THE SCATTERING MATRIX AND ASSOCIATED FORMULAS IN HAMILTONIAN MECHANICS

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ABSTRACT. We prove two new identities in scattering theory in Hamiltonian mechanics and discuss the analogy between these identities and their counterparts in quantum scattering theory. These identities involve the Poincaré scattering map, which is analogous to the scattering matrix. The first of our identities states that the Calabi invariant of the Poincaré scattering map can be expressed as the regularised phase space volume. This is analogous to the Birman-Krein formula. The second identity relates the Poincaré scattering map to the total time delay and is analogous to the Eisenbud-Wigner formula.

1. INTRODUCTION

1.1. **The scattering matrix and the Poincaré scattering map.** The scattering theory in quantum mechanics deals with the following abstract framework (see e.g. [32]): for self-adjoint operators H_0 and H in a Hilbert space, the large t asymptotics of the corresponding unitary groups e^{-itH_0} and e^{-itH} are compared. In the scattering theory in Hamiltonian mechanics (in its most general form), one considers two Hamiltonian functions H_0 and H on a non-compact symplectic manifold and compares the large time asymptotics of the two corresponding Hamiltonian flows. We refer to these two branches of scattering theory as "quantum" and "classical" cases for short.

One of the fundamental objects in the "quantum" scattering theory is the *scattering matrix*. In this paper we discuss the analogous "classical" object known as the *Poincaré scattering map*. The Poincaré scattering map $\widetilde{S}_E$ (defined in Section 2.3) is a symplectic diffeomorphism of the manifold of the orbits of H_0 with a constant energy E.

In this paper, we prove two identities for the Poincaré scattering map; one of them is completely new, the other one has appeared before in some concrete forms in physics literature. At the same time, we attempt to make a fairly complete exposition of the basic framework of the "classical" scattering theory with an emphasis on the Poincaré scattering map $\widetilde{S}_E$. We believe that this interesting object has not received the attention it deserves in the mathematical scattering theory literature, and the fact that $\widetilde{S}_E$ is the correct "classical" analogue of the scattering matrix is not widely appreciated even among the experts in the area.

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1.2. **The Birman-Krein and the Eisenbud-Wigner formulas.** In "quantum" scattering theory, the determinant of the scattering matrix is related to the spectral shift function by the Birman-Krein formula (A.3). We prove a new identity (3.1) which can be interpreted as the "classical" version of the Birman-Krein formula. Somewhat surprisingly, the description of the correct "classical" analogue of determinant requires the use of a rather advanced language of modern symplectic geometry. It turns out that the "classical" analogue of the determinant of the scattering matrix is given by the Calabi invariant of the Poincaré scattering map. The "classical" analogue of the spectral shift function is the regularised phase space volume. Like the "quantum" Birman-Krein formula, the identity (3.1) relates objects of a very different nature: the Poincaré scattering map $\widetilde{S}_E$, which describes dynamics for a fixed energy E, is related to the regularised phase space volume, which is defined without any reference to dynamics.

The Eisenbud-Wigner formula in "quantum" scattering theory relates the determinant of the scattering matrix to the total time delay, see (A.4). We prove the analogous "classical" identity (3.3).

Our proofs of these identities proceed entirely in classical terms; the analogy with the "quantum" case is used only as a motivation. The reader not interested in the "quantum" scattering theory can safely ignore all references to it.

"Quantum" scattering theory was initially motivated by the study of the Schrödinger equation, but found its most natural mathematical description in the framework of operator theory. In the same way, the natural framework for the study of "classical" scattering is Hamiltonian dynamics and symplectic geometry. For this reason, we discuss our results in Sections 2 and 3 in a fairly general context; applications to Newtonian mechanics are given in Section 4.

1.3. **The structure of the paper.** In Section 2 we describe the set-up of Hamiltonian scattering and introduce the main objects: the "classical" analogues of the wave operators and the scattering map, the Poincaré scattering map, the total time delay and the regularised phase space volume (the latter is the analogue of the "quantum" spectral shift function). In Section 3, we state our main results which relate the Poincaré scattering map to the regularised phase space volume and the time delay; these are the "classical" analogues of the Birman-Krein and the Eisenbud-Wigner formulas. In Section 4, we consider applications to classical mechanics. The proofs are presented in Sections 5–7. In Appendix A we collect the relevant formulas and definitions from "quantum" scattering theory for the purposes of comparison with the "classical" case. In Appendix B, we recall the necessary background information from symplectic geometry. In particular, we recall the definition of the Calabi invariant.

2. The set-up of Hamiltonian scattering theory

2.1. **Notation and assumptions.** Let $\mathcal{N}$ be a non-compact $2n$-dimensional symplectic manifold, $n \geqslant 1$, with a symplectic form ω. We will compare the large time behaviour of the

Hamiltonian flows associated with two Hamiltonian functions $H_0, H \in C^\infty(\mathcal{N})$. We use the following notation: X is the Hamiltonian vector field corresponding to H and $\Phi_t : \mathcal{N} \to \mathcal{N}$ is the Hamiltonian flow:

$$(i(X)\omega)(\cdot) \equiv \omega(X, \cdot) = -dH(\cdot); \quad \frac{d}{dt}\Phi_t(\cdot) = X(\Phi_t(\cdot)), \quad \Phi_0 = id.$$

For $E \in \mathbb{R}$, let

$$G(E) = \{x \in \mathcal{N} \mid H(x) \leqslant E\}, \quad \Sigma_E = \{x \in \mathcal{N} \mid H(x) = E\}. \tag{2.1}$$

Notation X_0, Φ_t^0, G_0, Σ_E^0 have the same meaning and refer to the Hamiltonian H_0.

The symplectic volume $\mathrm{vol}(\Omega)$ of a Borel set $\Omega \subset \mathcal{N}$ is defined as

$$\mathrm{vol}(\Omega) = \int_\Omega \frac{\omega^n}{n!}, \quad \omega^n = \omega \wedge \cdots \wedge \omega;$$

note the normalisation $1/n!$. The characteristic function of Ω is denoted by χ_Ω. If $\varphi : \mathcal{N} \to \mathcal{N}$ is a diffeomorphism and α is a differential form on $\mathcal{N}$, then $\varphi^*\alpha$ denotes the pullback of α by φ.

Fix $E \in \mathbb{R}$. We make the following assumptions:

Assumption 2.1. (i) E is a regular value of H, H_0: $dH(x) \neq 0$ for all $x \in \Sigma_E$ and $dH_0(x) \neq 0$ for all $x \in \Sigma_E^0$. Thus, Σ_E and Σ_E^0 are C^∞-smooth manifolds.

(ii) The maps $\Phi_t^0 : \Sigma_E^0 \to \Sigma_E^0$ and $\Phi_t : \Sigma_E \to \Sigma_E$ are well defined for all $t \in \mathbb{R}$, i.e. the trajectories do not run off to infinity in finite time. Thus, Φ_t^0 and Φ_t are groups of diffeomorphisms on Σ_E^0 and Σ_E.

(iii) *Non-trapping:* For any compact set $K \subset \Sigma_E^0$ there exists $T > 0$ such that for all $x \in K$ and all $|t| \geqslant T$, one has $\Phi_t^0(x) \notin K$.

(iv) The sets $G(E) \cap \mathrm{supp}(H - H_0)$ and $G_0(E) \cap \mathrm{supp}(H - H_0)$ are compact.

In concrete situations, Assumption 2.1(iv) can be considerably relaxed; we do not pursue this direction.

2.2. **Wave operators and the scattering map.**

For $x \in \Sigma_E^0$, let

$$W_\pm(x) = \lim_{t \to \pm\infty} \Phi_{-t} \circ \Phi_t^0(x). \tag{2.2}$$

If $K_0 \subset \Sigma_E^0$ is a compact, then, taking $K = \mathrm{supp}(H - H_0) \cup K_0$ in Assumption 2.1(iii), we see that the above limits exist and are attained at finite values of t:

$$W_+(x) = \Phi_{-t} \circ \Phi_t^0(x), \quad W_-(x) = \Phi_t \circ \Phi_{-t}^0(x), \quad \forall x \in K_0, \quad \forall t \geqslant T. \tag{2.3}$$

Since H_0 (resp. H) is constant on the orbits of Φ^0 (resp. Φ), we get

$$H(W_+(x)) = H(\Phi_{-t} \circ \Phi_t^0(x)) = H(\Phi_t^0(x)) = H_0(\Phi_t^0(x)) = H_0(x), \quad \forall x \in K_0, \quad \forall t \geqslant T$$

and in the same way, $H(W_-(x)) = H_0(x)$. It follows that $W_\pm(\Sigma_E^0) \subset \Sigma_E$. However, it is easy to construct examples such that $W_\pm(\Sigma_E^0) \neq \Sigma_E$. Thus, we make an additional assumption:

$$W_+(\Sigma_E^0) = W_-(\Sigma_E^0) = \Sigma_E. \tag{2.4}$$

This is analogous to the *completeness* assumption in quantum scattering, see (A.1). Since Φ_t and Φ_t^0 are symplectic diffeomorphisms of $\mathcal{N}$ for each t, it follows from (2.3) that $W_\pm : \Sigma_E^0 \to \Sigma_E$ are diffeomorphisms and that $W_\pm^*(\omega|_{\Sigma_E}) = \omega|_{\Sigma_E^0}$.

