Time delay and Calabi invariant in classical scattering theory

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Abstract

We define, prove the existence and obtain explicit expressions for classical time delay defined in terms of sojourn times for abstract scattering pairs (H_0, H) on a symplectic manifold. As a by-product, we establish a classical version of the Eisenbud-Wigner formula of quantum mechanics. Using recent results of V. Buslaev and A. Pushnitski on the scattering matrix in Hamiltonian mechanics, we also obtain an explicit expression for the derivative of the Calabi invariant of the Poincaré scattering map.

Our results are applied to dispersive Hamiltonians, to a classical particle in a tube and to Hamiltonians on the Poincaré ball.

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1 Introduction

Since the works of D. Bollé, H. Narnhofer, W. Thirring and collaborators in the 80's, it is known that one can define properly a notion of time delay in terms of sojourn times in classical scattering theory. However, most of the mathematical works on the topic (if not all) provide a complete description only for scattering pairs (H_0, H) where the free Hamiltonian is of the type $H_0(q,p) = |p|^2/2$ on $\mathbb{R}^{2n}$. Therefore, a legitimate interrogation is whether it is possible to define, to prove the existence and to obtain explicit expressions for classical time delay for a general class of scattering pairs in the modern set-up of symplectic geometry. Answering (affirmatively) to these questions is the purpose of the present paper.

Our interest in these issues has been aroused by recent articles on time delay in quantum mechanics [28, 29] and on the scattering matrix in Hamiltonian mechanics [8]. In [29], the authors prove that the existence of time delay defined in terms of sojourn times, as well as its identity with Eisenbud-Wigner time delay [33, 35], is a common feature of two-Hilbert spaces quantum scattering theory. Their proofs rely on abstract commutator methods and on an integral formula relating localisation operators to time operators [28]. Here, we use the classical counterpart of this formula, established in [14], to obtain similar results in classical scattering theory as well as an explicit expression for the derivative of the Calabi invariant of the Poincaré scattering map. Our approach takes its roots in the

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following observations: When $H_0(q,p) = |p|^2/2$ on $\mathbb{R}^{2n}$, the usual position observables $\Phi_j(q,p) := q^j$ satisfy the simple Poisson bracket identity

$$\big\{\{\Phi_j, H_0\}, H_0\big\} = 0. \tag{1.1}$$

In consequence, the time evolution of the observables Φ_j under the flow φ_t^0 of H_0 is lineal with growth rate $\{\Phi_j, H_0\} = p_j$. Accordingly, any trajectory $\{\varphi_t^0(q,p)\}_{t\in\mathbb{R}}$ with initial velocity $p \neq 0$ escapes from each ball $B_r := \{q \in \mathbb{R}^n \mid |q| \leq r\}$ as $|t| \to \infty$. Similarly, if $V := H - H_0$ is a suitable perturbation of H_0 and if the initial condition (q,p) is well chosen, the perturbed trajectory corresponding to the free trajectory $\{\varphi_t^0(q,p)\}_{t\in\mathbb{R}}$ also escapes from each ball B_r as $|t| \to \infty$. In such a case, the difference of sojourn times in B_r between the two trajectories may converge to a finite value, called the global time delay for (q,p), as $r \to \infty$. This is well known and has been established by various authors for different types of perturbations V (see for instance [5, 6, 7, 12, 20, 26, 27, 34]). Fine. But what happens when H_0 and H are abstract Hamiltonians on a given symplectic manifold M? If the dimension of M is finite, Darboux's theorem guarantees us that there exist, at least locally, canonical coordinates on M. However, these coordinates have usually nothing to do with the free Hamiltonian H_0, and are in consequence inappropriate for the definition of sojourn times. Therefore, our point of view is instead to retain as position observables merely functions Φ_j satisfying (1.1), as in the case $H_0(q,p) = |p|^2/2$. This choice is certainly not the most general one, but it turns out to be extremely rewarding as we shall explain below. Here, we just note three facts on its favour. First, it has been shown in [14, Sec. 4] that there exist natural position observables Φ satisfying (1.1) for many Hamiltonian systems (M, H_0) appearing in literature. Second, we know that this approach works in the quantum case [29]. Finally, the condition (1.1) is formulated in an invariant way on M, without any mention to the particular structure of H_0.

So, let H_0 and H be Hamiltonians on a symplectic manifold M with Poisson bracket $\{\,\cdot\,,\,\cdot\,\}$, assume that H_0 and H have complete flows $\{\varphi_t^0\}_{t\in\mathbb{R}}$ and $\{\varphi_t\}_{t\in\mathbb{R}}$, and let $\Phi := (\Phi_1, \ldots, \Phi_d)$ be a family of observables satisfying (1.1). Then, the vector $\nabla H_0 := \big(\{\Phi_1, H_0\}, \ldots, \{\Phi_d, H_0\}\big)$ and the set

$$\mathsf{Crit}(H_0, \Phi) := (\nabla H_0)^{-1}(\{0\}) \subset M$$

can be interpreted, respectively, as the velocity observable and the set of critical points associated to H_0 and Φ (see [28, Ass. 2.2 & Def. 2.5] for quantum analogues). Accordingly, the free trajectories $\{\varphi_t^0(m)\}_{t\in\mathbb{R}}$ with $m \in M \setminus \mathsf{Crit}(H_0, \Phi)$ escape from each set $\Phi^{-1}(B_r)$ as $|t| \to \infty$ (as in the case of $H_0(q,p) = |p|^2/2$, where $\mathsf{Crit}(H_0, \Phi) = \mathbb{R}^n \times \{0\}$ and $\Phi^{-1}(B_r) = B_r$). Therefore, we have propagation in $M \setminus \mathsf{Crit}(H_0, \Phi)$, and the wave maps $W_\pm := \lim_{t\to\pm\infty} \varphi_{-t} \circ \varphi_t^0$ exist and are well defined symplectomorphisms on $M \setminus \mathsf{Crit}(H_0, \Phi)$ if $V \equiv H - H_0$ is suitable (Theorem 2.8). Using a virial type argument, we then show in Lemma 2.10 that $W_\pm$ are complete, and thus that the scattering map $S := W_+^{-1} \circ W_-$ is also a well defined symplectomorphism on $M \setminus \mathsf{Crit}(H_0, \Phi)$. With these objects at hand, we introduce in Section 3 the symmetrised time delay τ_r, defined in terms of sojourn times in the sets $\Phi^{-1}(B_r)$, for the general scattering system (M, H_0, H). Then, we prove the existence of the limit $\tau := \lim_{r\to\infty} \tau_r$ and its identity with a difference of arrival times similar to Eisenbud-Wigner Formula in quantum mechanics (Theorem 3.3 and Remark 3.4). We also show in Corollary 3.5 that the usual (unsymmetrised) time delay exists and is equal to the symmetrised time delay if the scattering process preserves the norm of the velocity vector ∇H_0. Finally, we establish in Section 4 a link between our results on the whole manifold M and the results of [8] on fixed energy submanifolds $\Sigma_E^0 := H_0^{-1}(\{E\})$. Under appropriate assumptions on the energy $E \in \mathbb{R}$ and the perturbation V, we show that the abstract time delay τ_E defined in [8] as the difference of distance from a Poincaré section $\Gamma_E \subset \Sigma_E^0$ before and after scattering coincides with the restriction $\tau|_{\Gamma_E}$ if

$$\Gamma_E = \big\{m \in \Sigma_E^0 \mid (\Phi \cdot \nabla H_0)(m) = 0\big\}.$$

In other terms, if there exist position observables Φ satisfying (1.1), then there exist natural Poincaré sections Γ_E verifying the assumptions of [8], and our general time-dependent definition of time delay coincides, after restriction to Γ_E, with the abstract time-independent definition of time delay of [8]. This establishes a new relation between two complementary formulations of classical scattering theory. Furthermore, by using a theorem of [8] linking τ_E to the Calabi invariant $\mathrm{Cal}(\widetilde{S}_E)$ of the Poincaré scattering map $\widetilde{S}_E$, this leads to an explicit expression in terms of Φ, S and ∇H_0 for the derivative $\frac{\mathrm{d}}{\mathrm{d}E}\mathrm{Cal}(\widetilde{S}_E)$ of the Calabi invariant (Theorem 4.4).

To conclude, we point out several aspects of independent interest in the paper. In the first place, our results allow to treat three new classes of Hamiltonians systems: dispersive Hamiltonians $H_0(q,p) = h(p)$ on $\mathbb{R}^{2n}$, a classical particle in a tube and the kinetic energy Hamiltonian on the Poincaré ball. The first example generalises the case $H_0(q,p) = |p|^2/2$, the second example illustrates the fact that in general only the symmetrised time delay exists, and the last example shows that our results also apply to geodesic flows on manifolds with curvature. We also note that our treatment of classical scattering theory in Section 2 is model-independent, and therefore possibly of some use in other contexts. Finally, we note that the present paper provides a new example of results valid both in quantum and classical mechanics. Accordingly, we try to put into light throughout all of the paper the relation between both theories.

2 Classical scattering theory

In this section, we introduce a classical scattering pair (H_0, H) on a symplectic manifold M and a family of position type observables $\Phi \equiv (\Phi_1, \ldots, \Phi_d)$ satisfying the Poisson bracket relation (1.1). Then, we recall some results on H_0 following from the existence of the family Φ. Finally, we extend standard results on the scattering theory for $H_0(q,p) = |p|^2/2$, $H(q,p) = |p|^2/2 + V(q)$ and $\Phi(q,p) = q$ to the abstract triple (H_0, H, Φ).

Throughout the paper, we use the notations $\mathbb{R}_+ := (0,\infty)$ and $\mathbb{R}_- := (-\infty, 0)$, and we write ζ^* for the pullback of a diffeomorphism of manifolds $\zeta : M_1 \to M_2$.

2.1 Free Hamiltonian and position observables

Let M be a symplectic manifold, *i.e.* a smooth manifold endowed with a closed two-form ω such that the morphism $TM \ni X \mapsto \omega^\flat(X) := \iota_X\omega$ is an isomorphism. In infinite dimension, such a manifold is said to be a strong symplectic manifold (in opposition to a weak symplectic manifold, when the above map is only injective; see [2, Sec. 8.1]). When the dimension is finite, the dimension must be even, say equal to $2n$, and the $2n$-form $\omega^n := \omega \wedge \cdots \wedge \omega$ must be a volume form. The Poisson bracket is defined as follows: for each $f \in \mathsf{C}^\infty(M)$ we define the vector field $X_f := (\omega^\flat)^{-1}(\mathrm{d}f)$, *i.e.* $\mathrm{d}f(\,\cdot\,) = \omega(X_f, \cdot\,)$, and set $\{f,g\} := \omega(X_f, X_g)$ for each $f, g \in \mathsf{C}^\infty(M)$.

In the sequel, the function $H_0 \in \mathsf{C}^\infty(M)$ is an Hamiltonian with complete vector field X_{H_0}. So, the flow $\{\varphi_t^0\}$ associated to H_0 is defined for all $t \in \mathbb{R}$, it preserves the Poisson bracket, *i.e.*

$$\big\{f \circ \varphi_t^0, g \circ \varphi_t^0\big\} = \{f,g\} \circ \varphi_t^0, \quad t \in \mathbb{R},$$

and it satisfies the usual evolution equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} f \circ \varphi_t^0 = \big\{f, H_0\big\} \circ \varphi_t^0, \quad t \in \mathbb{R}.$$

In particular, the Hamiltonian H_0 is preserved along its flow, *i.e.*

$$H_0 \circ \varphi_t^0 = H_0, \quad t \in \mathbb{R}.$$

As in [14, Sec. 3], we consider an additional family $\Phi \equiv (\Phi_1, \dots, \Phi_d) \in \mathsf{C}^\infty(M; \mathbb{R}^d)$ of observables, and define the associated functions

$$\partial_j H_0 := \{\Phi_j, H_0\} \in \mathsf{C}^\infty(M) \qquad \text{and} \qquad \nabla H_0 \equiv \{\Phi, H_0\} := (\partial_1 H_0, \dots, \partial_d H_0) \in \mathsf{C}^\infty(M; \mathbb{R}^d),$$

and the corresponding set of critical points:

$$\mathsf{Crit}(H_0, \Phi) := (\nabla H_0)^{-1}(\{0\}) \subset M.$$

The set $\mathsf{Crit}(H_0, \Phi)$ is closed and contains the usual set $\mathsf{Crit}(H_0)$ of critical points of H_0, *i.e.*

$$\mathsf{Crit}(H_0, \Phi) \supset \mathsf{Crit}(H_0) := \big\{m \in M \mid X_{H_0}(m) = 0\big\} \equiv \big\{m \in M \mid (\mathrm{d}H_0)_m = 0\big\}.$$

Our first assumption is the following:

Assumption 2.1 (Position observables)**.** *One has* $\big\{\{\Phi_j, H_0\}, H_0\big\} = 0$ *for each* $j \in \{1, \dots, d\}$.

