm{e}^{-Lt} : \Psi(z) \to \Psi(S_t z). \tag{2.4}$$

Here, L is the Liouville operator. Explicitly we have

$$\begin{aligned} &L = L_0 + L_V \\ &L_0 = -(\boldsymbol{p}/\mu)\cdot\nabla_r, \qquad L_V = \nabla_r V(\boldsymbol{r})\cdot\nabla_p. \end{aligned} \tag{2.5}$$

L then satisfies the equation of motion

$$\mathrm{d}\Psi/\mathrm{d}t = \{H, \Psi\} = -L\Psi, \tag{2.6}$$

where $\{\,,\}$ is the Poisson bracket.

One can now describe bound states which must be linked to the boundedness of orbits in configuration space. One can also show the existence of scattering states and thus the existence of classical Möller operators under the conditions (a) and (b) on the potential. By close analogy with quantum mechanical scattering, these Möller operators

$$\Omega^{\pm} = s - \lim_{t\to\mp\infty} \mathrm{e}^{Lt}\, \mathrm{e}^{-L_0 t} \tag{2.7}$$

satisfy the following basic properties

$$\Omega^{\pm *}\Omega^{\pm} = I$$
$$\Omega^{\pm}\Omega^{\pm *} + B = I$$
$$e^{tL}\Omega^{\pm} = \Omega^{\pm} e^{tL_0}, \tag{2.8}$$

where $\Omega^{\pm *}$ is the adjoint of $\Omega^{\pm}$, I is the identity on $L^2(\Gamma)$, and B the projection operator onto the subspace of bound states. The first property expresses the fact that the $\Omega^{\pm}$ are partial isometries. The second property means that Ω^{+} and Ω^{-} form a complete set of scattering states. The third property is called intertwining.

Finally, one can define the classical scattering operator S as

$$S = \Omega^{-*}\Omega^{+}. \tag{2.9}$$

This operator is unitary, namely

$$SS^* = S^*S = I, \tag{2.10}$$

and satisfies the intertwining relation

$$SL_0 = L_0S. \tag{2.11}$$

The last property will play an important role in our further analysis.

For more details about this approach we refer to the literature (Hunziker 1968a, 1974).

3. Definition of classical two-particle time delay

In this section we first give a definition of classical two-particle time delay. We then write it in a form that contains only asymptotic states of the system. We will use arguments similar to the ones we employed in the corresponding quantum mechanical problem (Bollé and Osborn 1979).

Let $f_{\rm in}(z) \in L^2(\Gamma)$ be a function specifying the incoming state of the system at $t = 0$. Then there exists a state $\phi = \Omega^{+} f_{\rm in}$ such that the exact interacting state Ψ of the system satisfies

$$\Psi(t) = e^{-Lt}\phi \to e^{-L_0t}f_{\rm in} \equiv \Psi_{\rm in}(t) \qquad \text{for } t \to -\infty, \tag{3.1}$$

in the sense of the norm in $L^2(\Gamma)$. There also exists a function $f_{\rm out}(z) \in L^2(\Gamma)$ specifying the outgoing state of the system such that $\phi = \Omega^{-} f_{\rm out}$ and

$$\Psi(t) \to e^{-L_0t}f_{\rm out} \equiv \Psi_{\rm out}(t) \qquad \text{for } t \to +\infty. \tag{3.2}$$

Furthermore,

$$f_{\rm out} = S f_{\rm in}. \tag{3.3}$$

We now define time delay in terms of the exact state $\Psi(t)$ and the asymptotic states $\Psi_{\rm in}(t)$ and $\Psi_{\rm out}(t)$. We first look at a finite region Σ around the scattering centre in configuration space and define the following projection operator $P(\Sigma)$ in $L^2(\Gamma)$

$$P(\Sigma)f(z) = f(z) \qquad \text{for } \boldsymbol{r} \in \Sigma$$
$$= 0 \qquad \boldsymbol{r} \notin \Sigma. \tag{3.4}$$

Time delay for the region Σ is then defined as the time the interacting system, described by Ψ, is spending in the region Σ minus the time the asymptotic system, described by Ψ_{in} or Ψ_{out}, is spending in that region. This can be expressed in the following formula

$$\begin{aligned} T^{in}(f_{in}, \Sigma) &= \int_{-\infty}^{+\infty} dt[(\Psi(t), P(\Sigma)\Psi(t)) - (\Psi_{in}(t), P(\Sigma)\Psi_{in}(t))] \\ T^{out}(f_{in}, \Sigma) &= \int_{-\infty}^{+\infty} dt[(\Psi(t), P(\Sigma)\Psi(t)) - (\Psi_{out}(t), P(\Sigma)\Psi_{out}(t))]. \end{aligned} \tag{3.5}$$

The time delay we shall consider in detail is one that is fully symmetric with respect to the asymptotic states, namely

$$T(f_{in}, \Sigma) = \tfrac{1}{2}T^{in}(f_{in}, \Sigma) + \tfrac{1}{2}T^{out}(f_{in}, \Sigma). \tag{3.6}$$

Of course, we are interested in a quantity that is independent of the region Σ. Therefore, we will study the limit $\Sigma \to \mathbb{R}^3$ of these different time-delay forms. We will see that all these definitions (3.5)–(3.6) have limits and are equivalent. But, by analogy with the quantum case, we expect that this is no longer true in the many-particle classical time-delay problem.

In order to consider this limit, we first want to obtain an equivalent form for $T(f_{in}, \Sigma)$ in which the exact state $\Psi(t)$ is replaced by the asymptotic states $\Psi_{in}(t)$ and $\Psi_{out}(t)$. The following result allows this simplification:

Let f_{in}, $\Psi(t)$, $\Psi_{in}(t)$ and $\Psi_{out}(t)$ be defined as above. Set

$$\begin{aligned} \Delta^{+}(f_{in}, \Sigma) &= \int_{0}^{\infty} dt[(\Psi(t), P(\Sigma)\Psi(t)) - (\Psi_{out}(t), P(\Sigma)\Psi_{out}(t))] \\ \Delta^{-}(f_{in}, \Sigma) &= \int_{-\infty}^{0} dt[(\Psi(t), P(\Sigma)\Psi(t)) - (\Psi_{in}(t), P(\Sigma)\Psi_{in}(t))]; \end{aligned} \tag{3.7}$$

then we have that

$$\lim_{\Sigma \to \mathbb{R}^3} \Delta^{\pm}(f_{in}, \Sigma) = 0. \tag{3.8}$$

The proof of equation (3.8) rests on the fact that the t-integrands in equations (3.7) can be shown to have a Σ-independent absolutely integrable bound. Then the Lebesgue dominated convergence theorem allows one to interchange the Σ-limit and the t-integration. In that limit $\Sigma \to \mathbb{R}^3$, the integrand can be shown to be zero. Since the explicit details of this proof are completely analogous to the corresponding quantum mechanical result (Bollé and Osborn 1979) we don't repeat them here.