Next, since the definition of $W_\pm$ can also be written as $W_\pm(x) = \lim_{s\to\pm\infty} \Phi_{-t-s} \circ \Phi_{t+s}^0(x)$ for any $t \in \mathbb{R}$, we get the intertwining property

$$W_\pm \circ \Phi_t^0 = \Phi_t \circ W_\pm, \quad \forall t \in \mathbb{R}. \tag{2.5}$$

The completeness assumption (2.4), together with the intertwining property (2.5), ensures that the non-trapping Assumption 2.1(iii) holds true also for the flow Φ_t on Σ_E.

Assuming completeness (2.4), we can define the scattering map

$$S_E = W_+^{-1} \circ W_-. \tag{2.6}$$

By (2.3), one can write

$$S_E(x) = \Phi_{-t}^0 \circ \Phi_{2t} \circ \Phi_{-t}^0(x), \quad \forall x \in K_0, \quad \forall t,\ |t| \geqslant T. \tag{2.7}$$

It follows that $S_E : \Sigma_E^0 \to \Sigma_E^0$ is a diffeomorphism onto Σ_E^0 and

$$S_E^*(\omega|_{\Sigma_E^0}) = \omega|_{\Sigma_E^0}. \tag{2.8}$$

From (2.5) (or directly from (2.7)) it follows that

$$S_E \circ \Phi_t^0 = \Phi_t^0 \circ S_E, \quad \forall t \in \mathbb{R}. \tag{2.9}$$

The scattering map is often defined initially on the whole of $\mathcal{N}$ (or for some range of energies) and then restricted onto Σ_E^0.

The above constructions are very well known; see e.g. [14, 24, 13, 30]. The fact that the wave operators and the scattering map are symplectic transformations is particularly emphasized in the works by W. Thirring, see [30] or [22, 29].

2.3. **Symplectic reduction and the Poincaré scattering map.** One can consider the set of all orbits of Φ_t^0 on the constant energy surface Σ_E^0 as a symplectic manifold $\widetilde{\Sigma}_E^0$. Then the map S_E generates a quotient map $\widetilde{S}_E : \widetilde{\Sigma}_E^0 \to \widetilde{\Sigma}_E^0$ which is sometimes called the *Poincaré scattering map*; it is not difficult to see that $\widetilde{S}_E$ is a symplectic diffeomorphism. Let us discuss the details of this construction.

By Assumption 2.1(i)–(iii), the action of the group Φ^0 on Σ_E^0 is smooth, proper and free, and therefore (see [1, Proposition 4.1.23]) the orbit space admits a smooth manifold structure and the quotient map $\pi_0 : \Sigma_E^0 \to \widetilde{\Sigma}_E^0$ is a submersion. It is easy to construct charts on $\widetilde{\Sigma}_E^0$ by choosing sufficiently small $(2n-2)$-dimensional submanifolds of Σ_E^0 such that X_0 is non-tangential to these manifolds; see the proof of Lemma 5.1 below. If $x \in \Sigma_E^0$

is a point of an orbit $y \in \widetilde{\Sigma}_E^0$, then the tangent space $T_y\widetilde{\Sigma}_E^0$ can be identified with the quotient space $T_x\Sigma_E^0/\operatorname{span}\{X_0(x)\}$. There exists a unique symplectic form $\widetilde{\omega}_0$ on $\widetilde{\Sigma}_E^0$ such that $\pi_0^*\widetilde{\omega}_0 = \omega|_{\Sigma_E^0}$; see e.g. [1, Theorem 4.3.1 and Example 4.3.4(ii)]. It is not difficult to prove that if $\mathcal{N}$ is exact (i.e. there exists a 1-form α on $\mathcal{N}$ such that $\omega = d\alpha$), then $\widetilde{\Sigma}_E^0$ is also exact, see Lemma 5.1 below.

If $f : \Sigma_E^0 \to \mathbb{R}$ is a smooth function such that $f \circ \Phi_t^0 = f$ for all $t \in \mathbb{R}$, then f generates a smooth function $\widetilde{f} : \widetilde{\Sigma}_E^0 \to \mathbb{R}$ such that $\widetilde{f} \circ \pi_0 = f$. In a similar way, by (2.9), the scattering map S_E generates the diffeomorphism

$$\widetilde{S}_E : \widetilde{\Sigma}_E^0 \to \widetilde{\Sigma}_E^0, \quad \pi_0 \circ S_E = \widetilde{S}_E \circ \pi_0. \tag{2.10}$$

From (2.8) and (2.10) one easily obtains

$$\pi_0^*(\widetilde{S}_E^*\widetilde{\omega}_0 - \widetilde{\omega}_0) = 0.$$

Since π_0 is a surjection, it follows that $\widetilde{S}_E^*\widetilde{\omega}_0 = \widetilde{\omega}_0$, i.e. $\widetilde{S}_E$ is a symplectic diffeomorphism.

It is interesting to note that $\widetilde{S}_E$ does not have to be homotopic to the identity map, see Example 4.3 below.

Since the action of Φ on Σ_E is also free, smooth and proper, one can consider the symplectic manifold $\widetilde{\Sigma}_E$ of the orbits of Φ on Σ_E, with the natural projection $\pi : \Sigma_E \to \widetilde{\Sigma}_E$ and a symplectic form $\widetilde{\omega}$ on $\widetilde{\Sigma}_E$. By the intertwining property (2.5), there exist symplectic diffeomorphisms

$$\widetilde{W}_\pm : \widetilde{\Sigma}_E^0 \to \widetilde{\Sigma}_E, \quad \widetilde{W}_\pm \circ \pi_0 = \pi \circ W_\pm. \tag{2.11}$$

In the case $n = 1$ the above reduction produces a “manifold” of dimension zero, i.e. a discrete set of orbits. The Poincaré scattering map becomes just a permutation map on the set of these orbits. In this case, integration over the “volume forms” $\widetilde{\omega}^{n-1}$, $\widetilde{\omega}_0^{n-1}$, $n = 1$ will be understood simply as summation over this set of orbits.

Since we are going to discuss integration of forms over $\mathcal{N}$, Σ_E^0, Σ_E, $\widetilde{\Sigma}_E^0$, $\widetilde{\Sigma}_E$, we should fix orientation on these manifolds. Orientation on $\mathcal{N}$ is fixed in such a way that the form ω^n is positive on a positively oriented basis. In the same way, orientation on $\widetilde{\Sigma}_E^0$ is fixed in such a way that the form $\widetilde{\omega}_0^{n-1}$ is positive on a positively oriented basis. Orientation on Σ_E^0 is fixed such that if $(e_1, \dots, e_{2n-1})$ is a positively oriented basis in $T_x\Sigma_E^0$ and $\xi \in T_x\mathcal{N}$ is such that $d_xH_0(\xi) > 0$, then $(\xi, e_1, \dots, e_{2n-1})$ is a positively oriented basis in $T_x\mathcal{N}$. In other words, Σ_E^0 is considered as a boundary of G_0 with induced orientation. Orientation on $\widetilde{\Sigma}_E$ and Σ_E is fixed in a similar way to $\widetilde{\Sigma}_E^0$, Σ_E^0.

2.4. **Poincaré section.** The above procedure of symplectic reduction looks particularly simple if one makes

Assumption 2.2. There exists a smooth submanifold $\Gamma \subset \Sigma_E^0$ of dimension $2n-2$ such that:

(a) $X_0(x) \notin T_x\Gamma$ for all $x \in \Gamma$;

(b) for all $x \in \Sigma_E^0$, there exists a unique $z = z(x) \in \Gamma$ and a unique $t = t(x)$ such that $x = \Phi_t^0(z)$.

In this case, the elements $x \in \Sigma_E^0$ can be considered as pairs $(z, t) \in \Gamma \times \mathbb{R}$ such that $x = \Phi_t(z)$. It is easy to see that

$$\text{Assumption 2.1(i),(ii)} + \text{Assumption 2.2} \Rightarrow \text{Assumption 2.1(iii)}.$$

Let $i : \Gamma \to \Sigma_E^0$ be the natural embedding. Then $\gamma_0 = \pi_0 \circ i : \Gamma \to \widetilde{\Sigma}_E^0$ is a diffeomorphism and $\gamma_0^* \widetilde{\omega}_0 = \omega|_\Gamma$. Thus, Γ can be considered as a "concrete" realisation of the "abstract" manifold $\widetilde{\Sigma}_E^0$.