Assumption 2.1 is verified by many free Hamiltonian systems (M, ω, H_0) appearing in literature (see [14, Sec. 4] for both finite and infinite dimensional examples). It implies that the time evolution of the observables Φ_j under the flow $\{\varphi_t^0\}_{t\in\mathbb{R}}$ is lineal with growth rate $\partial_j H_0$; namely,

$$\big(\Phi_j \circ \varphi_t^0\big)(m) = \Phi_j(m) + t\big(\partial_j H_0\big)(m) \quad \text{for all } j \in \{1, \dots, d\},\ t \in \mathbb{R} \text{ and } m \in M. \tag{2.1}$$

Furthermore, one has for each $t \in \mathbb{R}$

$$\varphi_t^0\big(\mathsf{Crit}(H_0, \Phi)\big) = \mathsf{Crit}(H_0, \Phi) \qquad \text{and} \qquad \varphi_t^0\big(M \setminus \mathsf{Crit}(H_0, \Phi)\big) = M \setminus \mathsf{Crit}(H_0, \Phi), \tag{2.2}$$

and if $m \in M \setminus \mathsf{Crit}(H_0, \Phi)$, then one must have $\varphi_t^0(m) \neq m$ for all $t \neq 0$ due to Equation (2.1). So, each orbit $\{\varphi_t^0(m)\}_{t\in\mathbb{R}}$ either stays in $\mathsf{Crit}(H_0, \Phi)$ if $m \in \mathsf{Crit}(H_0, \Phi)$, or stays outside $\mathsf{Crit}(H_0, \Phi)$ and is not periodic if $m \notin \mathsf{Crit}(H_0, \Phi)$.

Assumption 2.1 also permits to relate the difference of the sojourn times (in the past and in the future) of a classical orbit $\{\varphi_t^0(m)\}_{t\in\mathbb{R}}$ in the dilated regions $\Phi^{-1}(B_r) \subset M$, $r > 0$, to a finite arrival time defined in terms of Φ and H_0. To see this, let $T : M \setminus \mathsf{Crit}(H_0, \Phi) \to \mathbb{R}$ be the C^∞-function given by

$$T := \Phi \cdot \frac{\nabla H_0}{|\nabla H_0|^2}, \tag{2.3}$$

and then observe the following (see [14, Sec. 3.1-3.2] for details):

(i) One has for each $t \in \mathbb{R}$

$$\big\{T, H_0\big\} \circ \varphi_t^0 \equiv \frac{\mathrm{d}}{\mathrm{d}t}\big(T \circ \varphi_t^0\big) = 1 \qquad \text{and} \qquad T \circ \varphi_t^0 = T + t$$

on $M \setminus \mathsf{Crit}(H_0, \Phi)$.

(ii) If we consider the observables Φ_j as the components of an abstract position observable Φ, then ∇H_0 can be seen as the velocity vector for the Hamiltonian H_0, and $-T(m)$ is equal to the time at which a particle in $\mathbb{R}^n$ with initial position $\Phi(m)$ and velocity $(\nabla H_0)(m)$ intersects the hyperplane (containing the origin) orthogonal to the unit vector $\frac{(\nabla H_0)(m)}{|(\nabla H_0)(m)|}$. For instance, if $\Phi(q, p) = q$ and $H_0(q, p) = |p|^2/2$ are the usual position and kinetic energy on $M = T^*\mathbb{R}^n$, then $-T(q, p) \equiv -q \cdot p/|p|^2$ is known in physics literature as the arrival time of the free particle (see *e.g.* [31, Sec. II.E]).

Accordingly, the observable T represents a time of arrival growing linearly under the flow $\{\varphi_t^0\}_{t\in\mathbb{R}}$ (in quantum mechanics, the relations $\{T, H_0\} = 1$ and $T \circ \varphi_t^0 = T + t$ are replaced by the canonical commutation relation $[T, H_0] = i$ and the Weyl relation $\mathrm{e}^{itH_0}\, T\, \mathrm{e}^{-itH_0} = T + t$, and the corresponding operator T is called a time operator for H_0; see [3] or [23] for details). It only remains to link the observable T to the sojourn times of the classical orbits in the regions $\Phi^{-1}(B_r)$. This is the content of the next theorem, proved in Section 3.2 of [14]:

Theorem 2.2. *Let H_0 and Φ satisfy Assumption 2.1. Then we have*

$$\lim_{r\to\infty} \frac{1}{2} \int_0^\infty \mathrm{d}t \left\{ (\chi_r^\Phi \circ \varphi_{-t}^0)(m) - (\chi_r^\Phi \circ \varphi_t^0)(m) \right\} = \begin{cases} T(m) & \text{if } m \in M \setminus \mathsf{Crit}(H_0, \Phi) \\ 0 & \text{if } m \in \mathsf{Crit}(H_0, \Phi), \end{cases}$$

with χ_r^Φ the characteristic function for the set $\Phi^{-1}(B_r)$.

We conclude the section by exhibiting three examples which will serve as connecting thread throughout the whole paper. However, we note that many other examples are certainly accessible as suggested by [14, Sec. 4] (for instance, it would be interesting to study the cases of the nonlinear Klein-Gordon and Schrödinger equations where the scattering theory is well defined, see [24, 25]). The notation $\langle y \rangle := \sqrt{1 + |y|^2}$ is used for any $y \in \mathbb{R}^n$.

Example 2.3 ($H_0(q,p) = h(p)$)**.** *Consider on $M := T^*\mathbb{R}^n \simeq \mathbb{R}^{2n}$ the canonical coordinates (q,p), with $q \equiv (q^1, \ldots, q^n)$ and $p \equiv (p_1, \ldots, p_n)$, and the canonical symplectic form $\omega := \sum_{j=1}^n \mathrm{d}q^j \wedge \mathrm{d}p_j$. Take a purely kinetic Hamiltonian $H_0(q,p) := h(p)$ with $h \in \mathsf{C}^\infty(\mathbb{R}^n; \mathbb{R})$, and let $\Phi_j(q,p) := q^j$ be the usual position functions. Then $\varphi_t^0(q,p) = \big(q + t(\nabla h)(p), p\big)$, $\nabla H_0 = \nabla h$, and Assumption 2.1 is satisfied:*

$$\big\{\{\Phi_j, H_0\}, H_0\big\}(q,p) = \big\{(\partial_j h)(p), h(p)\big\} = 0.$$

Furthermore, we have $\mathsf{Crit}(H_0) = \mathsf{Crit}(H_0, \Phi) = \mathbb{R}^n \times (\nabla h)^{-1}(\{0\})$.

Example 2.4 (Particle in a tube)**.** *Let $\Omega := \mathbb{R} \times \mathring{B}_1$ be a straight tube with section $\mathring{B}_1 := \big\{q_\perp \in \mathbb{R}^n \mid |q| < 1\big\}$, and endow $M := T^*\Omega \simeq \Omega \times \mathbb{R}^{n+1}$ with the coordinates $q \equiv (q^1, q_\perp) \in \Omega$ and $p \equiv (p_1, p_\perp) \in \mathbb{R}^{n+1}$ and with the symplectic form $\omega := \sum_{j=1}^{n+1} \mathrm{d}q^j \wedge \mathrm{d}p_j$. Then, consider the Hamiltonian given by the map*

$$H_0 : M \to \mathbb{R}, \quad (q,p) \mapsto |p|^2/2 + v_0\big(|q_\perp|^2\big),$$

where $v_0 \in \mathsf{C}^\infty\big((0,1)\big)$ satisfies

(i) $v_0 \equiv 0$ in a neighbourhood of $0 \in \mathbb{R}$,

(ii) $v_0'(x) \geq 0$ for all $x \in (0,1)$,

(iii) $\lim_{x\nearrow 1} v_0(x) = +\infty$.

The Hamiltonian H_0 models a classical particle in the tube Ω evolving under the influence of a confining potential v_0, which repels the particle near the boundary of Ω. The motion of the particle is uniform along the q^1-axis and given by the equation $\ddot{q}_\perp = -2q_\perp v_0'\big(|q_\perp|^2\big)$ in the transverse direction. To show the completeness of the corresponding Hamiltonian vector field

$$X_{H_0}(q,p) = p\, \frac{\partial}{\partial q}\bigg|_{(q,p)} - 2q_\perp v_0'\big(|q_\perp|^2\big)\, \frac{\partial}{\partial p_\perp}\bigg|_{(q,p)}, \quad (q,p) \in M,$$

one can for instance use the criterion [1, Prop. 2.1.20] with the (proper and C^∞) function

$$f : M \to \mathbb{R}, \quad (q,p) \mapsto H_0(q,p) + \big\langle q^1 \big\rangle. \tag{2.4}$$

As a function Φ, we take the longitudinal coordinate $\Phi(q,p) := q^1$. This gives $(\nabla H_0)(q,p) = p_1$ as velocity observable and implies that

$$\big\{\{\Phi, H_0\}, H_0\big\}(q,p) = \big\{p_1, |p|^2/2 + v_0\big(|q_\perp|^2\big)\big\} = 0.$$

So, Assumption 2.1 is satisfied and

$$\mathsf{Crit}(H_0) = \big(\mathbb{R} \times (v_0')^{-1}(\{0\})\big) \times \{0\} \subset \Omega \times \big(\{0\} \times \mathbb{R}^n\big) = \mathsf{Crit}(H_0, \Phi).$$

Example 2.5 (Poincaré ball)**.** *Consider the open unit ball $\mathring{B}_1 \equiv \big\{q \in \mathbb{R}^n \mid |q| < 1\big\}$ endowed with the Riemannian metric g given by*

$$g_q(X_q, Y_q) := \frac{4}{(1-|q|^2)^2}\,(X_q \cdot Y_q), \quad q \in \mathring{B}_1,\ X_q, Y_q \in T_q\mathring{B}_1 \simeq \mathbb{R}^n.$$

Let $T^*\mathring{B}_1 \simeq \big\{(q,p) \in \mathring{B}_1 \times \mathbb{R}^n\big\}$ be the cotangent bundle on $\mathring{B}_1$ with symplectic form $\omega := \sum_{j=1}^n \mathrm{d}q^j \wedge \mathrm{d}p_j$, and let

$$H_0 : T^*\mathring{B}_1 \to \mathbb{R}, \quad (q,p) \mapsto \frac{1}{2}\sum_{j,k=1}^n g^{jk}(q) p_j p_k = \frac{1}{8}|p|^2\big(1-|q|^2\big)^2$$

be the kinetic energy Hamiltonian. Then, we know from [14, Sec. 4.3(D)] that the Hamiltonian vector field X_{H_0} is complete on $M := T^*\mathring{B}_1 \setminus H_0^{-1}(\{0\}) \simeq \mathring{B}_1 \times \mathbb{R}^n \setminus \{0\}$ and that the function

$$\Phi : M \to \mathbb{R}, \quad (q,p) \mapsto \tanh^{-1}\left(\frac{2(p\cdot q)}{|p|(1+|q|^2)}\right)$$

is C^∞ and satisfies Assumption 2.1 with $\nabla H_0 = \sqrt{2H_0}$ and $\mathsf{Crit}(H) = \mathsf{Crit}(H, \Phi) = \varnothing$.