Using this result (3.8), the symmetric definition of time delay (3.6) can be written as

$$T(f_{in}, \Sigma) = T^{+}(f_{in}, \Sigma) + T^{-}(f_{in}, \Sigma) + \Delta^{+}(f_{in}, \Sigma) + \Delta^{-}(f_{in}, \Sigma), \tag{3.9}$$

where

$$T^{\pm}(f_{in}, \Sigma) = \tfrac{1}{2} \int_{0}^{\pm\infty} dt[(\Psi_{out}(t), P(\Sigma)\Psi_{out}(t)) - (\Psi_{in}(t), P(\Sigma)\Psi_{in}(t))]. \tag{3.10}$$

In the form (3.9) the exact states of the system only appear in the $\Delta^{\pm}$ and these terms vanish in the limit $\Sigma \to \mathbb{R}^3$.

Finally, we can easily introduce the S-matrix in equation (3.10) by employing the relations (3.1)–(3.3) and the intertwining property (2.11). We obtain

$$T^{\pm}(f_{\text{in}}, \Sigma) = \tfrac{1}{2} \int_0^{\pm\infty} \mathrm{d}t (\mathrm{e}^{-L_0 t} f_{\text{in}}, K(\Sigma)\, \mathrm{e}^{-L_0 t} f_{\text{in}}), \tag{3.11}$$

where

$$K(\Sigma) = S^* P(\Sigma) S - P(\Sigma). \tag{3.12}$$

From now on we omit the subscript 'in'.

In the next section, we will work out explicit values for these integrals (3.11).

4. Relation between time delay and the scattering operator

This section completes the study of the connection between classical time delay and the classical S-operator by calculating the limit $\Sigma \to \mathbb{R}^3$ of $T(f, \Sigma)$. Although the method we use resembles the one employed in the quantum mechanical case (Bollé and Osborn 1979), we will see that the details are very different.

Writing out the scalar product in equation (3.11) or (3.10) we get e.g. for the second term

$$\begin{aligned} -\tfrac{1}{2} \int_0^{\pm\infty} \mathrm{d}t \int \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{p} (\mathrm{e}^{-L_0 t} f)^*(\boldsymbol{r}, \boldsymbol{p}) (P(\Sigma)\, \mathrm{e}^{-L_0 t} f)(\boldsymbol{r}, \boldsymbol{p}) \\ = -\tfrac{1}{2} \int_0^{\pm\infty} \mathrm{d}t \int \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{p}\, f^*\Big(\boldsymbol{r} + \frac{\boldsymbol{p}}{\mu} t, \boldsymbol{p}\Big) \chi_\Sigma(\boldsymbol{r}) f\Big(\boldsymbol{r} + \frac{\boldsymbol{p}}{\mu} t, \boldsymbol{p}\Big) \end{aligned} \tag{4.1}$$

with $\chi_\Sigma(\boldsymbol{r})$ the characteristic function for the region Σ. The difficulty here is that the time dependence is implicit and not a multiplying phase factor like in quantum mechanics. To solve this difficulty we will consider a Fourier transformation with respect to the coordinate space part of phase space.

We assume that $f(\boldsymbol{r}, \boldsymbol{p})$ belongs to the Schwarz functions with compact support $\mathscr{S}(\Gamma) \subset L^2(\Gamma)$. We then define

$$(\mathscr{F} f)(\boldsymbol{\alpha}, \boldsymbol{p}) \equiv \tilde{f}(\boldsymbol{\alpha}, \boldsymbol{p}) = \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}\boldsymbol{r} \exp(\mathrm{i}\boldsymbol{\alpha} \cdot \boldsymbol{r}) f(\boldsymbol{r}, \boldsymbol{p}). \tag{4.2}$$

So we have that

$$(\mathscr{F}\, \mathrm{e}^{-L_0 t} f)(\boldsymbol{\alpha}, \boldsymbol{p}) = \exp[-\mathrm{i}(\boldsymbol{\alpha} \cdot \boldsymbol{p}) t/\mu] \tilde{f}(\boldsymbol{\alpha}, \boldsymbol{p}). \tag{4.3}$$

Fron now on we drop the $\tilde{}$ since the rest of our analysis takes place entirely in this partly Fourier transformed phase space indicated by $(\boldsymbol{\alpha}, \boldsymbol{p})$. Because this Fourier transform leaves the scalar product in equation (3.11) invariant, we can write out the RHS of this equation as

$$\begin{aligned} \tfrac{1}{2} \int_0^{\pm\infty} \mathrm{d}t\, \mathrm{d}\boldsymbol{\alpha}'\, \mathrm{d}\boldsymbol{p}' \exp[\mathrm{i}(\boldsymbol{\alpha}' \cdot \boldsymbol{p}') t/\mu] f^*(\boldsymbol{\alpha}', \boldsymbol{p}') \int \mathrm{d}\boldsymbol{\alpha}\, \mathrm{d}\boldsymbol{p}\, K(\Sigma; \boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}, \boldsymbol{p}) \\ \times \exp[-\mathrm{i}(\boldsymbol{\alpha} \cdot \boldsymbol{p}) t/\mu] f(\boldsymbol{\alpha}, \boldsymbol{p}) \end{aligned} \tag{4.4}$$

where

$$K(\Sigma; \boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}, \boldsymbol{p}) = (S^* P(\Sigma) S)(\boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}, \boldsymbol{p}) - P(\Sigma; \boldsymbol{\alpha}' - \boldsymbol{\alpha}) \delta(\boldsymbol{p}' - \boldsymbol{p}), \tag{4.5}$$

with $P(\Sigma, \boldsymbol{\alpha}'-\boldsymbol{\alpha})$ the Fourier transform of $\chi_\Sigma(\boldsymbol{r})$. These are the forms we are going to work with.