Using the above identification of Σ_E^0 and $\Gamma \times \mathbb{R}$, the free dynamics can be represented as $\Phi_s^0 : (z, t) \mapsto (z, t + s)$ and the scattering map as

$$S_E : (z, t) \mapsto (z', t'), \qquad z' = \widetilde{s}_E(z), \quad t' = t - \tau_E(z), \tag{2.12}$$

where $\widetilde{s}_E = \gamma_0^{-1} \circ \widetilde{S}_E \circ \gamma_0 : \Gamma \to \Gamma$ is a symplectic diffeomorphism, and $\tau_E : \Gamma \to \mathbb{R}$ is a smooth function. The map τ_E is often called *time delay*, or *sojourn time*. We note that the definition (2.12) of τ_E depends on the choice of Γ; there is no invariant way of defining a time delay function on $\widetilde{\Sigma}_E^0$.

The manifold Γ is, of course, the well known Poincaré section; see e.g. [1, §7.1]. The map $\widetilde{s}_E : \Gamma \to \Gamma$ in concrete cases appeared before in physics literature in [15, 11, 27] and in mathematical literature in [16, 3]. The connection of $\widetilde{s}_E$ with the "quantum" scattering matrix in the framework of semiclassical analysis has been discussed in physics literature, see e.g. [27] and in mathematical literature in [3]. One of the earliest rigourous works which established the connection between the "quantum" scattering matrix and the analogous classical objects was [31].

2.5. **Total time delay.** Although the definition of time delay τ_E above depends on the choice of Γ, the *total* (or average) *time delay* T_E can be defined (see (2.15) below) in an invariant way.

Let $\Omega_1 \subset \Omega_2 \subset \cdots \subset \mathcal{N}$ be a sequence of open pre-compact sets such that $\cup_{k=1}^\infty \Omega_k = \mathcal{N}$. Let us define the functions $u_k^0 : \Sigma_E^0 \to \mathbb{R}$ and $u_k : \Sigma_E \to \mathbb{R}$ by

$$u_k^0(x) = \int_{-\infty}^{\infty} \chi_{\Omega_k} \circ \Phi_t^0(x) dt, \quad x \in \Sigma_E^0, \tag{2.13}$$

$$u_k(x) = \int_{-\infty}^{\infty} \chi_{\Omega_k} \circ \Phi_t(x) dt, \quad x \in \Sigma_E. \tag{2.14}$$

It is straightforward to see that $u_k^0 \circ \Phi_t^0 = u_k^0$ and $u_k \circ \Phi_t = u_k$ for all $t \in \mathbb{R}$ and therefore u_k^0, u_k generate functions $\widetilde{u}_k^0 : \widetilde{\Sigma}_E^0 \to \mathbb{R}$, $\widetilde{u}_k : \widetilde{\Sigma}_E \to \mathbb{R}$ such that $\widetilde{u}_k^0 \circ \pi_0 = u_k^0$ and $\widetilde{u}_k \circ \pi = u_k$.

Theorem 2.3. *Suppose Assumption 2.1 and completeness* (2.4) *hold true, and let* $\Omega_1 \subset \Omega_2 \subset \cdots \subset \mathcal{N}$ *and* $\widetilde{u}_k^0$, $\widetilde{u}_k$ *be as defined above. Then the limit*

$$T_E = \lim_{k\to\infty} \left\{ \int_{\widetilde{\Sigma}_E} \widetilde{u}_k(y) \frac{\widetilde{\omega}^{n-1}(y)}{(n-1)!} - \int_{\widetilde{\Sigma}_E^0} \widetilde{u}_k^0(y) \frac{\widetilde{\omega}_0^{n-1}(y)}{(n-1)!} \right\} \tag{2.15}$$

exists and is independent of the choice of the sequence $\{\Omega_k\}$. *If, in addition, Assumption 2.2 holds true and* $\tau_E : \Gamma \to \mathbb{R}$ *is as defined by* (2.12), *then*

$$T_E = \int_\Gamma \tau_E(x) \frac{\omega^{n-1}(x)}{(n-1)!}. \tag{2.16}$$

T_E is the *total time delay*. The above statement (in various concrete forms) is well known; for completeness, we give a proof in Section 7. See [10] for a survey of time delay and [25] for a rigourous discussion of semiclassical aspects.

Remark 2.4. Since $\widetilde{W}_- : \widetilde{\Sigma}_E^0 \to \widetilde{\Sigma}_E$ (see (2.11)) is a symplectic diffeomorphism, the difference of the integrals in (2.15) can be rewritten as

$$\int_{\widetilde{\Sigma}_E} \widetilde{u}_k(y) \frac{\widetilde{\omega}^{n-1}(y)}{(n-1)!} - \int_{\widetilde{\Sigma}_E^0} \widetilde{u}_k^0(y) \frac{\widetilde{\omega}_0^{n-1}(y)}{(n-1)!} = \int_{\widetilde{\Sigma}_E^0} (\widetilde{u}_k \circ \widetilde{W}_-(y) - \widetilde{u}_k^0(y)) \frac{\widetilde{\omega}_0^{n-1}(y)}{(n-1)!}. \tag{2.17}$$

The quantity $\widetilde{u}_k \circ \widetilde{W}_-(y) - \widetilde{u}_k^0(y)$ and its limit

$$\lim_{k\to\infty} (\widetilde{u}_k \circ \widetilde{W}_-(y) - \widetilde{u}_k^0(y)) \tag{2.18}$$

(or similar objects with $\widetilde{W}_+$ instead of $\widetilde{W}_-$) is often interpreted as the time delay related to the orbit y. Note, however, that the limit (2.18) may not exist unless the sequence Ω_k is chosen in a special way; see [28, 12] for a discussion of this issue.

2.6. **Regularised phase space volume.** Suppose that Assumption 2.1(iv) holds true for some E. Let us denote

$$\xi(E) = \int_{\mathcal{N}} (\chi_{G_0(E)} - \chi_{G(E)}) \frac{\omega^n}{n!}. \tag{2.19}$$

It is interesting to note that if $\pm(H(x) - H_0(x)) \geqslant 0$ for all $x \in \mathcal{N}$, then $\pm\xi(E) \geqslant 0$. The "quantum" analogue of $\xi(E)$ is the spectral shift function. See the survey [26] for an extensive discussion of this analogy in semiclassical context.

3. Main results

We will use some notation and terminology from symplectic topology. We collect the required material in Appendix B; for the details, see [20]. In particular, we use the notion of the Calabi invariant. Let $\mathcal{M}$ be an exact non-compact symplectic manifold; the Calabi invariant CAL is a functional on a certain subset (which we denote by $\mathrm{Dom}(\mathrm{CAL}, \mathcal{M})$) of the set of symplectic diffeomorphisms of $\mathcal{M}$. We note that our sign conventions and normalisation of the Calabi invariant are different from those of [20]. In Appendix B (see Section B.3) we explain the analogy between CAL and the functional $-\mathrm{Im}\log\det$ on the set of unitary operators.

3.1. $\mathrm{CAL}(\widetilde{S}_E)$ and the regularised phase space volume.

Theorem 3.1. *Let $n \geqslant 2$; suppose that Assumption 2.1 and completeness* (2.4) *hold true for some $E \in \mathbb{R}$. Assume also that $\mathcal{N}$ is exact and that $\widetilde{\Sigma}^0_E$ is non-compact. Then the map $\widetilde{S}_E : \widetilde{\Sigma}^0_E \to \widetilde{\Sigma}^0_E$ belongs to* $\mathrm{Dom}(\mathrm{CAL}, \widetilde{\Sigma}^0_E)$ *and the identity*

$$\mathrm{CAL}(\widetilde{S}_E) = \xi(E) \tag{3.1}$$

holds true.

This should be compared to the Birman-Krein formula (A.3) in “quantum” scattering theory, bearing in mind the analogy between the Calabi invariant and the logarithm of determinant, see Section B.3.

The proof of Theorem 3.1 is given in Sections 5 and 6 entirely in the framework of Hamiltonian mechanics. The proof can probably be obtained, at least in some particular cases, by analysing the semiclassical asymptotics of the Birman-Krein formula. However, this route is likely to be much more technically difficult.

Similarly to the Birman-Krein formula, the relation (3.1) can be applied to a wide variety of concrete situations. In Section 4 we discuss applications to scattering of classical particles.