*The observable Φ can be interpreted (*e.g. *using isometries) as follows. Let $\widetilde{q}$ be the closest point to the origin $0 \in \mathring{B}_1$ on the geodesic curve generated by (q,p). Then $\Phi(q,p)$ is the geodesic distance between q and $\widetilde{q}$ together with a sign (positive if going from $\widetilde{q}$ to q goes in the same direction as p and negative otherwise).*

2.2 Wave maps and scattering map

From now on, we also consider a perturbed Hamiltonian $H \in \mathsf{C}^\infty(M)$ with complete flow $\{\varphi_t\}_{t\in\mathbb{R}}$, and suppose for a moment that the pair (H_0, H) is such that the wave maps exist, have common ranges and are invertible:

Assumption 2.6 (Wave maps)**.**

(i) The pointwise limits $W_\pm := \lim_{t\to\pm\infty} \varphi_{-t} \circ \varphi_t^0$ exist on some open sets $\mathcal{D}_\pm \subset M$.

(ii) The maps $W_\pm$ are invertible, with inverses $W_\pm^{-1} : \mathsf{Ran}(W_\pm) \to \mathcal{D}_\pm$.

(iii) The maps $W_\pm$ have common ranges equal to $\mathcal{R}$, i.e. *$\mathsf{Ran}(W_+) = \mathsf{Ran}(W_-) = \mathcal{R}$.*

The functions $W_\pm : \mathcal{D}_\pm \to \mathcal{R}$ are called the wave maps and the condition (ii) is often referred as completeness of the wave maps. Since the flows $\{\varphi_t^0\}_{t\in\mathbb{R}}$ and $\{\varphi_t\}_{t\in\mathbb{R}}$ are groups of diffeomorphisms on M, the wave maps $W_\pm$ verify the intertwining property

$$\big(\varphi_t \circ W_\pm\big)(m_\pm) = \big(W_\pm \circ \varphi_t^0\big)(m_\pm) \quad \text{for all } t \in \mathbb{R} \text{ and } m_\pm \in \mathcal{D}_\pm. \tag{2.5}$$

Due to points (ii) and (iii) of Assumption 2.6 the scattering map

$$S := W_+^{-1} \circ W_-$$

is well defined and invertible from $\mathcal{D}_-$ to $\mathcal{D}_+$. Furthermore, the intertwining property (2.5) implies that S commutes with the free evolution:

$$\big(\varphi_t^0 \circ S\big)(m_-) = \big(S \circ \varphi_t^0\big)(m_-) \quad \text{for all } t \in \mathbb{R} \text{ and } m_- \in \mathcal{D}_-. \tag{2.6}$$

In finite dimension, what precedes admits an interesting formulation (borrowed from [8, Sec. 2.3]) on submanifolds of fixed energy. To see this, let $E \in \mathbb{R}$ be a regular value of H_0, *i.e.* $H_0^{-1}(\{E\}) \cap \mathrm{Crit}(H_0) = \varnothing$. Then, $\Sigma_E^0 := H_0^{-1}(\{E\})$ is a regular submanifold of M of dimension $2n-1$, the family $\big\{\varphi_t^{0,E} := \varphi_t^0|_{\Sigma_E^0}\big\}_{t\in\mathbb{R}}$ is a group of diffeomorphisms on Σ_E^0 and the group action

$$\varphi^{0,E} : \mathbb{R} \times \Sigma_E^0 \to \Sigma_E^0, \quad (t,m) \mapsto \varphi_t^{0,E}(m)$$

is smooth. Now, if $\varphi^{0,E}$ is free and proper, then the quotient (orbit) space $\widetilde{\Sigma}_E^0 := \Sigma_E^0/\mathbb{R}$ is a smooth manifold of dimension $2(n-1)$ and the quotient map $\pi_E^0 : \Sigma_E^0 \to \widetilde{\Sigma}_E^0$ is a submersion [1, Prop. 4.1.23]. Furthermore, there exists a unique symplectic form $\widetilde{\omega}_E^0$ on $\widetilde{\Sigma}_E^0$ such that $(\pi_E^0)^*\widetilde{\omega}_E^0 = \omega|_{\Sigma_E^0}$ (see [1, Thm. 4.3.1 & Ex. 4.3.4(ii)]). If the situation is favourable enough, it may also happen that $\Sigma_E^0 \subset \mathcal{D}_-$ and that the restriction $S_E := S|_{\Sigma_E^0}$ is a diffeomorphism from Σ_E^0 onto Σ_E^0 such that

$$S_E^*\big(\omega|_{\Sigma_E^0}\big) = \omega|_{\Sigma_E^0}. \tag{2.7}$$

In such a case, the map $S_E : \Sigma_E^0 \to \Sigma_E^0$ is equivariant with respect to the action $\varphi^{0,E}$ due to (2.6), and thus induces a diffeomorphism $\widetilde{S}_E : \widetilde{\Sigma}_E^0 \to \widetilde{\Sigma}_E^0$ defined by the relation

$$\pi_E^0 \circ S_E = \widetilde{S}_E \circ \pi_E^0. \tag{2.8}$$

Furthermore, one obtains from (2.7) and (2.8) that

$$(\pi_E^0)^*\big((\widetilde{S}_E)^*\widetilde{\omega}_E^0 - \widetilde{\omega}_E^0\big) = 0,$$

meaning that $\widetilde{S}_E^*\widetilde{\omega}_E^0 = \widetilde{\omega}_E^0$, since π_E^0 is a surjection. This implies that $\widetilde{S}_E$ is a symplectomorphism of $\big(\widetilde{\Sigma}_E^0, \widetilde{\omega}_E^0\big)$. In the case $n = 1$, the above reduction leads to a manifold $\widetilde{\Sigma}_E^0$ of dimension zero, *i.e.* a discrete set of orbits. So, the map $\widetilde{S}_E$ reduces to a permutation map on the discrete set $\widetilde{\Sigma}_E^0$.

The map $\widetilde{S}_E$, called the Poincaré scattering map, will play an important role in Section 4. We refer to [11, 18, 30] and [19] for early works involving the Poincaré scattering map in physics and mathematics literature respectively.

2.3 Completeness of the wave maps

Conditions on the free Hamiltonian H_0 and the potential $V := H - H_0$ guaranteeing the validity of Assumption 2.6 will now be presented. These conditions are natural extensions of the compactness of the support of the potential and the virial condition appearing in the case $\Phi(q,p) = q$, $H_0(q,p) := |p|^2/2$ and $H(q,p) = |p|^2/2 + V(q)$ on $M = T^*\mathbb{R}^n$. As in Section 2.2, we always assume that the Hamiltonians H_0 and H have complete flows $\{\varphi_t^0\}_{t\in\mathbb{R}}$ and $\{\varphi_t\}_{t\in\mathbb{R}}$.

We start below with a result on the domain and the range of the wave maps $W_\pm$. For this, we need to introduce the sets of Φ-bounded trajectories

$$B_\Phi^\pm := \big\{m \in M \mid \exists\, R \geq 0 \text{ such that } \big|\Phi\big(\varphi_{\pm t}(m)\big)\big| \leq R \text{ for all } t \geq 0\big\}.$$

The sets $B_\Phi^\pm$ coincide with the usual sets of bounded trajectories [10, Def. 2.1.1] if the map $|\Phi| : M \to [0,\infty)$ is proper. If it is not the case, the inclusion $m \in B_\Phi^- \cap B_\Phi^+$ does not guarantee that the orbit $\{\varphi_t(m)\}_{t\in\mathbb{R}}$ stays in a compact subset of M (consider for instance the case $M = T^*\mathbb{R}^2$, $\Phi(q,p) = q_1$ and $H(q,p) := |p|^2/2$).

We also need the following assumption on the potential:

Assumption 2.7 (Potential). *The difference $V \equiv H - H_0$ is of bounded support in Φ,* i.e. *there exists a constant $R_V \geq 0$ such that $|\Phi(m)| \leq R_V$ for all $m \in \mathrm{supp}(V)$.*

In explicit situations, Assumption 2.7 can often be relaxed to some condition on the decay at infinity (see for instance [10, Sec. 2.6-2.7], [15], [16], [17, Sec. 3] and [32]).

Theorem 2.8 (Existence of wave maps). *Let H_0 and H satisfy Assumptions 2.1 and 2.7. Then $W_\pm$ exist and are symplectomorphisms from $M \setminus \mathsf{Crit}(H_0, \Phi)$ to $M \setminus B_\Phi^\pm$. Furthermore, one has $H \circ W_\pm = H_0$ on $M \setminus \mathsf{Crit}(H_0, \Phi)$ (and thus $H = H_0 \circ W_\pm^{-1}$ on $M \setminus B_\Phi^\pm$).*

Theorem 2.8 implies Assumptions 2.6(i)-(ii) with $\mathcal{D}_\pm = M \setminus \mathsf{Crit}(H_0, \Phi)$ and $\mathsf{Ran}(W_\pm) = M \setminus B_\Phi^\pm$, but it does not imply Assumption 2.6(iii) since we do not have the equality $\mathsf{Ran}(W_+) = \mathsf{Ran}(W_-)$. Theorem 2.8 also implies that the sets $B_\Phi^\pm$ are closed in M.

Proof. We give the proof for W_+, since the proof for W_- is similar.

(i) Let $K \subset M \setminus \mathsf{Crit}(H_0, \Phi)$ be compact. Then, there exists $T > 0$ such that $\big|\Phi\big(\varphi_t^0(m)\big)\big| > R_V + 1$ for all $t > T$ and $m \in K$. In particular, $\varphi_t^0(K) \cap \mathrm{supp}(V) = \varnothing$ for all $t > T$. Thus, one has $\varphi_t^0 = \varphi_{t-T}^0 \circ \varphi_T^0 = \varphi_{t-T} \circ \varphi_T^0$ on K for all $t > T$, which implies

$$\lim_{t\to\infty} \varphi_{-t} \circ \varphi_t^0 = \lim_{t\to\infty} \varphi_{-t} \circ \varphi_{t-T} \circ \varphi_T^0 = \varphi_{-T} \circ \varphi_T^0$$

on K. Thence, W_+ is a hamiltomorphism on any compact subset of $M \setminus \mathsf{Crit}(H_0, \Phi)$, and thus a symplectomorphism on $M \setminus \mathsf{Crit}(H_0, \Phi)$.

Let $m \in W_+\big(M \setminus \mathsf{Crit}(H_0, \Phi)\big)$. Then, there exist $m_0 \in M \setminus \mathsf{Crit}(H_0, \Phi)$ and $T > 0$ such that $m = W_+(m_0) = \big(\varphi_{-t} \circ \varphi_t^0\big)(m_0)$ for all $t > T$, meaning that $\varphi_t(m) = \varphi_t^0(m_0)$ for all $t > T$. However, since $m_0 \in M \setminus \mathsf{Crit}(H_0, \Phi)$, one has for each $t \in \mathbb{R}$

$$(\nabla H_0)\big(\varphi_t^0(m_0)\big) = (\nabla H_0)(m_0) \neq 0 \quad \text{and} \quad \big|\Phi\big(\varphi_t^0(m_0)\big)\big| \geq \big||t| \cdot |(\nabla H_0)(m_0)| - |\Phi(m_0)|\big|$$

due to (2.1)-(2.2). This implies that $m \in M \setminus B_\Phi^+$.