First, we want to make the following important observation. Property (2.11) states that the S-operator intertwines with L_0. If we write out the explicit form of this property in the $\boldsymbol{\alpha}, \boldsymbol{p}$ variables we find that the kernel of S, $S(\boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}, \boldsymbol{p}) \sim \delta(\boldsymbol{\alpha}' \cdot \boldsymbol{p}' - \boldsymbol{\alpha} \cdot \boldsymbol{p})$. We explicitly want to take out that δ-function by defining a classically reduced s^{R} matrix by the kernel relation

$$S(\boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}, \boldsymbol{p}) = \delta(\boldsymbol{\alpha}' \cdot \boldsymbol{p}' - \boldsymbol{\alpha} \cdot \boldsymbol{p}) \frac{(\boldsymbol{\alpha} \cdot \hat{p})^3}{(\boldsymbol{\alpha}' \cdot \boldsymbol{p}')^2} s^{\mathrm{R}}{}_{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'} \left(\boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha} \cdot \hat{p}} \hat{p} \right). \tag{4.6}$$

The s^{R} kernel on the RHS of equation (4.6) represents an operator that is the classical equivalent of the quantum mechanical reduced on-energy-shell s operator. The factors in front of it are chosen such that the operator relations which S obeys are also valid for s^{R} in exactly the same form. An example of such a relation that we need further on is the unitarity of S (equation (2.10)) that can be written as

$$(S^*Sf)(\boldsymbol{\alpha}, \boldsymbol{p}) = f(\boldsymbol{\alpha}, \boldsymbol{p}). \tag{4.7}$$

Introducing the reduced s^{R} kernels in equation (4.7), the statement of unitarity becomes

$$\begin{aligned} f(\boldsymbol{\alpha}, \boldsymbol{p}) = \int & \mathrm{d}\boldsymbol{\alpha}_1 \, \mathrm{d}\hat{p}_1 \, \mathrm{d}\boldsymbol{\alpha}_2 \, \mathrm{d}\hat{p}_2 \, s^{\mathrm{R}*}\left(\boldsymbol{\alpha}, \boldsymbol{p}; \boldsymbol{\alpha}_1, \frac{\boldsymbol{\alpha} \cdot \boldsymbol{p}}{\boldsymbol{\alpha}_1 \cdot \hat{p}_1} \hat{p}_1 \right) \\ & \times s^{R}\left(\boldsymbol{\alpha}_1, \frac{\boldsymbol{\alpha} \cdot \boldsymbol{p}}{\boldsymbol{\alpha}_1 \cdot \hat{p}_1} \hat{p}_1; \boldsymbol{\alpha}_2, \frac{\boldsymbol{\alpha} \cdot \boldsymbol{p}}{\boldsymbol{\alpha}_6 \cdot \hat{p}_2} \hat{p}_2 \right) f\left(\boldsymbol{\alpha}_2, \frac{\boldsymbol{\alpha} \cdot \boldsymbol{p}}{\boldsymbol{\alpha}_2 \cdot \hat{p}_2} \hat{p}_2 \right), \end{aligned} \tag{4.8}$$

where we have omitted the subscript $\boldsymbol{\alpha}' \cdot \boldsymbol{p}'$ for convenience.

With this information we continue our derivation of the time-delay relation. We first introduce the Abel limit in equation (4.4) in order to carry out the t-integration.

Starting from equation (4.4) or equivalently equation (3.11) and using the fact that $U_t = \mathrm{e}^{Lt}$ is a unitary group and the Möller operators $\Omega^{\pm}$ are isometric, it is straightforward to show that the t-integrand is bounded by $2\|f\|^2$ for all t. Furthermore, we can estimate the rate of convergence in t of that t-integrand by deriving an asymptotic expansion for

$$g(t) = \int \mathrm{d}\boldsymbol{p} \, \exp[-\mathrm{i}(\boldsymbol{\alpha} \cdot \boldsymbol{p})t/\mu] F(\boldsymbol{p})$$

in inverse powers of t by doing successive partial integrations (Hunziker 1968b, p12). We then find that the first term of this expansion goes like t^{-2}. So, we can conclude that the time integrand of equation (4.4) is $L^1(t)$. The dominated convergence theorem then allows us to introduce the Abel limit, namely

$$\begin{aligned} T^{\pm}(f, \Sigma) = \tfrac{1}{2} \lim_{\varepsilon \to 0^+} \int_0^{\pm\infty} & \mathrm{d}t \, \mathrm{e}^{\mp \varepsilon t} \int \mathrm{d}\boldsymbol{\alpha}' \, \mathrm{d}\boldsymbol{p}' \, \mathrm{d}\boldsymbol{\alpha} \, \mathrm{d}\boldsymbol{p} \, \exp[\mathrm{i}t(\boldsymbol{\alpha}' \cdot \boldsymbol{p}' - \boldsymbol{\alpha} \cdot \boldsymbol{p})/\mu] \\ & \times f^*(\boldsymbol{\alpha}', \boldsymbol{p}') K(\Sigma; \boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}, \boldsymbol{p}) f(\boldsymbol{\alpha}, \boldsymbol{p}). \end{aligned} \tag{4.9}$$

Using equation (4.5) we immediately see that the $\boldsymbol{\alpha}, \boldsymbol{p}$ integrals exist absolutely so that we can change the order of integration by Fubini's theorem and do the t-integral first.