3.2. The scattering matrix and the total time delay.

Theorem 3.2. *Suppose that Assumption 2.1 and completeness* (2.4) *hold true for some $E \in \mathbb{R}$. Suppose also that Assumption 2.1(iv) holds true for some $E_1 > E$. Then the derivative $\frac{d\xi}{dE}(E)$ exists and the identity*

$$T_E = -\frac{d\xi}{dE}(E) \tag{3.2}$$

holds true.

This result in various concrete forms appeared before in physics literature; see e.g. [22, 6, 19]. For completeness, we give a proof in Section 7. Combining Theorem 3.2 with Theorem 3.1, we get

$$\frac{d}{dE}\,\mathrm{CAL}(\widetilde{S}_E) = -T_E. \tag{3.3}$$

This should be compared to the Eisenbud-Wigner formula (A.4) in “quantum” scattering. A related result was obtained in [5] in the framework of Hilbert space classical scattering.

4. Application to classical mechanics

4.1. **The general case.** Let $\mathcal{N} = \mathbb{R}^{2n}$, $n \geqslant 2$, with the standard symplectic form $\omega = \sum_{i=1}^n dp_i \wedge dq_i$, $(q_1 \dots q_n, p_1 \dots p_n) = x \in \mathbb{R}^{2n}$. Of course, $\mathcal{N}$ is exact, $\omega = d(-\sum_i q_i dp_i)$. We denote by $\langle \cdot, \cdot \rangle$ the usual inner product in $\mathbb{R}^n$, and $|q|^2 = \langle q, q \rangle$. Let

$$H_0(q,p) = \frac{1}{2}|p|^2 + v_0(q),$$

where $v_0 \in C^\infty(\mathbb{R}^n)$ satisfies the following assumptions:

$$\sup_{q \in \mathbb{R}^n} (v_0(q) + \frac{1}{2}\langle q, \nabla v_0(q) \rangle) < \infty, \tag{4.1}$$

$$\inf_{q \in \mathbb{R}^n} v_0(q) > -\infty. \tag{4.2}$$

The quantity $v_0 + \frac{1}{2}\langle q, \nabla v_0 \rangle$ in (4.1) is known as the virial. Next, let $H(q,p) = H_0(q,p) + v(q)$, where $v \in C_0^\infty(\mathbb{R}^n)$. Let $E \in \mathbb{R}$ be such that

$$E \text{ is not a critical value of } v_0 \text{ or } v_0 + v; \tag{4.3}$$

$$E > \sup_{q \in \mathbb{R}^n} (v_0(q) + \frac{1}{2}\langle q, \nabla v_0(q) \rangle). \tag{4.4}$$

Fix any $R \in \mathbb{R}$ and consider

$$\Gamma = \{(q,p) \mid h_0(q,p) = E, \langle q, p \rangle = R\} \subset \Sigma_E^0. \tag{4.5}$$

Lemma 4.1. *Assume* (4.1) *through* (4.4)*. Then Assumption 2.1 and Assumption 2.2 hold true with* Γ *as in* (4.5).

Proof. Assumption 2.1(i) follows from (4.3). Assumption 2.1(ii) follows from (4.2), since $\dot{q} = p$ and $|p|^2 = 2(E - v_0) \leqslant C < \infty$.

Let us check Assumption 2.1(iii). For any trajectory $(q(t), p(t)) = \Phi_t^0(x)$, we have

$$\frac{d}{dt}|q(t)|^2 = 2\frac{d}{dt}\langle q(t), p(t) \rangle = 2|p(t)|^2 - 2\langle q(t), \nabla v_0(q(t)) \rangle \geqslant C > 0 \tag{4.6}$$

by (4.4), and so $|q(t)| \to \infty$ as $t \to \pm\infty$, as required.

Let us check Assumption 2.1(iv). We have

$$G_0(E) \cap \operatorname{supp}(H - H_0) = \{(q,p) \mid q \in \operatorname{supp} v, \frac{1}{2}|p|^2 \leqslant E - v_0(q)\};$$

using (4.2) we see that this set is compact. In the same way, $G(E) \cap \operatorname{supp}(H - H_0)$ is compact.

Let us check Assumption 2.2. In order to check that Γ is a smooth manifold in Σ_E^0, it suffices to verify that dH_0 and $d\langle q, p \rangle$ are linearly independent on Γ. Suppose that $dH_0 = \lambda d\langle q, p \rangle$ at some point $(q,p) \in \Gamma$. Then $\nabla v_0(q) = \lambda p$ and $p = \lambda q$, and so $E = \frac{1}{2}|p|^2 + v_0(q) = \frac{1}{2}\langle \nabla v_0(q), q \rangle + v_0(q) < E$ by (4.4) — contradiction.

Next, we need to check that X_0 is non-tangential to Γ. We have $X_0(q,p) = (p, -\nabla v_0(q))$. The tangent space $T_{(q,p)}\Gamma$ consists of vectors (ξ, η) such that $\langle \xi, p\rangle + \langle \eta, q\rangle = 0$ and $\langle \xi, \nabla v_0(q)\rangle + \langle \eta, p\rangle = 0$. For $(\xi,\eta) = X_0(q,p)$ we have

$$\langle \xi, p\rangle + \langle \eta, q\rangle = |p|^2 - \langle q, \nabla v_0(q)\rangle = 2(E - v_0(q)) - \langle q, \nabla v_0(q)\rangle > 0$$

by (4.4), and so $X_0(q,p)$ is not in $T_{(q,p)}\Gamma$.

Finally, by (4.6), for any trajectory $(q(t), p(t)) = \Phi_t^0(x)$, we have $\frac{d}{dt}\langle q(t), p(t)\rangle \geqslant C > 0$ and so there exists a unique $t \in \mathbb{R}$ such that $\langle q(t), p(t)\rangle = R$. ∎

Thus, (4.1)–(4.4) ensure that the wave operators $W_\pm : \Sigma_E^0 \to \Sigma_E$ exist. In order to ensure that completeness (2.4) holds true, we have to make more specific assumptions. Let us assume that

$$E > \sup_{q\in\mathbb{R}^n} (v_0(q) + v(q) + \tfrac{1}{2}\langle q, \nabla v_0(q)\rangle + \tfrac{1}{2}\langle q, \nabla v(q)\rangle). \tag{4.7}$$

Then by the same argument as in the proof of Lemma 4.1 (see (4.6)), we obtain that all trajectories of Φ_t leave $\operatorname{supp} v$ for large $|t|$ and therefore coincide with some trajectories of the free dynamics for large $\pm t > 0$. From here we get completeness (2.4).

To summarise: Suppose that (4.1)–(4.4), (4.7) hold true. Then Assumptions 2.1, (2.4) and Assumption 2.2 hold true and therefore Theorems 3.1 and 3.2 hold true.

We note without proof that under the above assumptions one can check that $\widetilde{S}_E \in \operatorname{Ham}^c(\widetilde{\Sigma}_E^0)$.

4.2. **The case $v_0 \equiv 0$.** In the case $v_0 \equiv 0$ it is easy to give explicit formulas for the phase space volume, time delay, and the Calabi invariant of $\widetilde{S}_E$.

The formula for the regularised phase space volume (2.19) is very well known (see e.g. [26] for a comprehensive discussion) and easy to compute:

$$\xi(E) = \varkappa_n 2^{n/2} \int_{\mathbb{R}^n} \big(E - (E - v(q))_+^{n/2}\big) d^n q, \quad E > 0, \tag{4.8}$$

where $\varkappa_n = \frac{\pi^{n/2}}{\Gamma(1+n/2)}$ is the volume of a unit ball in $\mathbb{R}^n$, $d^n q$ is the Lebesgue measure in $\mathbb{R}^n$, and $(a)_+ = (a + |a|)/2$.

Next, the formula for the time delay is also well known; see e.g. [21]. Let $x^- = (q^-, p^-) \in \Gamma$ and let $x^+ = (q^+, p^+) = S_E(x^-)$. Then the time delay function τ_E from (2.12) can be expressed as

$$\tau_E(x^-) = \frac{1}{2E}(\langle q^-, p^-\rangle - \langle q^+, p^+\rangle),$$

and the total time delay is

$$T_E = \int_\Gamma \tau_E(x^-) \frac{\omega^{n-1}(x^-)}{(n-1)!} = (2E)^{(n-3)/2} \int_{\mathbb{S}^{n-1}} d^{n-1}\hat{p}^- \int_{\langle q^-, p^-\rangle = R} d^{n-1} q^- \, (\langle q^-, p^-\rangle - \langle q^+, p^+\rangle),$$

where $\hat{p}^- = p^-/|p^-|$, and $d^{n-1}\hat{p}^-$ is the Lebesgue measure on the unit sphere in $\mathbb{R}^n$.