Assume now that $m \in M \setminus B_\Phi^+$. If $\big|\Phi\big(\varphi_t(m)\big)\big| \geq R_V + 1$ for all $t \geq 0$, one directly obtains $m = W_+(m) \in W_+\big(M \setminus \mathsf{Crit}(H_0, \Phi)\big)$. If not, consider the time $t_0 := \inf\big\{t \geq 0 \mid \big|\Phi\big(\varphi_t(m)\big)\big| > R_V + 1\big\}$ and observe that for each $\varepsilon \in (0, t_0)$

$$\begin{aligned}
(R_V + 1)^2 > \big|\Phi\big(\varphi_{t_0-\varepsilon}(m)\big)\big|^2 &= \Big|\Phi\big(\varphi_{t_0}(m)\big) - \int_0^\varepsilon \mathrm{d}s\, \{\Phi, H\}\big(\varphi_{t_0-s}(m)\big)\Big|^2 \\
&= \big|\Phi\big(\varphi_{t_0}(m)\big) - \varepsilon\,(\nabla H_0)\big(\varphi_{t_0}(m)\big)\big|^2 \\
&= (R_V + 1)^2 - 2\varepsilon\,(\Phi \cdot \nabla H_0)\big(\varphi_{t_0}(m)\big) + \varepsilon^2 \big|(\nabla H_0)\big(\varphi_{t_0}(m)\big)\big|^2.
\end{aligned}$$

So, one has $2(\Phi \cdot \nabla H_0)\big(\varphi_{t_0}(m)\big) > \varepsilon\big|(\nabla H_0)\big(\varphi_{t_0}(m)\big)\big|^2$, which implies $(\nabla H_0)\big(\varphi_{t_0}(m)\big) \neq 0$ and $(\Phi \cdot \nabla H_0)\big(\varphi_{t_0}(m)\big) > 0$. It follows that

$$\frac{\mathrm{d}}{\mathrm{d}t}\big|\Phi\big(\varphi_{t_0+t}(m)\big)\big|^2\Big|_{t=0} = \frac{\mathrm{d}}{\mathrm{d}t}\Big\{(R_V + 1)^2 + 2t(\Phi \cdot \nabla H_0)\big(\varphi_{t_0}(m)\big) + t^2\big|(\nabla H_0)\big(\varphi_{t_0}(m)\big)\big|^2\Big\}\Big|_{t=0} > 0.$$

So, $\varphi_{t_0+t}(m)$ remains out of the support of V for all $t \geq 0$, which implies $\varphi_{t+t_0}(m) = \big(\varphi_t^0 \circ \varphi_{t_0}\big)(m)$ for all $t \geq 0$. To conclude, let $m_0 \in M \setminus \mathsf{Crit}(H_0, \Phi)$ satisfy $\varphi_{t_0}^0(m_0) = \varphi_{t_0}(m)$ (such a m_0 exists, since $\varphi_{t_0}(m) \in M \setminus \mathsf{Crit}(H_0, \Phi)$ and $\varphi_{t_0}^0$ is a diffeomorphism of $M \setminus \mathsf{Crit}(H_0, \Phi)$ onto itself). Then the last formula gives $W_+(m_0) = \lim_{t\to\infty}\big(\varphi_{-t-t_0} \circ \varphi_t^0 \circ \varphi_{t_0}\big)(m) = m$, which implies $m \in W_+\big(M \setminus \mathsf{Crit}(H_0, \Phi)\big)$.

(ii) Take $m \in M \setminus \mathsf{Crit}(H_0, \Phi)$. Then we know from (i) that there exists $T > 0$ such that $\varphi_T^0(m) \notin \mathrm{supp}(V)$ and $W_+(m) = \big(\varphi_{-T} \circ \varphi_T^0\big)(m)$. This implies that $\big(H \circ W_+\big)(m) = H_0(m)$. □

In order to define the scattering map $S \equiv W_+^{-1} \circ W_-$, the ranges of the wave maps $W_\pm$ have to be equal (see Assumption 2.6(iii)). We present in the sequel two methods to prove this equality. The first one hinges on a virial identity, while the second one consists in showing that the symmetric difference of the ranges of $W_\pm$ is of (Liouville) measure zero. In the second case, completeness holds upon removing from M a relatively abstract set; namely, the preimage of a set of measure zero. In classical mechanics, this type of completeness is sometimes referred as asymptotic completeness [34, Sec. 3.4].

In the standard case, the virial method relies on the following observation: if there exists $\delta > 0$ such that

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\big(|\Phi|^2 \circ \varphi_t\big)(m) \equiv \big(\big\{\big\{|\Phi|^2, H\big\}, H\big\} \circ \varphi_t\big)(m) > \delta \quad \text{for all } t \in \mathbb{R} \text{ and } m \in M,$$

then $\lim_{|t|\to\infty} \big(|\Phi|^2 \circ \varphi_t\big)(m) = +\infty$ for all $m \in M$, and so $B_\Phi^\pm = \varnothing$. Accordingly, it is sufficient to prove that $\big\{\big\{|\Phi|^2, H\big\}, H\big\} > \delta$ on M to get, under Assumptions 2.1 and 2.7, the completeness of the wave maps. Now, a direct calculation shows that the expression for $\big\{\big\{|\Phi|^2, H\big\}, H\big\}$ (the virial identity) is

$$\frac{1}{2}\big\{\big\{|\Phi|^2, H\big\}, H\big\} = |\nabla H_0|^2 + |\{\Phi, V\}|^2 + \Phi \cdot \big\{\{\Phi, V\}, V\big\} + \big\{\Phi \cdot \{\Phi, V\}, H_0\big\} + \{\Phi \cdot \nabla H_0, V\}. \quad (2.9)$$

At this level of generality, finding scattering systems (M, H_0, H) for which this expression is bounded away from zero is rather daunting. However, if one assumes that $\{\Phi, V\} = 0$ (as in the standard case where V depends only on the position $\Phi(q,p) = q$), then Formula (2.9) reduces to the much more sympathetic equation:

$$\big\{\Phi \cdot \nabla H_0, H\big\} = |\nabla H_0|^2 + \Phi \cdot \big\{\nabla H_0, V\big\}.$$

Lemma 2.10 below provides conditions under which one recovers this simplified situation. For it, we need the following:

Assumption 2.9. *(i) H_0 is boundedly preserved by the flow of H,* i.e. *for each $m \in M$ there exists a constant $\mathsf{c}_m \geq 0$ such that $\big|H_0\big(\varphi_t(m)\big) - H_0(m)\big| \leq \mathsf{c}_m$ for all $t \in \mathbb{R}$.*

(ii) There exists an increasing function $\rho : [0,\infty) \to [0,\infty)$ with $\lim_{R\to\infty} \rho(R) = +\infty$ such that $|(\nabla H_0)(m)| \geq R$ implies $|H_0(m)| \geq \rho(R)$ for all $m \in M$ and $R \geq 0$.

If V is bounded, then (i) holds automatically, since $\big|H_0\big(\varphi_t(m)\big) - H_0(m)\big| = \big|V\big(\varphi_t(m)\big) - V(m)\big|$. On the other hand, (i) also holds for some unbounded V's. For example, if $H_0 \geq 0$ and V is bounded from below by $V_0 \in \mathbb{R}$, then (i) is verified with $\mathsf{c}_m = H_0(m) + H(m) - V_0$.

Lemma 2.10 (Completeness of wave maps)**.** *Let H_0 and H satisfy Assumptions 2.1 and 2.7. Suppose either that $\{\Phi, V\} = 0$ or that Assumption 2.9 holds. Assume there exists $\delta > 0$ such that $\{\Phi \cdot \nabla H_0, H\}(m) > \delta$ for all $m \in M$. Then, $B_\Phi^\pm = \varnothing$ and the maps*

$$W_\pm : M \setminus \mathsf{Crit}(H_0, \Phi) \to M \quad \text{and} \quad S = W_+^{-1} \circ W_- : M \setminus \mathsf{Crit}(H_0, \Phi) \to M \setminus \mathsf{Crit}(H_0, \Phi)$$

are well defined symplectomorphisms. In particular, Assumptions 2.6(i)-(iii) hold on the submanifold $M \setminus \mathsf{Crit}(H_0, \Phi)$.

Proof. If $\{\Phi, V\} = 0$, then the claim follows directly from the observations made before Assumption 2.9.

So, suppose that Assumption 2.9 holds. Since $\{\Phi \cdot \nabla H_0, H\} > \delta$, we have $\frac{\mathrm{d}}{\mathrm{d}t}(\Phi \cdot \nabla H_0)\big(\varphi_t(m)\big) > \delta$ for all $t \in \mathbb{R}$ and $m \in M$. In particular, there exist for all $m \in M$ and all $R \geq 0$ times $t_\pm \in \mathbb{R}_\pm$ such that either $\big|\Phi\big(\varphi_{t_\pm}(m)\big)\big| > R$ or $\big|(\nabla H_0)\big(\varphi_{t_\pm}(m)\big)\big| > R$. However, we know by Assumption 2.9(ii) that

if $\big|(\nabla H_0)\big(\varphi_{t_\pm}(m)\big)\big| > R$ then $\big|H_0\big(\varphi_{t_\pm}(m)\big)\big| > \rho(R)$. We also know from Assumption 2.9(i) that there exists $c_m \geq 0$ such that $\big|H_0\big(\varphi_{t_\pm}(m)\big) - H_0(m)\big| \leq c_m$. This implies that

$$\rho(R) < \big|H_0\big(\varphi_{t_\pm}(m)\big)\big| = \big|H_0\big(\varphi_{t_\pm}(m)\big) - H_0(m) + H_0(m)\big| \leq c_m + |H_0(m)|,$$

which is a contradiction since $\rho(R)$ is not bounded for R big enough. Thus, we must have the following: for all $m \in M$ and all $R \geq 0$ such that $\rho(R) \geq C_m + H_0(m)$, there exist times $t_\pm \in \mathbb{R}_\pm$ such that $\big|\Phi\big(\varphi_{t_\pm}(m)\big)\big| > R$. In particular, we have that $\lim_{|t|\to\infty} \big(|\Phi|^2 \circ \varphi_t\big)(m) = +\infty$ for all $m \in M$, which implies the claim. □

Let $U \subset \mathbb{R}$ be an open set such that $H_0^{-1}(U) \cap \mathsf{Crit}(H_0, \Phi) = \varnothing$. Then, $H_0^{-1}(U)$ is a submanifold of M preserved by the flow of H_0. But in general, $H_0^{-1}(U)$ is not preserved by the flow of H. However, if Theorem 2.8 applies, one has $H \circ W_\pm = H_0$ and $W_\pm\big(H_0^{-1}(U)\big) = H^{-1}(U) \setminus B_\Phi^\pm$ is also a submanifold of M. Therefore, the following corollary is a consequence of Theorem 2.8 and Lemma 2.10.

Corollary 2.11. *Let H_0 and H satisfy Assumptions 2.1 and 2.7. Suppose either that $\{\Phi, V\} = 0$ or that Assumption 2.9 holds. Let $U \subset \mathbb{R}$ be an open set such that*

(i) $H_0^{-1}(U) \cap \mathsf{Crit}(H_0, \Phi) = \varnothing$,

(ii) there exists $\delta > 0$ such that $\big\{\Phi \cdot \nabla H_0, H\big\}(m) > \delta$ for all $m \in H_0^{-1}(U)$.

Then, the sets $H_0^{-1}(U)$ and $H^{-1}(U)$ are submanifolds of M, and the maps

$$W_\pm : H_0^{-1}(U) \to H^{-1}(U) \quad \text{and} \quad S = W_+^{-1} \circ W_- : H_0^{-1}(U) \to H_0^{-1}(U)$$

are well defined symplectomorphisms. In particular, Assumptions 2.6(i)-(iii) hold on the submanifold $H_0^{-1}(U)$.

Before pursuing the Examples 2.3-2.5 of Section 2.1, we give a last result on scattering theory sometimes referred to as asymptotic completeness. It is is inspired by [34, Thm. 3.4.7(c)] (in the case $\Phi(q,p) = q$ and $H(q,p) = |p|^2/2 + V(q)$ on $M = T^*\mathbb{R}^n$) and basically states that the ranges of $W_\pm$ are equal up to a set of Liouville measure zero. We recall that the Liouville measure of a Borel subset $U \subset M$, with M of finite dimension, is given by

$$\mathrm{m}_\omega(U) := \int_U \frac{\omega^n}{n!}.$$

We also recall that the symmetric difference of sets X, Y is $X \triangle Y := (X \setminus Y) \cup (Y \setminus X)$.

Proposition 2.12 (Asymptotic completeness of wave maps)**.** *Assume that M has finite dimension. Let H_0 and H satisfy Assumptions 2.1 and 2.7. Suppose that for each $k \in \mathbb{N}$ the set*

$$A_k := \big\{m \in M \mid |\Phi(m)| \leq k \text{ and } |H(m)| \leq k\big\}$$

satisfies $\mathrm{m}_\omega(A_k) < \infty$. Then, $\mathrm{m}_\omega\big(\mathsf{Ran}(W_+) \triangle \mathsf{Ran}(W_-)\big) = 0$.

In the case $\Phi(q,p) = q$ and $H(q,p) = |p|^2/2 + V(q)$ on $M = T^*\mathbb{R}^n$, the condition $\mathrm{m}_\omega(A_k) < \infty$, is satisfied, for instance, if V is bounded.