The result is

$$T^{\pm}(f,\Sigma)=\frac{\mathrm{i}}{2}\int \mathrm{d}\boldsymbol{\alpha}'\,\mathrm{d}\boldsymbol{p}'\,\mathrm{d}\boldsymbol{\alpha}\,\mathrm{d}\boldsymbol{p}\,f^*(\boldsymbol{\alpha}',\boldsymbol{p}')\frac{K(\Sigma;\boldsymbol{\alpha}',\boldsymbol{p}';\boldsymbol{\alpha},\boldsymbol{p})}{(1/\mu)(\boldsymbol{\alpha}'\cdot\boldsymbol{p}'-\boldsymbol{\alpha}\cdot\boldsymbol{p})\pm\mathrm{i}0}f(\boldsymbol{\alpha},\boldsymbol{p}). \tag{4.10}$$

Taking the symmetric combination of T^+ and T^- gives us, according to equation (3.9), the following expression for time delay

$$T(f,\Sigma)=\mathrm{i}\mu\int \mathrm{d}\boldsymbol{\alpha}'\,\mathrm{d}\boldsymbol{p}'\,\mathrm{d}\boldsymbol{\alpha}\,\mathrm{d}\boldsymbol{p}\,f^*(\boldsymbol{\alpha}',\boldsymbol{p}')\frac{K(\Sigma;\boldsymbol{\alpha}'\boldsymbol{p}';\boldsymbol{\alpha},\boldsymbol{p})}{\boldsymbol{\alpha}'\cdot\boldsymbol{p}'K(\Sigma;\boldsymbol{\alpha}',\boldsymbol{p}';\boldsymbol{\alpha},\boldsymbol{p})-\boldsymbol{\alpha}\cdot\boldsymbol{p}}f(\boldsymbol{\alpha},\boldsymbol{p})$$
$$+\Delta^+(f,\Sigma)+\Delta^-(f,\Sigma), \tag{4.11}$$

where the integral is defined as a principal-value integral.

We next have to calculate this principal-value integral (4.11) in the limit $\Sigma\to\mathbb{R}^3$. We start by writing out the kernel K using equation (4.5)

$$T(f,\mathbb{R}^3)=\lim_{\Sigma\to\mathbb{R}^3}\mathrm{i}\mu\int \mathrm{d}\boldsymbol{\alpha}'\,\mathrm{d}\boldsymbol{p}'\,\mathrm{d}\boldsymbol{\alpha}\,\mathrm{d}\boldsymbol{p}\frac{1}{\boldsymbol{\alpha}'\cdot\boldsymbol{p}'-\boldsymbol{\alpha}\cdot\boldsymbol{p}}f^*(\boldsymbol{\alpha}',\boldsymbol{p}')$$
$$\times\left\{\int \mathrm{d}\boldsymbol{\alpha}_1\,\mathrm{d}\boldsymbol{p}_1\,\mathrm{d}\boldsymbol{\alpha}_2\,S^*(\boldsymbol{\alpha}',\boldsymbol{p}';\boldsymbol{\alpha}_1,\boldsymbol{p}_1)P(\Sigma;\boldsymbol{\alpha}_1-\boldsymbol{\alpha}_2)S(\boldsymbol{\alpha}_2,\boldsymbol{p}_1;\boldsymbol{\alpha},\boldsymbol{p})\right.$$
$$\left.-P(\Sigma;\boldsymbol{\alpha}'-\boldsymbol{\alpha})\delta(\boldsymbol{p}'-\boldsymbol{p})\right\}f(\boldsymbol{\alpha},\boldsymbol{p}). \tag{4.12}$$

We now take the region Σ to be a sphere of radius R. We then use the Fourier transform properties of this sphere, outlined in the Appendix. Especially, the first property (A4) can immediately be employed to calculate the second term of equation (4.12) in the limit $\Sigma\to\mathbb{R}^3$, i.e. $R\to\infty$. We obtain

$$\mathrm{i}\mu\int \mathrm{d}\boldsymbol{\alpha}'\,\mathrm{d}\boldsymbol{p}'\,f^*(\boldsymbol{\alpha}',\boldsymbol{p}')\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}'\cdot\boldsymbol{p}'}f(\boldsymbol{\alpha}',\boldsymbol{p}'). \tag{4.13}$$

In the first term of equation (4.12) we introduce the reduced s^{R} matrices defined by equation (4.6). We then remove the δ-functions by integration and finally apply property (A4). The result is

$$-\mathrm{i}\mu\int \mathrm{d}\boldsymbol{\alpha}'\,\mathrm{d}\hat{p}'\,\mathrm{d}\boldsymbol{\alpha}\,\mathrm{d}\hat{p}\,\mathrm{d}\boldsymbol{\alpha}_1\,\mathrm{d}\boldsymbol{p}_1\,f^*\left(\boldsymbol{\alpha}',\frac{\boldsymbol{\alpha}_1\cdot\boldsymbol{p}_1}{\boldsymbol{\alpha}'\cdot\hat{p}'}\hat{p}'\right)\left(\frac{\boldsymbol{\alpha}_1\cdot\hat{p}_1}{\boldsymbol{\alpha}'\cdot\hat{p}'}\right)^3$$
$$\times s^{\mathrm{R}*}\left(\boldsymbol{\alpha}',\frac{\boldsymbol{\alpha}_1\cdot\boldsymbol{p}_1}{\boldsymbol{\alpha}'\cdot\hat{p}'}\hat{p}';\boldsymbol{\alpha}_1,\boldsymbol{p}_1\right)\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}_1\cdot\boldsymbol{p}_1}$$
$$\times\left[s^{\mathrm{R}}\left(\boldsymbol{\alpha}_1,\boldsymbol{p}_1;\boldsymbol{\alpha},\frac{\boldsymbol{\alpha}_1\cdot\boldsymbol{p}_1}{\boldsymbol{\alpha}\cdot\hat{p}}\hat{p}\right)f\left(\boldsymbol{\alpha},\frac{\boldsymbol{\alpha}_1\cdot\boldsymbol{p}_1}{\boldsymbol{\alpha}\cdot\hat{p}}\hat{p}\right)\right], \tag{4.14}$$

where we have assumed that the derivative with respect to $\boldsymbol{\alpha}_1\cdot\boldsymbol{p}_1$ exists. We split up this result into two parts. The first part contains the derivative of the function f and can be written, using the transformation $p_1=(\boldsymbol{\alpha}'\cdot\hat{p}'/\boldsymbol{\alpha}_1\cdot\hat{p}_1)p'$,