Let us display formula (3.2) in the cases $n = 2, 3$:

$$T_E = 0 \qquad (n = 2),$$

$$T_E = 6\pi\sqrt{2}\int_{\mathbb{R}^3}\big(E - (E - v(q))_+^{1/2}\big)d^3q \qquad (n = 3).$$

Finally, let us give a formula for $\mathrm{CAL}(\widetilde{S}_E)$. As above, we have $S_E : \Sigma_E^0 \to \Sigma_E^0$, $x^- = (q^-, p^-) \mapsto (q^+, p^+)$; define

$$\rho(x^-) = \sum_{i,j=1}^{n} q_i^- q_j^+ \frac{\partial p_j^+}{\partial q_i^-}(q^-, p^-).$$

It is straightforward to see that this definition is independent of the choice of the coordinate system in $\mathbb{R}^n$.

Lemma 4.2. *Under the assumptions* (4.1)–(4.4), (4.7), *one has* $\rho \circ \Phi_t^0 = \rho$ *for all* $t \in \mathbb{R}$ *and*

$$\mathrm{CAL}(\widetilde{S}_E) = -\frac{1}{n(n-1)}\int_\Gamma \rho(x)\frac{\omega^{n-1}(x)}{(n-1)!} \tag{4.9}$$

$$= -\frac{(2E)^{(n-1)/2}}{n(n-1)}\int_{\mathbb{S}^{n-1}} d^{n-1}\hat{p}\int_{\langle q,p\rangle = R} d^{n-1}q\ \rho(q,p). \tag{4.10}$$

Remark. (1) Since $\rho \circ \Phi_t^0 = \rho$, there exists a function $\widetilde{\rho} : \widetilde{\Sigma}_E^0 \to \mathbb{R}$ such that $\widetilde{\rho} \circ \pi_0 = \rho$. Then (4.9) can be rewritten in an invariant form as

$$\mathrm{CAL}(\widetilde{S}_E) = -\frac{1}{n(n-1)}\int_{\widetilde{\Sigma}_E^0} \widetilde{\rho}(z)\frac{\widetilde{\omega}_0^{n-1}(z)}{(n-1)!}.$$

(2) It is possible to prove Lemma 4.2 by a direct calculation in local coordinates. Instead, below we give a proof which clarifies the main idea behind the definition of ρ and can be adapted to more general situations.

Proof. 1. Fix $\alpha = -\sum_{i=1}^n q_i dp_i$. Let us prove that the identity

$$(S_E^*\alpha) \wedge \alpha \wedge \omega^{n-1} = -\frac{1}{n}\rho\omega^n \tag{4.11}$$

holds true in some open neighbourhood of Σ_E^0. Here S_E should be understood as an extension of the map $S_E : \Sigma_E^0 \to \Sigma_E^0$ into a neighbourhood of Σ_E^0. More precisely, if the hypothesis of the Lemma is fulfilled for the energy E, then it is clearly also fulfilled for an open interval of energies $(E_1, E_2) \ni E$. Then S_E can be extended to $\{x \mid E_1 < H_0(x) < E_2\}$ by using the same construction.

In order to check (4.11), we note that

$$S_E^*\alpha = -\sum_{i=1}^n q_i^+ dp_i^+ = -\sum_{i,k=1}^n q_i^+ \frac{\partial p_i^+}{\partial q_k^-} dq_k^- - \sum_{i,k=1}^n q_i^+ \frac{\partial p_i^+}{\partial p_k^-} dp_k^-,$$

and therefore

$$(S_E^*\alpha)\wedge\alpha\wedge\omega^{n-1}=(\sum_{k,i=1}^n q_i^+\frac{\partial p_i^+}{\partial q_k^-}dq_k^-+\sum_{k,i=1}^n q_i^+\frac{\partial p_i^+}{\partial p_k^-}dp_k^-)\wedge(\sum_{j=1}^n q_j^-\,dp_j^-)\wedge\omega^{n-1}$$
$$=(\sum_{k,i=1}^n q_i^+\frac{\partial p_i^+}{\partial q_k^-}dq_k^-)\wedge(\sum_{j=1}^n q_j^-\,dp_j^-)\wedge\omega^{n-1}=\frac{1}{n}\sum_{i,j=1}^n q_i^+q_j^-\frac{\partial p_i^+}{\partial q_j^-}dq_j^-\wedge dp_j^-\wedge\omega^{n-1}$$
$$=-\frac{1}{n}\sum_{i,j=1}^n q_i^+q_j^-\frac{\partial p_i^+}{\partial q_j^-}\omega^{n-1}=-\frac{1}{n}\rho\omega^n,$$

as required.

2. By inspection,

$$\alpha(X_0)=0 \text{ and } (\Phi_0^t)^*\alpha=\alpha. \tag{4.12}$$

This is crucial for our proof. Since S commutes with Φ_t^0 (see (2.9)), it follows that

$$(\Phi_t^0)^*S^*\alpha=S^*(\Phi_t^0)^*\alpha=S^*\alpha.$$

Using these relations and applying $(\Phi_t^0)^*$ to both sides of (4.11), we get $\rho\circ\Phi_t^0=\rho$.

3. Let us prove that

$$(S_E^*\alpha)\wedge\alpha\wedge\omega^{n-2}=-\frac{1}{n-1}\rho\omega^{n-1}\quad\text{on } \Sigma_E^0. \tag{4.13}$$

Choose a vector field Y in the neighbourhood of Σ_E^0 such that $dH_0(Y)=-1$. Then $i(X_0)\omega=-dH_0=0$ on Σ_E^0 and

$$i(Y)i(X_0)\omega=\omega(X_0,Y)=-dH_0(Y)=1,$$
$$i(Y)i(X_0)\omega=(n-1)(i(Y)i(X_0)\omega))\wedge\omega^{n-2}=(n-1)\omega^{n-2} \text{ on } \Sigma_E^0.$$

By the same argument, one obtains

$$i(Y)i(X_0)\omega^n=n\omega^{n-1} \text{ on } \Sigma_E^0. \tag{4.14}$$

Using these identities and (4.12), we get

$$i(Y)i(X_0)(S^*\alpha)\wedge\alpha\wedge\omega^{n-1}=i(Y)((S^*\alpha)\wedge\alpha\wedge(i(X_0)\omega^{n-1}) \tag{4.15}$$
$$=(S^*\alpha)\wedge\alpha\wedge i(Y)i(X_0)\omega^{n-1}=(n-1)(S^*\alpha)\wedge\alpha\wedge\omega^{n-2} \text{ on } \Sigma_E^0.$$

Applying $i(Y)i(X_0)$ to both sides of (4.11) and using (4.14), (4.15), one obtains (4.13).

4. By the definition (2.12) of $\widetilde{s}_E$, we have $S_E(z)=\Phi^0_{-\tau(z)}\circ\widetilde{s}_E(z)$, $z\in\Gamma$. It follows that

$$d_zS_E(\xi)=d_z(\Phi_t^0\circ\widetilde{s}_E)(\xi)|_{t=-\tau(z)}-X_0(S_E(z))d_z\tau(d_z\widetilde{s}_E(\xi)),$$

for any $\xi\in T_z\Gamma$. By (4.12), we get

$$\alpha(d_zS_E(\xi))=\alpha(d_z(\Phi_t^0\circ\widetilde{s}_E)(\xi))|_{t=-\tau(z)}=\alpha(d_zs_E(\xi)).$$

It follows that

$$\widetilde{s}_E^*\alpha = (S_E^*\alpha)|_\Gamma. \tag{4.16}$$

5. According to formula (B.4) for CAL, we have

$$\mathrm{CAL}(\widetilde{S}_E) = \mathrm{CAL}(\widetilde{s}_E) = \frac{1}{n!}\int_\Gamma (\tilde{s}_E^*\alpha)\wedge\alpha\wedge\omega^{n-2}.$$

From here, using (4.16) and (4.13), one obtains (4.9). Formula (4.10) is just (4.9) with ω^{n-1} expanded. ∎

4.3. **The case of rotationally symmetric** v**.** Let $v_0 \equiv 0$ and let v be rotationally symmetric, $v(x) = v_1(|x|)$. Then formula (4.9) can be recast in terms of the usual variables of scattering theory: the impact parameter s and the scattering angle ϕ (see [17, Section 18]). For $(q, p) \in \mathbb{R}^{2n}$, $p \neq 0$, the impact parameter $s > 0$ is defined by

$$s = \left| q - \frac{\langle q, p\rangle p}{|p|^2}\right|.$$

Due to the conservation of angular momentum, the impact parameter is the integral of motion for both dynamics Φ^0, Φ. If $(q^+, p^+) = S_E(q^-, p^-)$, then the scattering angle ϕ is defined such that

$$\cos\phi = \frac{\langle p^+, p^-\rangle}{|p^+|^2}. \tag{4.17}$$

Of course, this does not yet define ϕ uniquely. In order to fix ϕ, let us note that due to the rotational symmetry, ϕ depends only on E and s. Thus, for a fixed energy E let us define ϕ as a continuous function of $s \in (0, \infty)$ such that (4.17) holds true and

$$\sin\phi = \frac{\langle p^+, q^-\rangle}{|p^+||q^-|},$$

where q^- is chosen such that $\langle q^-, p^-\rangle = 0$. In other words, $\phi(s) \geqslant 0$ for small repulsive potentials ($v \geqslant 0$) and $\phi(s) \leqslant 0$ for small attractive potentials ($v \leqslant 0$).