Proof. For each $k \in \mathbb{N}$, let $A_k^\pm := \bigcap_{\pm t \geq 0} \varphi_t(A_k)$. Then, simple calculations using the identity $H \circ \varphi_t = H$ show that $B_\Phi^\pm = \bigcup_{k\in\mathbb{N}} A_k^\pm$. Furthermore, one deduce from Schwarzschild's capture theorem [2, Thm. 7.1.15] that $\mathrm{m}_\omega(A_k^+ \cap A_k^-) = \mathrm{m}_\omega(A_k^+) = \mathrm{m}_\omega(A_k^-)$ for each $k \in \mathbb{N}$. Therefore, $m_\omega\big(A_k^\pm \setminus A_k^\mp\big) = 0$ for each $k \in \mathbb{N}$, and one gets from Theorem 2.8 and the sub-additivity of m_ω that

$$m_\omega\big(\mathsf{Ran}(W_+) \setminus \mathsf{Ran}(W_-)\big) = m_\omega\big(B_\Phi^- \setminus B_\Phi^+\big) \leq \sum_{k\in\mathbb{N}} m_\omega\big(A_k^- \setminus B_\Phi^+\big) \leq \sum_{k\in\mathbb{N}} m_\omega\big(A_k^- \setminus A_k^+\big) = 0.$$

Repeating the argument with W_+ and W_- interchanged yields the conclusion. □

Example 2.13 ($H_0(q,p) = h(p)$, continued)**.** *Let $V \in \mathsf{C}^\infty_{\mathsf{c}}(\mathbb{R}^n;\mathbb{R})$ be a C^∞ function with compact support and let $H \in \mathsf{C}^\infty(M;\mathbb{R})$ be the perturbed Hamiltonian given by $H(q,p) := h(p) + V(q)$. To show the completeness of the corresponding vector field X_H, one has to impose some condition on h. So, we assume that $|(\nabla h)(p)| \leq \alpha\, \mathrm{e}^{\beta\langle p\rangle}$ for some constants $\alpha, \beta \geq 0$ and all $p \in \mathbb{R}^n$, but we also note that many other cases can be covered (such as when h is a proper map). Under this assumption, the completeness of X_H follows from [1, Prop. 2.1.20] with the (proper and C^∞) function $M \ni (q,p) \mapsto \mathrm{e}^{\beta\langle p\rangle} + \langle q\rangle \in \mathbb{R}$. Since Assumption 2.7 is satisfied, Theorem 2.8 implies that the wave maps $W_\pm$ exist and are symplectomorphisms from $\mathbb{R}^n \times \mathbb{R}^n \setminus (\nabla h)^{-1}(\{0\})$ to $M \setminus B^\pm_\Phi$. Furthermore, the commutation $\{\Phi, V\} = 0$ implies that*

$$\big\{\Phi \cdot \nabla H_0, H\big\}(q,p) = |(\nabla h)(p)|^2 - q^{\mathsf{T}} \cdot (\mathsf{Hess}\, h)(p)\,(\nabla V)(q) \geq |(\nabla h)(p)|^2 - n\, \mathsf{c}_V \max_{1\leq i,j\leq n} \big|(\partial_i\partial_j h)(p)\big|,$$

where $(\mathsf{Hess}\, h)(p)$ is the Hessian matrix of h at p and $\mathsf{c}_V := \sup_{q\in\mathbb{R}^n} |q| \cdot |(\nabla V)(q)|$. Therefore, if there exist continuous functions $g_1, g_2 : \mathsf{Ran}(h) \to [0,\infty)$ such that

$$|(\nabla h)(p)|^2 \geq g_1\big(h(p)\big) \quad \text{and} \quad \max_{1\leq i,j\leq n} \big|(\partial_i\partial_j h)(p)\big| \leq g_2\big(h(p)\big) \quad \text{for all } p \in \mathbb{R}^n$$

(which occurs for instance when $h(p) = |p|^2/2$ or $h(p) = \sqrt{1+p^2}$), then the open sets

$$U_\delta := \big\{x \in \mathbb{R} \mid g_1(x) - n\, \mathsf{c}_V g_2(x) > \delta\big\}, \quad \delta > 0,$$

satisfy the conditions (i) and (ii) of Corollary 2.11. Thus, the maps

$$W_\pm : H_0^{-1}(U_\delta) \to H^{-1}(U_\delta) \quad \text{and} \quad S = W_+^{-1} \circ W_- : H_0^{-1}(U_\delta) \to H_0^{-1}(U_\delta)$$

are well defined symplectomorphisms, and Assumption 2.6 holds on the submanifold $H_0^{-1}(U_\delta)$.

Example 2.14 (Particle in a tube, continued)**.** *Let $V \in \mathsf{C}^\infty_{\mathsf{c}}(\Omega;\mathbb{R})$ be a C^∞ function with compact support and let $H \in \mathsf{C}^\infty(M;\mathbb{R})$ be the perturbed Hamiltonian given by $H(q,p) := H_0(q,p) + V(q)$. Then, Assumption 2.7 is satisfied and we know from [1, Prop. 2.1.20] (once more applied with the function (2.4)) that X_H is complete. So, Theorem 2.8 implies that the wave maps $W_\pm$ exist and are symplectomorphisms from $\Omega \times \big(\mathbb{R}\setminus\{0\} \times \mathbb{R}^n\big)$ to $M \setminus B^\pm_\Phi$. Now, we cannot apply Corollary 2.11 to obtain the identity of the ranges of $W_\pm$, since the virial identity*

$$\big\{\Phi \cdot \nabla H_0, H\big\}(q,p) = p_1^2 - q^1\big(\partial_1 V\big)(q)$$

does not involve observables comparable with the free energy $H_0(q,p)$. Instead, we set $K_V := \sup_{q\in\Omega} \big|q^1\big(\partial_1 V\big)(q)\big|$ and define the open set

$$M_\delta := \big\{(q,p) \in M \mid |(\nabla H_0)(q,p)|^2 > K_V + \delta\big\}, \quad \delta > 0,$$

Then, φ_t^0 is a diffeomorphism on M_δ for each $t \in \mathbb{R}$ and $\big|\big\{\Phi \cdot \nabla H_0, H\big\}\big| > \delta$ on M_δ. So, for each $(q,p) \in M_\delta$ there exists $T > 0$ such that $W_-(q,p) = \big(\varphi_T \circ \varphi^0_{-T}\big)(q,p)$ and

$$\lim_{|t|\to\infty} \big(|\Phi|^2 \circ \varphi_t \circ W_-\big)(q,p) = \lim_{|t'|\to\infty} \big(|\Phi|^2 \circ \varphi_{t'} \circ \varphi^0_{-T}\big)(q,p) = +\infty.$$

This implies that $W_-(M_\delta) \subset M \setminus \big\{B^-_\Phi \cup B^+_\Phi\big\}$, and thus

$$S := W_+^{-1} \circ W_- : M_\delta \to \big(W_+^{-1} \circ W_-\big)(M_\delta)$$

is a well defined symplectomorphism.

Example 2.15 (Poincaré ball, continued)**.** *Let $V \in \mathsf{C}^\infty(\mathring{B}_1;\mathbb{R})$ with $\mathrm{supp}(V) \subset B_{R_V}$ for some $R_V \in [0,1)$ and let $H \in \mathsf{C}^\infty(M;\mathbb{R})$ be the perturbed Hamiltonian given by $H(q,p) := H_0(q,p)+V(q)$. Then, Assumption 2.7 is satisfied (since $|\Phi| \leq \tanh^{-1}(2R_V)$ on $\mathrm{supp}(V)\times\mathbb{R}^n$) and we know from Gordon's Theorem [13] that X_H is complete. So, Theorem 2.8 implies that the wave maps $W_\pm$ exist and are symplectomorphisms from $\mathring{B}_1 \times \mathbb{R}^n \setminus \{0\}$ to $M \setminus B_\Phi^\pm$. Now, direct calculations using the inclusion $\mathrm{supp}(V) \subset B_{R_V}$ and the bound $|\Phi| \leq \tanh^{-1}(2R_V)$ on $\mathrm{supp}(V)\times\mathbb{R}^n$ show that*

$$\big\{\Phi\cdot\nabla H_0, H\big\} = 2H_0 + \sqrt{2H_0}\big\{\Phi, V\big\} + \Phi\big\{\sqrt{2H_0}, V\big\}$$

with $\big|\sqrt{2H_0}\big\{\Phi,V\big\}\big|$ and $\big|\Phi\big\{\sqrt{2H_0},V\big\}\big|$ bounded on M. Therefore, there exists a constant $K_V \geq 0$ such that $\big\{\Phi\cdot\nabla H_0, H\big\} \geq 2H_0 - K_V$ on M. Moreover, Assumption 2.9 is satisfied due to the boundedness of V and the identity $\nabla H_0 = \sqrt{2H_0}$. So, the open intervals $U_\delta := \big(\frac{K_V+\delta}{2},\infty\big)$, $\delta>0$, satisfy the conditions (i) and (ii) of Corollary 2.11, and the maps

$$W_\pm : H_0^{-1}(U_\delta) \to H^{-1}(U_\delta) \quad \text{and} \quad S = W_+^{-1}\circ W_- : H_0^{-1}(U_\delta) \to H_0^{-1}(U_\delta)$$

are well defined symplectomorphisms. In particular, Assumption 2.6 holds on the submanifold $H_0^{-1}(U_\delta)$.

3 Time delay in classical scattering theory

In this section, we consider for general scattering systems (M, H_0, H) the symmetrised time delay defined in terms of sojourn times in the dilated regions $\Phi^{-1}(B_r)$. Under appropriate assumptions, we prove its existence and relate it to the time of arrival T defined in (2.3). When the scattering process preserves the norm of the velocity observable ∇H_0, we show that the original (unsymmetrised) time delay also exists and coincides with the symmetrised time delay. We refer to [5, 7], [6, Sec. II.B], [9, Sec. 4.1], [12, Sec. III], [20, Ch. 10], [26, 27] and [34, Sec. 3.4] for previous works on classical time delay for $H_0(q,p) = |p|^2/2$ and $H(q,p) = |p|^2/2 + V(q)$ on $M = T^*\mathbb{R}^n$.

So, let

$$T_r^0(m_-) := \int_{\mathbb{R}} \mathrm{d}t\, \big(\chi_r^\Phi \circ \varphi_t^0\big)(m_-)$$

be the sojourn time in the region $\Phi^{-1}(B_r)$ of the free trajectory starting from $m_- \in \mathcal{D}_-$ at time $t=0$, and let

$$T_r(m_-) := \int_{\mathbb{R}} \mathrm{d}t\, \big(\chi_r^\Phi \circ \varphi_t \circ W_-\big)(m_-)$$

be the corresponding sojourn time of the perturbed trajectory starting from $W_-(m_-)$ at time $t=0$. The free sojourn time $T_r^0(m_-)$ is finite for each $m_- \in \mathcal{D}_- \setminus \mathrm{Crit}(H_0,\Phi)$ due to Equation (2.1). The finiteness of the perturbed sojourn time $T_r(m_-)$ is shown in Lemma 3.1 below under some additional assumptions. Under these assumptions, one can define the symmetrised time delay in $\Phi^{-1}(B_r)$ for the scattering system (M,H_0,H) with starting point m_- :

$$\tau_r(m_-) := T_r(m_-) - \frac{1}{2}\big\{T_r^0(m_-) + \big(T_r^0\circ S\big)(m_-)\big\}.$$

The time $\tau_r(m_-)$ can be interpreted as the time spent the perturbed trajectory $\big\{\big(\varphi_t\circ W_-\big)(m_-)\big\}_{t\in\mathbb{R}}$ within $\Phi^{-1}(B_r)$ minus the time spent by the corresponding free trajectory (before and after scattering) within the same region.

In the next lemma, we use the auxiliary time

$$\tau_r^{\mathrm{free}}(m_-) := \frac{1}{2}\int_0^\infty \mathrm{d}t\,\big\{\big(\chi_r^\Phi\circ\varphi_t^0\circ S\big)(m_-) - \big(\chi_r^\Phi\circ\varphi_{-t}^0\circ S\big)(m_-) - \big(\chi_r^\Phi\circ\varphi_t^0\big)(m_-) + \big(\chi_r^\Phi\circ\varphi_{-t}^0\big)(m_-)\big\}, \tag{3.1}$$

which is finite for all $m_- \in \mathcal{D}_-$ due to Theorem 2.2. The definition of τ_r^{free} is inspired by a similar definition in the context of quantum scattering theory [29, Sec. 4].