$$-\mathrm{i}\mu\int \mathrm{d}\boldsymbol{\alpha}'\,\mathrm{d}\boldsymbol{p}'\,f^*(\boldsymbol{\alpha}',\boldsymbol{p}')\int \mathrm{d}\boldsymbol{\alpha}_1\,\mathrm{d}\hat{p}_1\,\mathrm{d}\boldsymbol{\alpha}\,\mathrm{d}\hat{p}\,s^{\mathrm{R}*}\left(\boldsymbol{\alpha}',\boldsymbol{p}';\boldsymbol{\alpha}_1,\frac{\boldsymbol{\alpha}'\cdot\boldsymbol{p}'}{\boldsymbol{\alpha}_1\cdot\hat{p}_1}\hat{p}_1\right)$$
$$\times s^{\mathrm{R}}\left(\boldsymbol{\alpha}_1,\frac{\boldsymbol{\alpha}'\cdot\boldsymbol{p}'}{\boldsymbol{\alpha}_1\cdot\hat{p}_1}\hat{p}_1,\boldsymbol{\alpha},\frac{\boldsymbol{\alpha}'\cdot\boldsymbol{p}'}{\boldsymbol{\alpha}\cdot\hat{p}}\hat{p}\right)\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}'\cdot\boldsymbol{p}'}f\left(\boldsymbol{\alpha},\frac{\boldsymbol{\alpha}'\cdot\boldsymbol{p}'}{\boldsymbol{\alpha}\cdot\hat{p}}\hat{p}\right). \tag{4.15}$$

Applying unitarity of the s^{R} matrices given by equation (4.8) we see that this contribution (4.15) cancels expression (4.13). This is what we expect physically, since otherwise our time delay expression would depend on the shape of the function f specifying the incoming state.

The second part of expression (4.14) becomes, after putting $p_1 = (\boldsymbol{\alpha}' \cdot \hat{p}'/\boldsymbol{\alpha}_1 \cdot \hat{p}_1)p'$,

$$-\mathrm{i}\mu \int \mathrm{d}\boldsymbol{\alpha}' \,\mathrm{d}\boldsymbol{p}' \,\mathrm{d}\boldsymbol{\alpha}\, \mathrm{d}\hat{p}\, f^*(\boldsymbol{\alpha}', \boldsymbol{p}') \int \mathrm{d}\boldsymbol{\alpha}_1 \,\mathrm{d}\hat{p}_1 \bigg[s^{\mathrm{R}*}\bigg(\boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}_1, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha}_1 \cdot \hat{p}_1}\hat{p}_1\bigg) \times \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}' \cdot \boldsymbol{p}'} s^{\mathrm{R}}\bigg(\boldsymbol{\alpha}_1, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha}_1 \cdot \hat{p}_1}\hat{p}_1; \boldsymbol{\alpha}, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha} \cdot \hat{p}}\hat{p}\bigg)\bigg] f\bigg(\boldsymbol{\alpha}, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha} \cdot \hat{p}}\hat{p}\bigg). \tag{4.16}$$

Combining the results (4.12)–(4.16) we have shown that time delay is given by

$$T(f, \mathbb{R}^3) = -\mathrm{i}\mu \int \mathrm{d}\boldsymbol{\alpha}' \,\mathrm{d}\boldsymbol{p}' \,\mathrm{d}\boldsymbol{\alpha} \,\mathrm{d}\boldsymbol{p}\, \delta(\boldsymbol{\alpha}' \cdot \boldsymbol{p}' - \boldsymbol{\alpha} \cdot \boldsymbol{p}) \frac{(\boldsymbol{\alpha} \cdot \hat{p})^3}{(\boldsymbol{\alpha}' \cdot \boldsymbol{p}')^2} f^*(\boldsymbol{\alpha}', \boldsymbol{p}') \times \int \mathrm{d}\boldsymbol{\alpha}_1 \,\mathrm{d}\hat{p}_1 \bigg[s^{\mathrm{R}*}\bigg(\boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}_1, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha}_1 \cdot \hat{p}_1}\hat{p}_1\bigg) \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}' \cdot \boldsymbol{p}'} \times s^{\mathrm{R}}\bigg(\boldsymbol{\alpha}_1, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha}_1 \cdot \hat{p}_1}\hat{p}_1; \boldsymbol{\alpha}, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha} \cdot \hat{p}}\hat{p}\bigg)\bigg] f(\boldsymbol{\alpha}, \boldsymbol{p}). \tag{4.17}$$

From this result, we see that $T(f, \mathbb{R}^3)$ contains the same δ-function as the S-matrix (compare equation (4.6)). In fact, if we look back at the definition of $T(f, \Sigma)$ for finite Σ, given by equations (3.5) and (3.6), and write out the time-integrand of these equations explicitly, it is clear that the factor $\exp[(\mathrm{i}/\mu)(\boldsymbol{\alpha}' \cdot \boldsymbol{p}' - \boldsymbol{\alpha} \cdot \boldsymbol{p})t]$ also leads to this δ-function. Therefore we are justified in defining a reduced time delay operator q^{R} by

$$T(f, \Sigma) = \int \mathrm{d}\boldsymbol{\alpha}' \,\mathrm{d}\boldsymbol{p}' \,\mathrm{d}\boldsymbol{\alpha} \,\mathrm{d}\boldsymbol{p}\, \delta(\boldsymbol{\alpha}' \cdot \boldsymbol{p}' - \boldsymbol{\alpha} \cdot \boldsymbol{p}) \frac{(\boldsymbol{\alpha} \cdot \hat{p})^3}{(\boldsymbol{\alpha}' \cdot \boldsymbol{p}')^2} f^*(\boldsymbol{\alpha}', \boldsymbol{p}') \times q^{\mathrm{R}}_{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}\bigg(\Sigma; \boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}, \frac{\boldsymbol{\alpha}' \ \boldsymbol{p}'}{\boldsymbol{\alpha} \cdot \hat{p}}\hat{p}\bigg) f(\boldsymbol{\alpha}, \boldsymbol{p}). \tag{4.18}$$