Formula for ϕ is well known (see e.g. [17, Section 18]):
(4.18)

$$\phi(s) = \pi - 2\int_{r_{min}}^\infty \frac{sdr}{r^2}\left(1 - \frac{v_1(r)}{E} - \frac{s^2}{r^2}\right)^{-1/2}, \quad r_{min}(s) = \max\left\{r : 1 - \frac{v_1(r)}{E} - \frac{s^2}{r^2} = 0\right\}.$$

It is easy to compute that

$$\rho = \rho(s) = \sqrt{2E}s^2\frac{d\phi}{ds},$$

and therefore

$$\mathrm{CAL}(\widetilde{S}_E) = -\varkappa_n\varkappa_{n-1}(2E)^{n/2}\int_0^\infty s^n\frac{d\phi}{ds}ds = n\varkappa_n\varkappa_{n-1}(2E)^{n/2}\int_0^\infty s^{n-1}\phi(s)ds. \tag{4.19}$$

Substituting (4.18) into (4.19), and using (4.8), it is not difficult to check directly the validity of Theorem 3.1 in this case.

Example 4.3. Let us give an example where the Poincaré scattering map is not homotopic to the identity map. Let $n = 2$, $v_0 = 0$ and v be of the form $v(q) = v_1(|q|)$, $v_1 \geqslant 0$, $v_1(r) = 0$ for $r \geqslant 1$, $v_1'(r) < 0$ for all $r \in (0, 1)$. Let $E \in (0, v_1(0))$. Under these assumptions, (4.7) may or may not hold true. However, using the separation of variables, one can directly check that the completeness condition (2.4) holds true.

In order to make our notation more succinct, let us identify $\mathbb{R}^2$ with $\mathbb{C}$ in the usual way. Then the trajectories $q = q(t)$, $p = p(t)$ of the free dynamics Φ^0 can be parameterised by $\theta \in [0, 2\pi)$ and $\sigma \in \mathbb{R}$ so that

$$q(t) = i\sigma e^{i\theta} + t\sqrt{2E}e^{i\theta}, \quad p(t) = p(0) = \sqrt{2E}e^{i\theta}.$$

Of course, $|\sigma|$ is the impact parameter.

It is easy to see that $\sigma\sqrt{2E}$, θ are symplectic coordinates on $\widetilde{\Sigma}_E^0$, and so $\widetilde{\Sigma}_E^0$ can be identified with a cylinder $T^*\mathbb{S}^1$ (as in Example B.3). Due to the conservation of angular momentum, the Poincaré scattering map has the form

$$\widetilde{S}_E : (\sigma, \theta) \mapsto (\sigma, \theta + \varphi(\sigma))$$

where $\varphi(\sigma) = 0$ for $\sigma \leqslant -1$ and $\varphi(\sigma) = 2\pi$ for $\sigma \geqslant 1$. Here φ is the scattering angle with a different normalisation. Since the map $\widetilde{S}_E$ "twists" the cylinder $T^*\mathbb{S}^1$, it is easy to see that $\widetilde{S}_E$ is not homotopic to the identity map: $\widetilde{S}_E \notin \mathrm{Symp}_0^c(T^*\mathbb{S}^1)$.

5. Auxiliary statements

5.1. **Exactness of $\widetilde{\Sigma}_E^0$.** Recall that $\mathcal{N}$ is called exact if there exists a 1-form α on $\mathcal{N}$ such that $d\alpha = \omega$. Here we prove that exactness of $\mathcal{N}$ implies exactness of $\widetilde{\Sigma}_E^0$. In the course of the proof, we construct an atlas on $\widetilde{\Sigma}_E^0$.

Lemma 5.1. *Let Assumption 2.1 (i)–(iii) hold true and suppose that $\mathcal{N}$ is exact. Then the 1-form α on $\mathcal{N}$ such that $d\alpha = \omega$ can be chosen in such a way that*

$$i(X_0)\alpha = 0 \quad \text{on } \Sigma_E^0. \tag{5.1}$$

Moreover, there exists a 1-form $\widetilde{\alpha}$ on $\widetilde{\Sigma}_E^0$ such that $d\widetilde{\alpha} = \widetilde{\omega}_0$ and $\pi_0^*\widetilde{\alpha} = \alpha|_{\Sigma_E^0}$.

Proof. 1. First let us construct an atlas on $\widetilde{\Sigma}_E^0$. Fix $y_0 \in \widetilde{\Sigma}_E^0$ and choose $x_0 \in y_0$. Using local coordinates around x_0, it is easy to construct a manifold $\Gamma_0 \subset \Sigma_E^0$ of dimension $2n-2$ such that $x_0 \in \Gamma_0$ and $X_0(x) \notin T_x\Gamma_0$ for all $x \in \Gamma_0$. By Assumption 2.1(iii), there exists $T > 0$ such that for all $|t| \geqslant T$, one has $\Phi_t^0(\overline{\Gamma}_0) \cap \overline{\Gamma}_0 = \emptyset$; here $\overline{\Gamma}_0$ is the closure of Γ_0 in Σ_E^0. It follows that the orbit $\Phi_t^0(x_0)$ can intersect Γ_0 only finitely many times. By reducing Γ_0 if necessary, we can ensure that $\Phi_t^0(x_0) \notin \overline{\Gamma}_0$ for all $t \neq 0$.

Next, since we may assume Γ_0 to be pre-compact, there exists $\epsilon > 0$ such that for all $0 < |t| < \epsilon$, one has $\Phi_t^0(\overline{\Gamma}_0) \cap \overline{\Gamma}_0 = \emptyset$. Since the closed set $K = \{\Phi_t^0(x_0) \mid \epsilon \leqslant |t| \leqslant T\}$

has empty intersection with $\overline{\Gamma}_0$, there exists an open neighbourhood of K which has empty intersection with $\overline{\Gamma}_0$. It follows that one can choose a subset $\Gamma \subset \Gamma_0$ (which is itself a manifold of dimension $2n-2$) such that $\Phi_t^0(\Gamma) \cap \Gamma = \emptyset$ for all $t \neq 0$. Thus, we have constructed a "local Poincaré section", i.e. Γ parameterises $\{\Phi_t^0(x) \mid t \in \mathbb{R},\ x \in \Gamma\} \subset \Sigma_E^0$ rather than the whole manifold Σ_E^0.

Such a manifold Γ can be constructed for any point $y_0 \in \widetilde{\Sigma}_E^0$; then the corresponding sets $\pi_0(\Gamma)$ form an open cover of $\widetilde{\Sigma}_E^0$. Let us choose a locally finite subcover $\{\pi_0(\Gamma_j)\}$ of this cover and a smooth partition of unity $\{\widetilde{\zeta}_j\}$ on $\widetilde{\Sigma}_E^0$ subordinate to this subcover (i.e. for each j, $\operatorname{supp}\widetilde{\zeta}_j$ lies entirely within one of the sets $\pi_0(\Gamma_j)$). Clearly, we have an associated partition of unity $\{\zeta_j\}$ on Σ_E^0, $\zeta_j = \widetilde{\zeta}_j \circ \pi_0$.

Of course, if Assumption 2.2 holds true, then the above atlas can be chosen to consist of just one map.

2. Since $\mathcal{N}$ is exact, there exists a 1-form β on $\mathcal{N}$ such that $d\beta = \omega$. Let us construct $F \in C^\infty(\mathcal{N})$ such that $\alpha = \beta + dF$ has the required properties. We will construct F using the atlas described above.

For each j, let us construct a function F_j on $\Omega_j = \{\Phi_t^0(x) \mid t \in \mathbb{R},\ x \in \Gamma_j\}$ such that $\beta(X_0) + dF_j(X_0) = 0$ on Ω_j. This can be done by setting $F_j = 0$ on Γ_j and then extending F_j onto Ω_j by integrating the differential equation

$$\frac{d}{dt} F_j \circ \Phi_t^0(x) = -\beta(X_0 \circ \Phi_t^0(x)) \tag{5.2}$$

along the orbits of Φ^0.