Lemma 3.1. *Let H_0 and H satisfy Assumptions 2.1 and 2.6, and let $m_- \in \mathcal{D}_- \setminus \mathsf{Crit}(H_0, \Phi)$ satisfy $S(m_-) \notin \mathsf{Crit}(H_0, \Phi)$. Suppose also that there exist functions $g_\pm \in \mathsf{L}^1(\mathbb{R}_\pm, \mathrm{d}t)$ such that*

$$\big|\big(\chi_r^\Phi \circ W_- - \chi_r^\Phi\big)\big(\varphi_t^0(m_-)\big)\big| \leq g_-(t) \quad \text{for all } r > 0 \text{ and } t \in \mathbb{R}_- \tag{3.2}$$

and

$$\big|\big(\chi_r^\Phi \circ W_+ - \chi_r^\Phi\big)\big((S \circ \varphi_t^0)(m_-)\big)\big| \leq g_+(t) \quad \text{for all } r > 0 \text{ and } t \in \mathbb{R}_+. \tag{3.3}$$

Then, $T_r(m_-)$ is finite for each $r > 0$, and

$$\lim_{r\to\infty} \big\{\tau_r(m_-) - \tau_r^{\text{free}}(m_-)\big\} = 0.$$

Before moving on to the proof of the lemma, we make a digression to show that the conditions (3.2)-(3.3) are automatically verified if Assumption 2.7 holds:

Remark 3.2. *If Assumptions 2.1, 2.6 and 2.7 hold, then we know from the proof of Theorem 2.8 that there exists $T > 0$ such that $\big(W_+ \circ S\big)(m_-) = \big(\varphi_{-T} \circ \varphi_T^0 \circ S\big)(m_-)$ and $\big(S \circ \varphi_t^0\big)(m_-) = \big(\varphi_{t-T} \circ \varphi_T^0 \circ S\big)(m_-)$ for all $t > T$. This implies for all $t > T$ that*

$$\big(W_+ \circ S \circ \varphi_t^0\big)(m_-) = \big(\varphi_t \circ W_+ \circ S\big)(m_-) = \big(\varphi_{t-T} \circ \varphi_T^0 \circ S\big)(m_-) = \big(S \circ \varphi_t^0\big)(m_-),$$

and thus (3.3) *is satisfied for some g_+ of compact support. So, both* (3.2) *and* (3.3) *hold, since a similar argument applies to* (3.2).

Proof of Lemma 3.1. Direct computations using the identities

$$\big(\varphi_t \circ W_-\big)(m_-) = \big(W_- \circ \varphi_t^0\big)(m_-) = \big(W_+ \circ S \circ \varphi_t^0\big)(m_-)$$

imply that

$$\begin{aligned} I_r(m_-) &:= T_r(m_-) - \frac{1}{2}\big\{T_r^0(m) + \big(T_r^0 \circ S\big)(m_-)\big\} - \tau_r^{\text{free}}(m_-) \\ &= \int_{\mathbb{R}_+} \mathrm{d}t\, \big(\chi_r^\Phi \circ W_+ - \chi_r^\Phi\big)\big((S \circ \varphi_t^0)(m_-)\big) + \int_{\mathbb{R}_-} \mathrm{d}t\, \big(\chi_r^\Phi \circ W_- - \chi_r^\Phi\big)\big(\varphi_t^0(m_-)\big). \end{aligned} \tag{3.4}$$

It follows by (3.2) and (3.3) that

$$|I_r(m_-)| \leq \int_{\mathbb{R}_+} \mathrm{d}t\, g_+(t) + \int_{\mathbb{R}_-} \mathrm{d}t\, g_-(t) < \infty,$$

and thus $|I_r(m_-)|$ is bounded by a constant independent of r. So, $T_r(m_-)$ is finite for each $r > 0$, since all the other terms of (3.4) are finite for each $r > 0$. Moreover, one obtains that $\lim_{r\to\infty} I_r(m_-) = 0$ by using Lebesgue's dominated convergence theorem and the fact that $\lim_{r\to\infty} \chi_r^\Phi(m) = 1$ for each $m \in M$. □

The next theorem shows the existence of the symmetrised time delay $\tau_r(m_-)$ as $r \to \infty$. It is a direct consequence of Definition (3.1), Lemma 3.1 and Theorem 2.2.

Theorem 3.3 (Symmetrised time delay)**.** *Let H_0 and H satisfy Assumptions 2.1 and 2.6, and let $m_- \in \mathcal{D}_- \setminus \mathsf{Crit}(H_0, \Phi)$ satisfy $S(m_-) \notin \mathsf{Crit}(H_0, \Phi)$ and* (3.2)-(3.3)*. Then, one has*

$$\lim_{r\to\infty} \tau_r(m_-) = T(m_-) - (T \circ S)(m_-). \tag{3.5}$$

Taking into account the definition (2.3) of T, one can rewrite (3.5) as

$$\lim_{r\to\infty} \tau_r(m_-) = \frac{\Phi(m_-)\cdot(\nabla H_0)(m_-)}{|(\nabla H_0)(m_-)|^2} - \frac{(\Phi\circ S)(m_-)\cdot(\nabla H_0\circ S)(m_-)}{|(\nabla H_0\circ S)(m_-)|^2}.$$

Remark 3.4. *It is worth making a couple of observations on the result of Theorem 3.3:*

(i) For fixed $r > 0$, the l.h.s. of Formula (3.5) *is equal to the symmetrised time delay in $\Phi^{-1}(B_r)$ for the scattering system (M, H_0, H) with starting point m_-. On the other hand, the r.h.s. of Formula* (3.5) *is equal to the arrival time $-(T\circ S)(m_-)$ of the particle after scattering minus the arrival time $-T(m_-)$ of the particle before scattering. Therefore, Formula* (3.5) *shows in a very general set-up that this difference of arrival times is equal to the limit of the symmetrised time delay in $\Phi^{-1}(B_r)$ as $r\to\infty$.*

(ii) Denote by $\tau(m_-) := \lim_{r\to\infty}\tau_r(m_-)$ the global time delay obtained in Theorem 3.3. Then, the linear evolution $T\circ\varphi_t^0 = T+t$ of T under the free flow φ_t^0, together with the commutation (2.6) *of S with φ_t^0, implies that*

$$\tau(m_-) = \big\{(T - T\circ S)\circ\varphi_t^0\big\}(m_-) = \big(\tau\circ\varphi_t^0\big)(m_-)$$

for all $t\in\mathbb{R}$, meaning that τ is a first integral of the free motion. This property corresponds in the quantum case to the fact that the time delay operator is decomposable in the spectral representation of the free Hamiltonian (see [29, Rem. 4.4]).

(iii) Formula (3.5) *can be considered as classical version of the Eisenbud-Wigner formula of quantum mechanics. Indeed, if one replaces m_- by an appropriate incoming state φ in a Hilbert space $\mathcal{H}$, (H_0, H) by a pair of self-adjoint operators in $\mathcal{H}$, T by a time operator (acting as the differential operator $i\frac{\mathrm{d}}{\mathrm{d}H_0}$ in the spectral representation of H_0) and S by the unitary scattering operator for (H_0, H), one recovers the general Eisenbud-Wigner formula established in Theorem 4.3 of [29]:*

$$\lim_{r\to\infty}\tau_r(\varphi) = \langle\varphi, T\varphi\rangle_{\mathcal{H}} - \langle S\varphi, TS\varphi\rangle_{\mathcal{H}} = -\langle\varphi, S^*[T,S]\varphi\rangle_{\mathcal{H}} = -\left\langle\varphi, iS^*\frac{\mathrm{d}S}{\mathrm{d}H_0}\varphi\right\rangle_{\mathcal{H}}.$$

In the next corollary, we show that the unsymmetrised time delay

$$\tau_r^{\mathrm{in}}(m_-) := T_r(m_-) - T_r^0(m_-)$$

exists and is equal to the symmetrised time delay in the limit $r\to\infty$ if the scattering process preserves the norm of the velocity vector ∇H_0 (the superscript "in", borrowed from [29, Sec. 4], refers to "incoming" time delay). This result is the classical analogue of Theorem 5.4 of [29] in quantum scattering theory. In the proof, we use the notations $\cos(x,y) := \frac{x\cdot y}{|x||y|}$ and $\sin(x,y)^2 := 1-\cos(x,y)^2$ for vectors $x, y\in\mathbb{R}^d$.

Corollary 3.5 (Unsymmetrised time delay)**.** *Let H_0 and H satisfy Assumptions 2.1 and 2.6, and let $m_-\in\mathcal{D}_-\setminus\mathsf{Crit}(H_0,\Phi)$ satisfy* (3.2)-(3.3)*. Suppose also that*

$$|(\nabla H_0)(m_-)|^2 = |(\nabla H_0\circ S)(m_-)|^2. \tag{3.6}$$

Then, one has

$$\lim_{r\to\infty}\tau_r^{\mathrm{in}}(m_-) = \lim_{r\to\infty}\tau_r(m_-) = T(m_-) - (T\circ S)(m_-). \tag{3.7}$$

Note that the assumption $S(m_-) \notin \mathrm{Crit}(H_0, \Phi)$ of Lemma 3.1 and Theorem 3.3 is, here, automatically verified for each $m_- \in \mathcal{D}_- \setminus \mathrm{Crit}(H_0, \Phi)$ due to the hypothesis (3.6).

Proof. The identity

$$\tau_r^{\mathrm{in}}(m_-) = \tau_r(m_-) + \frac{1}{2}\big\{(T_r^0 \circ S)(m_-) - T_r^0(m_-)\big\},$$

together with Theorem 3.3, implies that is enough to show that

$$\lim_{\nu \searrow 0} \big\{ \big(T_{1/\nu}^0 \circ S\big)(m_-) - T_{1/\nu}^0(m_-)\big\} = 0.$$

Now, we know from the proof of [14, Lemma 2.4] that for any $x \in \mathbb{R}^d$ and $y \in \mathbb{R}^d \setminus \{0\}$ one has

$$\int_{\mathbb{R}_+} \mathrm{d}t\, \chi_{1/\nu}(x \pm ty) = \frac{\sqrt{1 - \nu^2 |x|^2 \sin(x,y)^2}}{|y|\nu} \mp \frac{x \cdot y}{|y|^2}$$

if $\nu > 0$ is small enough. So, a direct calculation using Formula (2.1) and the hypothesis (3.6) gives

$$\begin{aligned}
&\big(T_{1/\nu}^0 \circ S\big)(m_-) - T_{1/\nu}^0(m_-) \\
&= \frac{2\sqrt{1 - \nu^2 |(\Phi \circ S)(m_-)|^2 \sin\big((\Phi \circ S)(m_-), (\nabla H_0 \circ S)(m_-)\big)^2}}{|(\nabla H_0 \circ S)(m_-)|\,\nu} \\
&\quad - \frac{2\sqrt{1 - \nu^2 |\Phi(m_-)|^2 \sin\big(\Phi(m_-), (\nabla H_0)(m_-)\big)^2}}{|(\nabla H_0)(m_-)|\,\nu} \\
&= \frac{2}{|(\nabla H_0 \circ S)(m_-)|\,\nu} \Big\{ \sqrt{1 - \nu^2 |(\Phi \circ S)(m_-)|^2 \sin\big((\Phi \circ S)(m_-), (\nabla H_0 \circ S)(m_-)\big)^2} - 1 \Big\} \\
&\quad - \frac{2}{|(\nabla H_0)(m_-)|\,\nu} \Big\{ \sqrt{1 - \nu^2 |\Phi(m_-)|^2 \sin\big(\Phi(m_-), (\nabla H_0)(m_-)\big)^2} - 1 \Big\},
\end{aligned}$$

which implies that

$$\begin{aligned}
&\lim_{\nu \searrow 0} \big\{ \big(T_{1/\nu}^0 \circ S\big)(m_-) - T_{1/\nu}^0(m_-)\big\} \\
&= \frac{2}{|(\nabla H_0 \circ S)(m_-)|} \frac{\mathrm{d}}{\mathrm{d}\nu} \sqrt{1 - \nu^2 |(\Phi \circ S)(m_-)|^2 \sin\big((\Phi \circ S)(m_-), (\nabla H_0 \circ S)(m_-)\big)^2} \Big|_{\nu=0} \\
&\quad - \frac{2}{|(\nabla H_0)(m_-)|} \frac{\mathrm{d}}{\mathrm{d}\nu} \sqrt{1 - \nu^2 |\Phi(m_-)|^2 \sin\big(\Phi(m_-), (\nabla H_0)(m_-)\big)^2} \Big|_{\nu=0} \\
&= 0 - 0.
\end{aligned}$$