Comparing this equation with equation (4.17) we see that the connection between time delay and the S-operator can be expressed in terms of the kernels q^{R} and s^{R} as follows

$$q^{\mathrm{R}}_{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}\bigg(\boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha} \cdot \hat{p}}\hat{p}\bigg) = -\mathrm{i} \int \mathrm{d}\boldsymbol{\alpha}_1 \,\mathrm{d}\hat{p}_1\, s^{\mathrm{R}*}_{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}\bigg(\boldsymbol{\alpha}', \boldsymbol{p}'; \boldsymbol{\alpha}_1, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha}_1 \cdot \hat{p}_1}\hat{p}_1\bigg) \times \frac{\mathrm{d}}{\mathrm{d}(\boldsymbol{\alpha}' \cdot \boldsymbol{p}')/\mu} s^{\mathrm{R}}_{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}\bigg(\boldsymbol{\alpha}_1, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha}_1 \cdot \hat{p}_1}\hat{p}_1; \boldsymbol{\alpha}, \frac{\boldsymbol{\alpha}' \cdot \boldsymbol{p}'}{\boldsymbol{\alpha} \cdot \hat{p}}\hat{p}\bigg), \tag{4.19}$$

where we have written again the $\boldsymbol{\alpha} \cdot \boldsymbol{p}$ subscript on the s^{R}-matrices. On the basis of this kernel relation (4.19), we can also state that the following operator relation is valid

$$\tilde{q}^{\mathrm{R}}_{\boldsymbol{\alpha} \cdot \boldsymbol{p}} = \tilde{s}^{\mathrm{R}*}_{\boldsymbol{\alpha} \cdot \boldsymbol{p}}\, \mathrm{d}/\mathrm{d}[\mathrm{i}(\boldsymbol{\alpha} \cdot \boldsymbol{p})/\mu]\, \tilde{s}^{\mathrm{R}}_{\boldsymbol{\alpha} \cdot \boldsymbol{p}} \tag{4.20}$$

where we have introduced again the $\tilde{}$.

Doing an inverse Fourier transformation with respect to α (recall equations (4.2)–(4.3)), the results (4.17)–(4.20) can finally be written in the form

$$\lim_{\Sigma\to\mathbb{R}^3} T(f,\Sigma)=(f, S^*(\mathrm{d}S/\mathrm{d}L_0)f). \tag{4.21}$$

The final result (4.21) expressing classical time delay in terms of the classical S-operator is the analogue of the corresponding quantum relation (Amrein *et al* 1977, Bollé and Osborn 1979, Martin 1976)

$$\lim_{\Sigma\to\mathbb{R}^3} T(f,\Sigma)=(f, S^*(\mathrm{d}S/\mathrm{di}H_0)f). \tag{4.22}$$

5. Discussion

In the foregoing sections we have derived the relation between classical time delay and the classical S-operator in a two-particle system with short-range interactions, within the context of the Hilbert-space approach to classical mechanics. The method we have used is based upon the explicit properties of the projection operator $P(\Sigma)$ onto a finite region Σ, taken to be a sphere of radius R. It would certainly be possible to establish the final result (4.21) on the basis of methods analogous to other rigorous quantum mechanical treatments like e.g. the work of Martin (Amrein *et al* 1977, Martin 1976). However, the big advantage of the method we have used here is that its quantum mechanical analogue is the only one up to now that has been shown to work in the quantum mechanical many-particle scattering problem (Bollé and Osborn 1979). So we are confident that with this method the same type of results can be obtained for classical many-particle systems.

In the two-particle problem we have discussed here, all three definitions of time delay (recall equations (3.5) and (3.6)) have limits when $\Sigma\to\mathbb{R}^3$ and are equivalent. Indeed, result (A21) of the Appendix tells us that the free reference time is independent of the choice of incoming or outgoing asymptotic state. But by analogy with the quantum case, we expect that this is no longer the case in the many-particle problem.

The results we have derived here can of course be transcribed into the language of phase space. In connection with such a phase-space approach to time delay, some recent results have appeared. Narnhofer (1980) has discussed a definition of time delay based on geometrical considerations which work in classical as well as in quantum mechanics. Bollé and Osborn (1980, see also Osborn *et al* 1980) have derived Levinson-type theorems for classical two-particle scattering in any dimension in terms of time delay and have used these theorems to discuss the high-temperature expansion for the classical second virial coefficient. After the present work was finished we received a paper (Narnhofer and Thirring 1980) in which the quasiclassical phase shift is identified as the generator of the classical canonical S-transformation, illuminating the connection between resonances of that phase shift and trajectories with large time delays or loopings.

Finally, comparing equations (4.21) and (4.22), we see that the time delay relation is valid for any (scattering) system irrespective of the fact that the underlying dynamics is classical or quantum mechanical. For a two-body quantum problem considered in a specific partial wave, the time delay is proportional to the energy derivative of the phase shift. Thus we can then state that time-delay theory provides a method of defining a universal phase-shift-like functional that is a characteristic of the (classical or quantum mechanical) scattering system. It would of course be interesting to study the further properties of this classical 'phase shift'.

Appendix 1.

This Appendix studies some properties of the projection operator $P(\Sigma)$ in the limit when $\Sigma \to \mathbb{R}^3$.

We assume that the operators act on the set of functions $f(\boldsymbol{\alpha}, \boldsymbol{p}) \in \mathcal{S}(\boldsymbol{\alpha}, \boldsymbol{p})$. The kernel $P(\Sigma; \boldsymbol{\alpha}' - \boldsymbol{\alpha})$ is defined as the Fourier transform of the characteristic function of the region Σ, $\chi_\Sigma(\boldsymbol{r})$, namely

$$P(\Sigma; \boldsymbol{\alpha}' - \boldsymbol{\alpha}) = \frac{1}{(2\pi)^3} \int \mathrm{d}\boldsymbol{r} \exp[\mathrm{i}(\boldsymbol{\alpha}' - \boldsymbol{\alpha}) \cdot \boldsymbol{r}] \chi_\Sigma(\boldsymbol{r}). \tag{A1}$$