Now let us define $F = \sum_j \zeta_j F_j$ on Σ_E^0 and extend F onto the whole of $\mathcal{N}$ as a smooth function. Then on Σ_E^0 we have

$$i(X_0)\alpha = i(X_0)\beta + i(X_0)dF = \sum_j \zeta_j\ (i(X_0)\beta + i(X_0)dF_j) + \sum_j F_j\ i(X_0)d\zeta_j. \tag{5.3}$$

The first sum in the r.h.s. of (5.3) vanishes by the construction of F_j. Next, by the construction of ζ_j we have

$$0 = \frac{d}{dt}\zeta_j \circ \Phi_t^0(x)|_{t=0} = d\zeta_j(X_0(x)),$$

and so the second sum in the r.h.s. of (5.3) also vanishes. Thus, α satisfies (5.1).

3. Let us prove that there exists a 1-form $\widetilde{\alpha}$ on $\widetilde{\Sigma}_E^0$ such that $\pi_0^*\widetilde{\alpha} = \alpha$. First note that, by Cartan's formula for Lie derivative,

$$L_{X_0}\alpha = di(X_0)\alpha + i(X_0)d\alpha = 0 + i(X_0)\omega = -dH_0 = 0$$

on Σ_E^0, where we have used (5.1). It follows that

$$(\Phi_t^0)^*\alpha|_{\Sigma_E^0} = \alpha|_{\Sigma_E^0} \quad \text{for all } t \in \mathbb{R}. \tag{5.4}$$

Next, let $x, y \in \Sigma_E^0$ and let $\xi \in T_x\Sigma_E^0$, $\eta \in T_y\Sigma_E^0$ be such that $\pi_0(x) = \pi_0(y)$ and $d_x\pi_0(\xi) = d_y\pi_0(\eta)$. This means that for some $t, c \in \mathbb{R}$, one has $y = \Phi_t^0(x)$ and $\eta = d_x\Phi_t^0(\xi) + cX_0(y)$. Then, using (5.1) and (5.4), we obtain

$$\alpha_y(\eta) = \alpha_y(d_x\Phi_t^0(\xi) + cX_0(y)) = \alpha_y(d_x\Phi_t^0(\xi)) = \alpha_x(\xi).$$

Thus, $\alpha : T\Sigma_E^0 \to \mathbb{R}$ is constant on the pre-images of any point under the map $d\pi_0 : T\Sigma_E^0 \to T\widetilde{\Sigma}_E^0$. This shows that one can define a smooth 1-form $\widetilde{\alpha}$ on $\widetilde{\Sigma}_E^0$ such that $\pi_0^*\widetilde{\alpha} = \alpha$.

4. Let us prove that $d\widetilde{\alpha} = \widetilde{\omega}_0$. We have

$$\pi_0^*\widetilde{\omega}_0 = \omega = d\alpha = d\pi_0^*\widetilde{\alpha} = \pi_0^* d\widetilde{\alpha},$$

and so $\pi_0^*(\widetilde{\omega}_0 - d\widetilde{\alpha}) = 0$. Since π_0 is a surjection, it follows that $d\widetilde{\alpha} = \widetilde{\omega}_0$. ∎

5.2. **Separation of variables in integrals over Σ_E^0.** We will need the following version of Fubini's theorem:

Lemma 5.2. *Let μ be a 1-form on Σ_E^0 and $\Omega \subset \Sigma_E^0$ be an open pre-compact set. Define*

$$\delta(x) = \int_{-\infty}^{\infty} \chi_\Omega \circ \Phi_t^0(x)\ (i(X_0)\mu) \circ \Phi_t^0(x) dt, \quad x \in \Sigma_E^0,$$

and let $\widetilde{\delta} : \widetilde{\Sigma}_E^0 \to \mathbb{R}$ be the corresponding function such that $\widetilde{\delta} \circ \pi_0 = \delta$. Then

$$\int_\Omega \mu \wedge \omega^{n-1} = \int_{\widetilde{\Sigma}_E^0} \widetilde{\delta}\ \widetilde{\omega}_0^{n-1}.$$

We note that this lemma, with obvious modifications, can (and will) also be applied to integrals over Σ_E and $\widetilde{\Sigma}_E$ instead of Σ_E^0, $\widetilde{\Sigma}_E^0$.

Proof. 1. Let ζ_j, $\widetilde{\zeta}_j$, Γ_j be as in the proof of Lemma 5.1. It suffices to prove that

$$\int_\Omega \zeta_j \mu \wedge \omega^{n-1} = \int_{\widetilde{\Sigma}_E^0} \widetilde{\zeta}_j\ \widetilde{\delta}\ \widetilde{\omega}_0^{n-1}. \tag{5.5}$$

Next, as in Section 2.4, we have a map $\gamma_j : \Gamma_j \to \widetilde{\Sigma}_E^0$ which is a symplectic diffeomorphism onto its range. Using this map, we can rewrite the integral in the r.h.s. of (5.5) as the integral over Γ_j. Thus, it suffices to prove that

$$\int_\Omega \zeta_j \mu \wedge \omega^{n-1} = \int_{\Gamma_j} \zeta_j(x)\omega^{n-1}(x) \int_{-\infty}^{\infty} \chi_\Omega \circ \Phi_t^0(x)\ (i(X_0)\mu) \circ \Phi_t^0(x) dt. \tag{5.6}$$

2. Let us prove (5.6). Consider the map $\phi : \mathbb{R} \times \Gamma_j \to \Sigma_E^0$, $\phi(t, x) = \Phi_t^0(x)$. We have

$$\int_\Omega \zeta_j \mu \wedge \omega^{n-1} = \int_{\mathbb{R}\times\Gamma_j} (\zeta_j \circ \phi)(\chi_\Omega \circ \phi)(\phi^*\mu) \wedge (\phi^*\omega)^{n-1}. \tag{5.7}$$

Since Φ_t^0 is a symplectic map, we get for any $\xi, \eta \in T_x\Gamma_j$:

$$(\phi^*\omega)_{(t,x)}(\xi, \eta) = \omega_{\Phi_t^0(x)}(d_x\Phi_t^0(\xi), d_x\Phi_t^0(\eta)) = \omega_x(\xi, \eta).$$

Further, let $(t, x_1, \dots, x_{2n-2})$ be local coordinates on $\mathbb{R}\times\Gamma_j$ and let $\frac{\partial}{\partial t}, \frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_{2n-2}}$ be the corresponding basis in the tangent space $T_{(t,x)}(\mathbb{R}\times\Gamma_j)$. For any $\xi\in T_x\Gamma_j$, we have

$$(\phi^*\omega)_{(t,x)}(\frac{\partial}{\partial t}, \xi) = \omega_x(X_0(x), d_x\Phi_t^0(\xi)) = -d_xH_0(d_x\Phi_t^0(\xi)) = 0,$$

and so

$$((\phi^*\mu)\wedge(\phi^*\omega)^{n-1})_{(t,x)}(\frac{\partial}{\partial t}, \frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_{2n-2}}) = \mu_{\Phi_t^0(x)}(X_0(\Phi_t^0(x)))\omega_x^{n-1}(\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_{2n-2}}).$$

It follows that we can separate integration over Γ_j and over $\mathbb{R}$ in (5.7), which yields the required identity (5.6). ∎

6. Proof of Theorem 3.1

6.1. **A generating function of $\widetilde{S}_E$.** Here we use the notion of a generating function of a symplectic map; see Appendix B. Let α be a 1-form on $\mathcal{N}$ as in Lemma 5.1. Let us define a function Δ on Σ_E by

$$\Delta(x) = -\int_{-\infty}^{\infty}(i(X)\alpha)\circ\Phi_t(x)dt, \quad x\in\Sigma_E. \tag{6.1}$$

Note that by (5.1), for all sufficiently large $|t|$ one has

$$(i(X)\alpha)\circ\Phi_t(x) = (i(X_0)\alpha)\circ\Phi_t(x) = 0$$

and so the integration in (6.1) is actually performed over a bounded set of t. It follows that $\Delta\in C^\infty(\Sigma_E)$.

It follows directly from the definition that Δ is constant on the orbits of Φ_t and therefore there exists $\widetilde{\Delta}\in C^\infty(\widetilde{\Sigma}_E)$ such that $\widetilde{\Delta}\circ\pi = \Delta$. Since $\Sigma_E\cap\operatorname{supp}(H-H_0)$ is compact, it follows that $\operatorname{supp}\widetilde{\Delta}$ is compact and so $\widetilde{\Delta}\in C_0^\infty(\widetilde{\Sigma}_E)$.