□

Taking into account the definition (2.3) of T and the hypothesis (3.6), one can rewrite (3.7) as

$$\lim_{r \to \infty} \tau_r^{\mathrm{in}}(m_-) = \lim_{r \to \infty} \tau_r(m_-) = \frac{\Phi(m_-) \cdot (\nabla H_0)(m_-) - (\Phi \circ S)(m_-) \cdot (\nabla H_0 \circ S)(m_-)}{|(\nabla H_0)(m_-)|^2}.$$

Remark 3.6. *In general, one cannot expect the existence of the unsymmetrised time delay as $r \to \infty$, since the sojourn times in regions defined in terms of Φ have no reason to be comparable before and after scattering (even though S commutes with φ_t^0 !). This occurs only in particular situations, as when the scattering process preserves the norm of the velocity vector ∇H_0. This is in fact exactly what tells us Corollary 3.5: if the scattering process preserves $|\nabla H_0|$, then the unsymmetrised time delay also exists and is equal to the symmetrised time delay in the limit $r \to \infty$. We refer to the Examples 3.7 and 3.8 below for an illustration of this observation.*

Example 3.7 ($H_0(q,p) = h(p)$, continued)**.** *We know that Assumptions 2.1, 2.6 and 2.7 hold on the manifold $H_0^{-1}(U_\delta)$, with $S : H_0^{-1}(U_\delta) \to H_0^{-1}(U_\delta)$ (see Example 2.13). It follows that each $(q_-,p^-) \in H_0^{-1}(U_\delta)$ satisfy $S(q_-,p^-) \notin \mathsf{Crit}(H_0,\Phi)$ and* (3.2)-(3.3) *(see Remark 3.2). So, Theorem 3.3 applies, and the global time delay exists and satisfies*

$$\lim_{r\to\infty} \tau_r(q_-,p^-) = T(q_-,p^-) - T(q_+,p^+) = \frac{q_- \cdot (\nabla h)(p^-)}{|(\nabla h)(p^-)|^2} - \frac{q_+ \cdot (\nabla h)(p^+)}{|(\nabla h)(p^+)|^2},$$

where $(q_+,p^+) := S(q_-,p^-)$. Now, if there exists a diffeomorphism $h_0 : (0,\infty) \to \mathsf{Ran}(h_0)$ such that $h(p) = h_0(p^2)$ for all $p \in \mathbb{R}^n$ (such as when $h(p) = p^2/2$), then $|(\nabla h)(p)|^2 = \big(f \circ h\big)(p)$ with $f \in \mathsf{C}^\infty\big(\mathsf{Ran}(h_0)\big)$ given by $f(x) := 4h_0^{-1}(x)\big|h_0'\big(h_0^{-1}(x)\big)\big|^2$. Therefore, one has for any $(q_-,p^-) \in H_0^{-1}(U_\delta)$

$$|(\nabla H_0)(q_-,p^-)|^2 = \big(f \circ H_0\big)(q_-,p^-) = \big(f \circ H_0 \circ S\big)(q_-,p^-) = |(\nabla H_0 \circ S)(q_-,p^-)|^2$$

due to the identities $H \circ W_\pm = H_0$ and $H = H_0 \circ W_\pm^{-1}$ of Theorem 2.8. So, Corollary 3.5 applies, and the unsymmetrised time delay exists and satisfies

$$\lim_{r\to\infty} \tau_r^{\mathrm{in}}(q_-,p^-) = \lim_{r\to\infty} \tau_r(q_-,p^-) = \frac{q_- \cdot (\nabla h)(p^-) - q_+ \cdot (\nabla h)(p^+)}{|(\nabla h)(p^-)|^2}.$$

Example 3.8 (Particle in a tube, the end)**.** *We know that Assumptions 2.1 and 2.7 hold on M_δ and that $S : M_\delta \to \big(W_+^{-1} \circ W_-\big)(M_\delta)$ has the required properties (see Example 2.14). It follows that each $(q_-,p^-) \in M_\delta$ satisfy $S(q_-,p^-) \notin \mathsf{Crit}(H_0,\Phi)$ and* (3.2)-(3.3) *(see Remark 3.2). So, Theorem 3.3 applies and the global time delay in the tube exists and satisfies*

$$\lim_{r\to\infty} \tau_r(q_-,p^-) = T(q_-,p^-) - T(q_+,p^+) = \frac{q_-^1 p_1^-}{(p_1^-)^2} - \frac{q_+^1 p_1^+}{(p_1^+)^2},$$

where $(q_+,p^+) := S(q_-,p^-)$. Note that although the scattering process preserves the free energy H_0, it does not preserve the norm of the longitudinal momentum alone since rearrangements between the transverse and longitudinal momenta occur during the scattering. So, we do not have $(p_1^-)^2 \neq (p_1^+)^2$ in general, and thus (in agreement with Corollary 3.5) the unsymmetrised time delay has no reason to exist.

Example 3.9 (Poincaré ball, continued)**.** *We know that Assumptions 2.1, 2.6 and 2.7 hold on the manifold $H_0^{-1}(U_\delta)$, with $S : H_0^{-1}(U_\delta) \to H_0^{-1}(U_\delta)$ (see Example 2.15). Furthermore, one has for each $(q_-,p^-) \in H_0^{-1}(U_\delta)$*

$$|(\nabla H_0)(q_-,p^-)|^2 = 2H_0(q_-,p^-) = 2(H_0 \circ S)(q_-,p^-) = |(\nabla H_0 \circ S)(q_-,p^-)|^2.$$

So, Corollary 3.5 applies, and both time delays exist and satisfy

$$\begin{aligned}
\lim_{r\to\infty} \tau_r^{\mathrm{in}}(q_-,p^-) = \lim_{r\to\infty} \tau_r(q_-,p^-) &= T(q_-,p^-) - T(q_+,p^+) \\
&= \frac{\Phi(q_-,p^-) - \Phi(q_+,p^+)}{\sqrt{2H_0(q_-,p^-)}} \\
&= \frac{2\left\{\tanh^{-1}\left(\frac{2(p^-\cdot q_-)}{|p^-|(1+|q_-|^2)}\right) - \tanh^{-1}\left(\frac{2(p^+\cdot q_+)}{|p^+|(1+|q_+|^2)}\right)\right\}}{|p^-|(1-|q_-|^2)},
\end{aligned}$$

with $(q_+,p^+) := S(q_-,p^-)$.

4 Calabi invariant of the Poincaré scattering map

In this section, we relate the Calabi morphism (evaluated at the Poincaré scattering map) to the time delay by combining the results of Section 3 with the ones of [8]. As in the previous sections, we always assume that the Hamiltonians H_0 and H have complete flows $\{\varphi_t^0\}_{t\in\mathbb{R}}$ and $\{\varphi_t\}_{t\in\mathbb{R}}$.

So, let $E \in \mathbb{R}$ be such that $H_0^{-1}(\{E\}) \cap \mathrm{Crit}(H_0, \Phi) = \varnothing$. Then, $\Sigma_E^0 := H_0^{-1}(\{E\})$ is a regular submanifold of M of dimension $2n-1$, and the map

$$\Psi_E : \Sigma_E^0 \to \mathbb{R}, \quad m \mapsto (\Phi \cdot \nabla H_0)(m)$$

is C^∞. Furthermore, for each $\alpha \in \mathbb{R}$, the set $\Gamma_{E,\alpha} := \Psi_E^{-1}(\{\alpha\}) \subset \Sigma_E^0$ satisfies the following:

Lemma 4.1 (Transversal section)**.** *Let H_0 satisfy Assumption 2.1 and take $E \in \mathbb{R}$ such that $H_0^{-1}(\{E\}) \cap \mathrm{Crit}(H_0, \Phi) = \varnothing$. Then, for each $\alpha \in \mathbb{R}$, the set $\Gamma_{E,\alpha}$ is a regular submanifold of Σ_E^0 of dimension $2(n-1)$ such that*

(a) $X_{H_0}(m) \notin T_m\Gamma_{E,\alpha}$ for all $m \in \Gamma_{E,\alpha}$,

(b) for all $m \in \Sigma_E^0$, there exists a unique $m_0 = m_0(m) \in \Gamma_{E,\alpha}$ and a unique $t_0 = t_0(m) \in \mathbb{R}$ such that $m = \varphi_{t_0}^0(m_0)$.

Note that the first two assertions imply that $\Gamma_{E,\alpha}$ is (in Σ_E^0) a local transversal section of the vector field $X_{H_0}|_{\Sigma_E^0}$ (see [1, Def. 7.1.1]).

Proof. Take $m \in \Gamma_{E,\alpha}$ and let $\gamma : \mathbb{R} \to \Sigma_E^0$ be the integral curve of X_{H_0} at m given by $\gamma(t) := \varphi_t^0(m)$. Then, we have $(\Psi_E \circ \gamma)(t) = \Psi_E(m) + t\,|(\nabla H_0)(m)|^2$ due to Assumption 2.1 and Equation (2.1). So, the differential $(\mathrm{d}\Psi_E)_m : T_m\Sigma_E^0 \to T_{\Psi_E(m)}\mathbb{R}$ satisfies for each germ $f \in \mathsf{C}^\infty_{\Psi_E(m)}(\mathbb{R})$ at $\Psi_E(m)$ the equalities

$$\begin{aligned}\big[(\mathrm{d}\Psi_E)_m\big(X_{H_0}(m)\big)\big](f) = \frac{\mathrm{d}}{\mathrm{d}t}(f\circ\Psi_E)(\gamma(t))|_{t=0} &= \frac{\mathrm{d}}{\mathrm{d}t} f\big(\Psi_E(m) + t\,|(\nabla H_0)(m)|^2\big)|_{t=0} \\ &= |(\nabla H_0)(m)|^2 f'\big(\Psi_E(m)\big) \\ &= |(\nabla H_0)(m)|^2 \frac{\partial}{\partial t}\Big|_{\Psi_E(m)}(f),\end{aligned}$$

and thus $(\mathrm{d}\Psi_E)_m\big(X_{H_0}(m)\big) = |(\nabla H_0)(m)|^2 \frac{\partial}{\partial t}\big|_{\Psi_E(m)}$. Since $|(\nabla H_0)(m)| \neq 0$, this implies that $(\mathrm{d}\Psi_E)_m$ is surjective, and so $\Gamma_{E,\alpha} \equiv \Psi_E^{-1}(\{\alpha\})$ is a regular submanifold of Σ_E^0 of codimension 1 by the regular level set theorem. Moreover, we also obtain that $X_{H_0}(m) \notin \ker\big((\mathrm{d}\Psi_E)_m\big)$, which implies that $X_{H_0}(m) \notin T_m\Gamma_{E,\alpha}$ since $\ker\big((\mathrm{d}\Psi_E)_m\big) = T_m\Gamma_{E,\alpha}$ (see the remark after [1, Prop. 1.6.18]).

To prove (b), take $m \in \Sigma_E^0$ and observe that

$$\varphi_t^0(m) \in \Gamma_{E,\alpha} \iff \Psi_E\big(\varphi_t^0(m)\big) = \alpha \iff \Psi_E(m) + t\,|(\nabla H_0)(m)|^2 = \alpha \iff t = \frac{\alpha - \Psi_E(m)}{|(\nabla H_0)(m)|^2}.$$

Thus, the time $t_0 := \frac{\Psi_E(m)-\alpha}{|(\nabla H_0)(m)|^2} \in \mathbb{R}$ and the point $m_0 := \varphi_{-t_0}^0(m) \in \Gamma_{E,\alpha}$ are unique and satisfy $m = \varphi_{t_0}^0(m_0)$. □

Lemma 4.1 implies in particular that the submanifold

$$\Gamma_E := \Gamma_{E,0} \equiv \big\{m \in \Sigma_E^0 \mid (\Phi \cdot \nabla H_0)(m) = 0\big\}$$

is a Poincaré section in the sense of [8, Assumption 2.2]. The rest of the assumptions of [8] are verified in the following lemma:

Lemma 4.2. *Assume that M is exact (that is, with ω exact) and satisfies $\dim(M) \geq 4$. Suppose also that*

(H1) Assumption 2.1 holds,

(H2) V has compact support,

(H3) $\{\Phi, V\} = 0$ or Assumption 2.9 holds,

(H4) $U \subset \mathbb{R}$ is an open set such that

(i) $H_0^{-1}(U) \cap \mathrm{Crit}(H_0, \Phi) = \varnothing$,

(ii) there exists $\delta > 0$ such that $\{\Phi \cdot \nabla H_0, H\}(m) > \delta$ for all $m \in H_0^{-1}(U)$.