Taking Σ to be a sphere of radius R, a straightforward calculation of the integral gives

$$P_R(\boldsymbol{\alpha}' - \boldsymbol{\alpha}) = (R/2\pi|\boldsymbol{\alpha}' - \boldsymbol{\alpha}|)^{3/2} J_{3/2}(|\boldsymbol{\alpha}' - \boldsymbol{\alpha}|R), \tag{A2}$$

where $J_{3/2}$ is a Bessel function of the first kind. Of course, we know that

$$\lim_{R\to\infty} (f', P_R f) = (f', f). \tag{A3}$$

The first property we want to prove is then

$$\lim_{R\to\infty} \int \mathrm{d}\boldsymbol{\alpha}' \, \mathrm{d}\boldsymbol{p}' \, \mathrm{d}\boldsymbol{\alpha} \, f^*(\boldsymbol{\alpha}', \boldsymbol{p}') \frac{P_R(\boldsymbol{\alpha}' - \boldsymbol{\alpha})}{(\boldsymbol{\alpha}' - \boldsymbol{\alpha}) \cdot \boldsymbol{p}'} f(\boldsymbol{\alpha}, \boldsymbol{p}')$$

$$= -\int \mathrm{d}\boldsymbol{\alpha}' \, \mathrm{d}\boldsymbol{p}' \, f^*(\boldsymbol{\alpha}', \boldsymbol{p}') \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}' \cdot \boldsymbol{p}'} f(\boldsymbol{\alpha}', \boldsymbol{p}'), \tag{A4}$$

where this integral has a well-defined meaning as a principal value integral.

Introducing the variable $\boldsymbol{z} = R(\boldsymbol{\alpha} - \boldsymbol{\alpha}')$ we can write

$$(\boldsymbol{\alpha} - \boldsymbol{\alpha}') \cdot \boldsymbol{p}' = p'(z/R) \cos\theta, \tag{A5}$$

where θ is the angle between $(\boldsymbol{\alpha} - \boldsymbol{\alpha}')$ and $\boldsymbol{p}'$. Using equation (A2) the integral on the LHS of equation (A4) becomes

$$-\int \mathrm{d}\boldsymbol{\alpha}' \, \mathrm{d}\boldsymbol{p}' \, \mathrm{d}\boldsymbol{z} \, f^*(\boldsymbol{\alpha}', \boldsymbol{p}') \frac{J_{3/2}(z)}{(2\pi z)^{3/2}} \frac{f(\boldsymbol{\alpha}' + \boldsymbol{z}/R, \boldsymbol{p}')}{p'(z/R)\cos\theta}. \tag{A6}$$

To evaluate the $\boldsymbol{z}$ integral, we introduce a spherical coordinate system $(z/R, \theta, \phi)$ and write expression (A6) as

$$-\int \mathrm{d}\boldsymbol{\alpha}' \, \mathrm{d}\boldsymbol{p}' \, \mathrm{d}z \, f^*(\boldsymbol{\alpha}', \boldsymbol{p}') \frac{J_{3/2}(z)}{(2\pi z)^{3/2}} F_{z/R}(\boldsymbol{\alpha}', \boldsymbol{p}') \tag{A7}$$

where

$$F_{z/R}(\boldsymbol{\alpha}', \boldsymbol{p}') = \tfrac{1}{2} \int_{-1}^{+1} \mathrm{d}\cos\theta \frac{1}{p'(z/R)\cos\theta} \bar{f}_{z/R}(\boldsymbol{\alpha}', \cos\theta, \boldsymbol{p}') \tag{A8}$$

$$\bar{f}_{z/R}(\boldsymbol{\alpha}', \cos\theta, \boldsymbol{p}') = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\phi \, f(\boldsymbol{\alpha}' + \boldsymbol{z}/R, \boldsymbol{p}'). \tag{A9}$$

Examination of these formulae indicates that $F_{z/R}$ is the average value of the function $(p'(z/R)\cos\theta)^{-1} f(\boldsymbol{\alpha}'+z/R, \boldsymbol{p}')$ summed over the surface of a sphere centred at $\boldsymbol{\alpha}'$ with radius z/R. The function $\bar{f}_{z/R}$ is the non-singular part of the average and the integral (A8) is the singular part.

It is clear that in domains excluding $z=0$, $F_{z/R}(\boldsymbol{\alpha}', \boldsymbol{p}')$ is integrable over dz. Furthermore we will show that $F_{z/R}(\boldsymbol{\alpha}', \boldsymbol{p}')$ is continuous in z/R in the neighbourhood of 0, so that we can use the weak convergence of P_R (equation (A3)) to conclude that expression (A7) can be written in the limit $R\to\infty$ as

$$-\int \mathrm{d}\boldsymbol{\alpha}'\,\mathrm{d}\boldsymbol{p}'\, f^*(\boldsymbol{\alpha}', \boldsymbol{p}')F_0(\boldsymbol{\alpha}', \boldsymbol{p}'). \tag{A10}$$

Let us examine then the behaviour of $F_{z/R}(\boldsymbol{\alpha}', \boldsymbol{p}')$. Defining

$$x = p'(z/R)\cos\theta \tag{A11}$$

we get for equation (A8)

$$F_{z/R}(\boldsymbol{\alpha}', \boldsymbol{p}') = \frac{R}{2p'z}\int_{-p'z/R}^{p'z/R} \mathrm{d}x\,\frac{1}{x}\bar{f}_{z/R}\left(\boldsymbol{\alpha}', \frac{xR}{p'z}, \boldsymbol{p}'\right). \tag{A12}$$

This principal value integral can be written as

$$\frac{1}{2a}\int_{-a}^{+a}\mathrm{d}x\,\frac{g(x)}{x} = \frac{1}{2a}\int_{-a}^{+a}\frac{g(x)-g(0)}{x}\,\mathrm{d}x = \frac{g(x_1)-g(0)}{x_1} \qquad x_1\in[-a, +a], \tag{A13}$$

where we have used the mean value theorem and where g is a differentiable function. As $a\to 0$, we simply get that (A13) is equal to the derivative of g at $x=0$. Recalling equation (A5) we obtain then for (A12) in the limit $R\to\infty$

$$F_0(\boldsymbol{\alpha}', \boldsymbol{p}') = \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}'\cdot\boldsymbol{p}'}f(\boldsymbol{\alpha}', \boldsymbol{p}'). \tag{A14}$$

Substituting this result in equation (A10) proves our first property (A4).