Then, all the assumptions of Theorems 3.1 and 3.2 of [8] are verified for each $E \in U$.

Note that the exactness of M necessarily implies the noncompactness of M [21, Rem. V.9.4]. Note also that Assumption 2.7 follows from the compactness of the support of V.

Proof. The hypotheses (H1)-(H4) imply that Corollary 2.11 applies. Thus, each $E \in U$ is a regular value of H_0 and H (Assumption 2.1(i) of [8]) and $W_+\big(H_0^{-1}(\{E\})\big) = W_-\big(H_0^{-1}(\{E\})\big) = H^{-1}(\{E\})$ (Equation (2.4) of [8]). The flows of H_0 and H are complete (Assumption 2.1(ii) of [8]). The fact that $H_0^{-1}(U) \cap \mathrm{Crit}(H_0, \Phi) = \varnothing$ implies for each $E \in U$ the non-trapping condition of Assumption 2.1(iii) of [8]; that is, for any compact set $K \subset \Sigma_E^0$ there exists $T > 0$ such that for all $m \in K$ and all $|t| \geq T$, one has $\varphi_t^0(m) \notin K$. Finally, the sets $H^{-1}\big((-\infty, E]\big) \cap \mathrm{supp}(V)$ and $H_0^{-1}\big((-\infty, E]\big) \cap \mathrm{supp}(V)$ are compact for any $E \in \mathbb{R}$ (Assumption 2.1(iv) of [8]) due to Assumption (H2). □

Remark 4.3. *In the proof of Lemma 4.2 we did not check the assumption of noncompactness of $\widetilde{\Sigma}_E^0$ made in [8, Thm. 3.1] because we believe it is unnecessary. Indeed, under the other assumptions of [8, Thm. 3.1], the authors of [8] show in their Lemma 5.1 that $\widetilde{\Sigma}_E^0$ is exact. Therefore, $\widetilde{\Sigma}_E^0$ is necessarily noncompact, since any exact symplectic manifold is noncompact (see [21, Rem. V.9.4]).*

Under the assumptions of Lemma 4.2, we know from [8] that the results of the last paragraph of Section 2.2 hold for any $E \in U$: The orbit space $\widetilde{\Sigma}_E^0 = \Sigma_E^0/\mathbb{R}$ is a symplectic manifold of dimension $2(n-1)$ with symplectic form $\widetilde{\omega}_E^0$ and the restricted scattering map $S_E := S|_{\Sigma_E^0}$ induces a symplectomorphism $\widetilde{S}_E$ of $\big(\widetilde{\Sigma}_E^0, \widetilde{\omega}_E^0\big)$. Furthermore, the Poincaré section Γ_E can be considered as a "concrete realisation of the abstract manifold $\widetilde{\Sigma}_E^0$", due to the existence of a diffeomorphism $\gamma_E^0 : \Gamma_E \to \widetilde{\Sigma}_E^0$ satisfying $(\gamma_E^0)^* \widetilde{\omega}_E^0 = \omega|_{\Gamma_E}$ ($\gamma_E^0 = \pi_E^0 \circ i$, with $i : \Gamma_E \to \Sigma_E^0$ the natural embedding). Since each element $m \in \Sigma_E^0$ can be identified with a pair $(m_0, t_0) \in \Gamma_E \times \mathbb{R}$ satisfying $\varphi_{t_0}^0(m_0)$ due to Lemma 4.1(b), we obtain an identification of $\Sigma_E^0 \simeq \Gamma_E \times \mathbb{R}$ which permits to represent the free flow as $\varphi_t^0 : (m_0, t_0) \mapsto (m_0, t_0 + t)$ and the map S_E as

$$S_E : (m_0, t_0) \mapsto \big(\widetilde{s}_E(m_0), t_0 - \tau_E(m_0)\big),$$

where $\widetilde{s}_E := (\gamma_E^0)^{-1} \circ \widetilde{S}_E \circ \gamma_E^0 : \Gamma_E \to \Gamma_E$ is a symplectomorphism and $\tau_E \in \mathrm{C}^\infty(\Gamma_E; \mathbb{R})$. Using the expressions for (m_0, t_0) obtained in the proof of Lemma 4.1(b) we thus obtain that

$$\varphi^0_{(T \circ S_E)(m)}\big(\widetilde{s}_E(m_0), t_0 - \tau_E(m_0) - (T \circ S_E)(m)\big) = S_E(m) = \varphi^0_{-\tau_E(m_0)}\big(\widetilde{s}_E(m_0), t_0\big),$$

meaning that $\tau_E(m_0) = -(T \circ S_E)(m_0)$. Since $T(m_0) = 0$ for each $m_0 \in \Gamma_E$, it follows from Theorem 3.3 that

$$\lim_{r \to \infty} \tau_r(m_0) = 0 - (T \circ S_E)(m_0) = \tau_E(m_0) \quad \text{for all } m_0 \in \Gamma_E. \tag{4.1}$$

This means that, when evaluated at points $m_0 \in \Gamma_E$, the global time delay $\lim_{r\to\infty} \tau_r(m_0)$ defined in terms of sojourn times in $\Phi^{-1}(B_r) \subset M$ coincides with the time delay $\tau_E(m_0)$ defined on Σ_E^0 as the difference of time intervals from the Poincaré section Γ_E before and after scattering. In other terms, the choice of the position observables Φ provides natural Poincaré sections Γ_E suitable for the application of the (fixed energy) theory of [8].

Now, we introduce as in [8, Sec. 2.5 & 2.6] the average time delay on Γ_E

$$\mathcal{T}_E := \int_{\Gamma_E} \tau_E(m_0)\, \frac{\omega^{n-1}(m_0)}{(n-1)!} = -\int_{\Gamma_E} \frac{(\Phi\circ S)(m_0)\cdot(\nabla H_0\circ S)(m_0)}{|(\nabla H_0\circ S)(m_0)|^2}\, \frac{\omega^{n-1}(m_0)}{(n-1)!}$$

and the regularised phase space volume[1]

$$\xi(E) := \int_M \Big(\chi_{H_0^{-1}((-\infty,E])}(m) - \chi_{H^{-1}((-\infty,E])}(m)\Big)\frac{\omega^n(m)}{n!}.$$

Then, the nice Theorems 3.1 and 3.2 of [8] state that

$$\mathrm{Cal}\big(\widetilde{S}_E\big) = \xi(E) \qquad \text{and} \qquad \mathcal{T}_E = -\frac{\mathrm{d}}{\mathrm{d}E}\xi(E), \tag{4.2}$$

where $\mathrm{Cal} : \mathrm{Dom}(\mathrm{Cal}, M) \to \mathbb{R}$ is the Calabi invariant as defined in [8, Sec. B.2] (the difference with respect to the usual definition is that $\mathrm{Dom}(\mathrm{Cal}, M)$ is here a subset of compactly supported symplectomorphisms whereas it is usually the set of compactly supported hamiltomorphisms, see [22, Eq. (10.4)] or [4]).

By combining Equations (4.1) and (4.2) one gets the following:

Theorem 4.4 (Calabi invariant)**.** *Under the assumptions of Lemma 4.2, one has for each $E \in U$*

$$\frac{\mathrm{d}}{\mathrm{d}E}\mathrm{Cal}\big(\widetilde{S}_E\big) = -\int_{\Gamma_E} \lim_{r\to\infty} \tau_r(m_0)\, \frac{\omega^{n-1}(m_0)}{(n-1)!} = \int_{\Gamma_E} \frac{(\Phi\circ S)(m_0)\cdot(\nabla H_0\circ S)(m_0)}{|(\nabla H_0\circ S)(m_0)|^2}\, \frac{\omega^{n-1}(m_0)}{(n-1)!}.$$

Theorem 4.4 implies that the derivative of the Calabi invariant evaluated at $\widetilde{S}_E$ is equal to the average of the global time delay $\lim_{r\to\infty}\tau_r$ on Γ_E (or equivalently, the average of the arrival time $T\circ S$ on Γ_E). Accordingly, it provides a simple and explicit expression for $\frac{\mathrm{d}}{\mathrm{d}E}\mathrm{Cal}\big(\widetilde{S}_E\big)$ in terms of Φ, S and ∇H_0 on Γ_E. Note that Theorem 4.4 also holds with $\lim_{r\to\infty}\tau_r$ replaced by $\lim_{r\to\infty}\tau_r^{\mathrm{in}}$ if $|\nabla H_0|^2 = |\nabla H_0\circ S|^2$ on Γ_E (see Corollary 3.5).

Example 4.5 ($H_0(q,p) = h(p)$, the end)**.** *If the dimension of $M \simeq \mathbb{R}^{2n}$ is bigger or equal to 4 and V has compact support, then we know from Example 3.7 that all the assumptions of Lemma 4.2 are verified on the open set $U_\delta \subset \mathbb{R}$. So, Theorem 4.4 applies, and one has for each $E \in U_\delta$*

$$\frac{\mathrm{d}}{\mathrm{d}E}\mathrm{Cal}\big(\widetilde{S}_E\big) = \int_{\{(q,p)\in\mathbb{R}^{2n}\,|\,h(p)=E,\ q\cdot(\nabla h)(p)=0\}} \frac{q_+\cdot(\nabla h)(p^+)}{|(\nabla h)(p^+)|^2}\, \frac{\omega^{n-1}(q,p)}{(n-1)!},$$

with $(q_+,p^+) := S(q,p)$. In the particular case $h(p) = |p|^2/2$, one thus obtains

$$\frac{\mathrm{d}}{\mathrm{d}E}\mathrm{Cal}\big(\widetilde{S}_E\big) = (2E)^{(n-3)/2}\int_{\mathbb{S}^{n-1}} \mathrm{d}^{n-1}\widehat{p}\int_{q\cdot p=0} \mathrm{d}^{n-1}q\,\big(q_+\cdot p^+\big),$$

where $\widehat{p} := p/|p|$ and $\mathrm{d}^{n-1}\widehat{p}$ is the spherical measure on $\mathbb{S}^{n-1}$. This corresponds to the case treated in [8, Sec. 4.2] (when the parameter $R \in \mathbb{R}$ of [8, Eq. (4.5)] is taken to be zero).

[1] Here, we follow the conventions of [8, Sec. 2.3] for the integrals on M and Σ_E^0 : The orientation on M is fixed in such a way that the form ω^n is positive on a positively oriented basis, and the orientation on Σ_E^0 is fixed such that if $(e_1,\ldots,e_{2n-1})$ is a positively oriented basis in $T_m\Sigma_E^0$ and $v \in T_mM$ is such that $(\mathrm{d}H_0)_m(v) > 0$, then $(v, e_1,\ldots,e_{2n-1})$ is a positively oriented basis in T_mM.

Example 4.6 (Poincaré ball, the end)**.** *If the dimension of* $M \simeq \mathring{B}_1 \times \mathbb{R}^n \setminus \{0\}$ *is bigger or equal to* 4 *and* V *has compact support, then we know from Example 3.9 that all the assumptions of Lemma 4.2 are verified on the open set* $U_\delta \subset \mathbb{R}$*. So, Theorem 4.4 applies, and one has for each* $E \in U_\delta$

$$\frac{\mathrm{d}}{\mathrm{d}E}\,\mathrm{Cal}\big(\widetilde{S}_E\big) = (2E)^{-1/2} \int_{\{(q,p)\in \mathring{B}_1\times\mathbb{R}^n\setminus\{0\}\,||p|^2(1-|q|^2)^2=8E,\ p\cdot q=0\}} \Phi(q_+,p^+)\,\frac{\omega^{n-1}(q,p)}{(n-1)!},$$

with $\Phi(q,p) = \tanh^{-1}\left(\frac{2(p\cdot q)}{|p|(1+|q|^2)}\right)$ *and* $(q_+,p^+) := S(q,p)$*.*

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