The second property we want to show is

$$\int_{-\infty}^{+\infty}\mathrm{d}t(\Psi_{\mathrm{in}}(t), P_R\Psi_{\mathrm{in}}(t)) \xrightarrow[R\to\infty]{} 2\mu R\int \mathrm{d}\boldsymbol{r}'\,\mathrm{d}\boldsymbol{p}'\, f^*(\boldsymbol{r}', \boldsymbol{p}')\frac{1}{p'}f(\boldsymbol{r}', \boldsymbol{p}') + \mathrm{O}\left(\frac{1}{R}\right). \tag{A15}$$

Writing out the LHS of expression (A15) by using equations (3.1), (4.2) and (4.3) gives us

$$2\pi\mu\int \mathrm{d}\boldsymbol{\alpha}'\,\mathrm{d}\boldsymbol{p}'\,\mathrm{d}\boldsymbol{\alpha}\, f^*(\boldsymbol{\alpha}', \boldsymbol{p}')\delta((\boldsymbol{\alpha}'-\boldsymbol{\alpha})\cdot\boldsymbol{p}')P_R(\boldsymbol{\alpha}'-\boldsymbol{\alpha})f(\boldsymbol{\alpha}, \boldsymbol{p}'). \tag{A16}$$

Introducing $\boldsymbol{q} = \boldsymbol{\alpha}-\boldsymbol{\alpha}'$ and choosing a coordinate system for $\boldsymbol{q}$ whose z-axis $\|\boldsymbol{p}'$, the δ-function in expression (A16) tells us that $\boldsymbol{q}$ is a vector lying in the x–y plane. Therefore we get, introducing the explicit expression for P_R (equation (A2)),

$$2\pi\mu\int \mathrm{d}\boldsymbol{\alpha}'\,\mathrm{d}\boldsymbol{p}'\, f^*(\boldsymbol{\alpha}', \boldsymbol{p}')\frac{1}{p'}\int_0^\infty q\,\mathrm{d}q\left(\frac{R}{2\pi q}\right)^{3/2} J_{3/2}(qR)\int_0^{2\pi}\mathrm{d}\phi\, f(\boldsymbol{\alpha}'+\boldsymbol{q}, \boldsymbol{p}'). \tag{A17}$$

Finally taking $qR = z$ and doing a partial integration in z, we obtain for expression (A17)

$$2\pi\mu \int d\boldsymbol{\alpha}'\, d\boldsymbol{p}'\, f^*(\boldsymbol{\alpha}', \boldsymbol{p}') \frac{1}{p'} \frac{R}{(2\pi)^{3/2}} \left\{ \left[-z^{-1/2} J_{1/2}(z) \int_0^{2\pi} d\phi\, f\left(\boldsymbol{\alpha}' + \frac{z}{R}, \boldsymbol{p}'\right) \right]_{z=0}^{z=\infty} + \int_0^{\infty} dz\, z^{-1/2} J_{1/2}(z) \frac{d}{dz} \int_0^{2\pi} d\phi\, f\left(\boldsymbol{\alpha}' + \frac{z}{R}, \boldsymbol{p}'\right) \right\}. \tag{A18}$$

In the limit $R \to \infty$, it is easy to check that the first term of (A18) leads to a contribution

$$2\mu R \int d\boldsymbol{\alpha}'\, d\boldsymbol{p}' \frac{1}{p'} f^*(\boldsymbol{\alpha}', \boldsymbol{p}') f(\boldsymbol{\alpha}', \boldsymbol{p}'). \tag{A19}$$

The second term of (A18) gives zero in that limit because of the Riemann–Lebesgue lemma. Finally, taking the inverse Fourier transform with respect to $\boldsymbol{\alpha}$ of the functions f in (A19) verifies our property (A15). Remark that this property just tells us that the free transit time through the sphere R is given by $2R$ divided by the radial velocity.

In the same way we can show that

$$\int_{-\infty}^{+\infty} dt (\Psi_{\text{out}}(t), P_R \Psi_{\text{out}}(t)) \underset{R \to \infty}{\longrightarrow} 2\mu R \int d\boldsymbol{r}'\, d\boldsymbol{p}'\, f^*_{\text{out}}(\boldsymbol{r}', \boldsymbol{p}') \frac{1}{p'} f_{\text{out}}(\boldsymbol{r}', \boldsymbol{p}') + O\left(\frac{1}{R}\right). \tag{A20}$$

Introducing equations (3.3) and (2.4) in this relation (A20), and applying conservation of energy, we easily see that the RHS of equations (A15) and (A20) are equal so that we finally obtain

$$\int_{-\infty}^{+\infty} dt (\Psi_{\text{in}}(t), P_R \Psi_{\text{in}}(t)) - \int_{-\infty}^{+\infty} dt (\Psi_{\text{out}}(t), P_R \Psi_{\text{out}}(t)) = O(R^{-1}). \tag{A21}$$

References

Amrein W O, Jauch J M and Sinha K B 1977 *Scattering Theory in Quantum Mechanics* (Reading, Mass.: Benjamin)

Bollé D 1979a *Ann. Phys., NY* **121** 131–46

—— 1979b *Phys. Lett.* **74** A 26–8

Bollé D and Osborn T A 1979 *J. Math. Phys.* **20** 1121–34

—— 1980 *J Math. Phys.* to be published

Hunziker W 1968a *Commun. Math. Phys.* **8** 282–99

—— 1968b in *Lectures in Theoretical Physics* ed. A O Barut and W E Brittin (New York: Gordon and Breach) vol X-A, pp 1–48

—— 1974 in *Scattering in Mathematical Physics* ed. J A LaVita and J P Marchand (Boston: Reidel) pp 79–96

Martin Ph A 1976 *Commun. Math. Phys.* **47** 221–7

Narnhofer H 1980 *Phys. Rev. D.* **22** 2387–90

Narnhofer H and Thirring W 1980 *The Canonical Scattering Transformation in Classical Mechanics* Universität Wien preprint

Osborn T A 1977 *Phys. Rev.* A **16** 334–50

Osborn T A, Froese R G and Howes S F 1980 *Phys. Rev.* A**22** 101–10