Lemma 6.1. *Under the assumptions of Theorem 3.1, we have* $\widetilde{S}_E\in\operatorname{Dom}(\mathrm{CAL}, \widetilde{\Sigma}_E^0)$ *and*

$$n\,\mathrm{CAL}(\widetilde{S}_E) = \int_{\widetilde{\Sigma}_E}\widetilde{\Delta}(x)\frac{\widetilde{\omega}^{n-1}(x)}{(n-1)!}. \tag{6.2}$$

Proof. 1. First recall the well known formula for the derivative of reduced action. Let $T>0$ and

$$f_T(x) = \int_0^T(i(X)\alpha)\circ\Phi_t(x)dt, \quad x\in\Sigma_E;$$

then

$$df_T = \Phi_T^*\alpha - \alpha + TdH. \tag{6.3}$$

On Σ_E, we have $H=E$ and so the last term in the r.h.s. of (6.3) vanishes.

2. Let us check that the function $\Delta_0 = \Delta\circ W_-\in C^\infty(\Sigma_E^0)$ satisfies the identity

$$\alpha - S_E^*\alpha = d\Delta_0 \quad \text{on } \Sigma_E^0. \tag{6.4}$$

Let $K \subset \Sigma_E^0$ be a compact set. We can choose $T > 0$ sufficiently large so that for all $x \in K$,

$$S_E(x) = \Phi^0_{-T} \circ \Phi_{2T} \circ \Phi^0_{-T}(x)$$

and

$$\Delta(x) = -\int_{-T}^{T} (i(X)\alpha) \circ \Phi_t(x) dt = -f_{2T} \circ \Phi_{-T}(x).$$

Thus, using (5.4) and (6.3), we have on K:

$$\begin{aligned} S_E^* \alpha &= (\Phi^0_{-T})^* (\Phi_{2T})^* (\Phi^0_{-T})^* \alpha = (\Phi^0_{-T})^* (df_{2T} + \alpha) \\ &= d(f_{2T} \circ \Phi^0_{-T}) + \alpha = d(f_{2T} \circ \Phi_{-T} \circ W_-) + \alpha = -d(\Delta \circ W_-) + \alpha = -d\Delta_0 + \alpha, \end{aligned}$$

which proves (6.4).

3. Let $\widetilde{\Delta}_0 \in C_0^\infty(\widetilde{\Sigma}_E^0)$ be a function such that $\widetilde{\Delta}_0 \circ \pi_0 = \Delta_0$. Using the formula $\alpha = \pi_0^* \widetilde{\alpha}$ and (2.10), we can rewrite (6.4) as

$$\pi_0^* (\widetilde{\alpha} - \widetilde{S}_E^* \widetilde{\alpha}) = \pi_0^* d\widetilde{\Delta}_0.$$

Since π_0 is a surjection, it follows that

$$\widetilde{\alpha} - \widetilde{S}_E^* \widetilde{\alpha} = d\widetilde{\Delta}_0 \quad \text{on } \widetilde{\Sigma}_E^0, \tag{6.5}$$

i.e. $\widetilde{\Delta}_0$ is an $\widetilde{\alpha}$-generating function of $\widetilde{S}_E$. Thus, $\widetilde{S}_E \in \mathrm{Dom}(\mathrm{CAL}, \widetilde{\Sigma}_E^0)$ and, according to the definition (B.3),

$$n\, \mathrm{CAL}(\widetilde{S}_E) = \int_{\widetilde{\Sigma}_E^0} \widetilde{\Delta}_0(x) \frac{\widetilde{\omega}_0^{n-1}(x)}{(n-1)!}. \tag{6.6}$$

4. Let $\widetilde{W}_-$ be as in (2.11). Since $\widetilde{W}_-^* \widetilde{\omega} = \widetilde{\omega}_0$, by a change of variable in the integral (6.6) we obtain (6.2). ∎

6.2. **Application of Stokes' formula.** Below we apply Stokes' formula to rewrite the integral (2.19) in the definition of ξ. The following statement is used in the proof of Theorem 3.1 but it might be of an independent interest.

Proposition 6.2. *Let α be a 1-form on $\mathcal{N}$ as in Lemma 5.1; then the identity*

$$\xi(E) = -\frac{1}{n!} \int_{\Sigma_E} \alpha \wedge \omega^{n-1} \tag{6.7}$$

holds true.

Proof. 1. We first note that

$$\alpha \wedge \omega^{n-1}|_{\Sigma_E^0} = 0. \tag{6.8}$$

Indeed, $i(X_0)\alpha|_{\Sigma_E^0} = 0$ by (5.1), and $i(X_0)\omega = -dH_0 = 0$ on Σ_E^0 since Σ_E^0 is a constant energy surface. Thus, $i(X_0)(\alpha \wedge \omega^{n-1})|_{\Sigma_E^0} = 0$; since $\alpha \wedge \omega^{n-1}$ has a maximal rank on Σ_E^0, it follows that (6.8) holds true.

2. Let $\Omega \subset \mathcal{N}$ be a compact set with a smooth boundary such that $\mathrm{supp}(H - H_0) \cap G(E) \subset \Omega$ and $\mathrm{supp}(H - H_0) \cap G_0(E) \subset \Omega$. Since

$$\Sigma_E \setminus \Omega = \Sigma_E^0 \setminus \Omega,$$

by (6.8) the integrand in (6.7) vanishes outside Ω. Thus, the integration in (6.7) is in fact performed over $\Sigma_E \cap \Omega$ and so the r.h.s. is finite.

3. Writing $G = G(E)$ and $G_0 = G_0(E)$ for brevity, we get

$$\xi(E) = \int_{\mathcal{N}} (\chi_{G_0} - \chi_G) \frac{\omega^n}{n!} = \int_{\mathcal{N} \cap \Omega} (\chi_{G_0} - \chi_G) \frac{\omega^n}{n!} = \int_{G_0 \cap \Omega} \frac{\omega^n}{n!} - \int_{G \cap \Omega} \frac{\omega^n}{n!}.$$

We have $d(\alpha \wedge \omega^{n-1}) = \omega^n$ and therefore, by the Stokes' formula,

$$\begin{aligned} n!\xi(E) &= \int_{\partial(G_0 \cap \Omega)} \alpha \wedge \omega^{n-1} - \int_{\partial(G \cap \Omega)} \alpha \wedge \omega^{n-1} \\ &= \int_{\Sigma_E^0 \cap \Omega} \alpha \wedge \omega^{n-1} - \int_{\Sigma_E \cap \Omega} \alpha \wedge \omega^{n-1} = - \int_{\Sigma_E} \alpha \wedge \omega^{n-1} \end{aligned}$$

since the integrals over $G_0 \cap \partial\Omega$ and $G \cap \partial\Omega$ cancel out. ∎

6.3. **The rest of the proof of Theorem 3.1.** By (6.2) and (6.7), it remains to prove that

$$- \int_{\Sigma_E} \alpha \wedge \omega^{n-1} = \int_{\widetilde{\Sigma}_E} \widetilde{\Delta}(x) \widetilde{\omega}^{n-1}(x).$$

This follows from Lemma 5.2 with $\mu = \alpha$, $\Omega = \Sigma_E$.

7. Time delay: Proof of Theorems 2.3 and 3.2

7.1. **Proof of Theorem 2.3.** 1. Our first aim is to prove that the r.h.s. of (2.17) is independent of k for all sufficiently large k. Denote $K_0 = \mathrm{supp}(H - H_0) \cap \Sigma_E^0$ and $\widetilde{K}_0 = \pi_0(K_0)$. It is easy to see that $\mathrm{supp}(\widetilde{u}_k \circ \widetilde{W}_- - \widetilde{u}_k^0) \subset \widetilde{K}_0$ and therefore the integration in the r.h.s. of (2.17) is actually performed over $\widetilde{K}_0$.

By Assumption 2.1(iii), there exists $T > 0$ such that for all $|t| \geqslant T$ one has

$$\Phi_t^0(K_0) \cap K_0 = \emptyset. \tag{7.1}$$

Then we have

$$\begin{aligned} \Phi_t \circ W_-(x) &= \Phi_t^0(x), \quad t \leqslant -T, \quad \forall x \in K_0, \\ \Phi_t \circ W_-(x) &= \Phi_t^0 \circ S_E(x), \quad t \geqslant T \quad \forall x \in K_0. \end{aligned}$$

Let us choose ℓ sufficiently large so that for all $|t| \leqslant T$, we have

$$\Phi_t^0(K_0) \subset \Omega_\ell, \quad \Phi_t \circ W_-(K_0) \subset \Omega_\ell. \tag{7.2}$$

Then for all $x \in K_0$ and all $k \geqslant \ell$:

$$u_k \circ W_-(x) - u_k^0(x) = \int_0^\infty (\chi_{\Omega_k} \circ \Phi_t^0 \circ S_E(x) - \chi_{\Omega_k} \circ \Phi_t^0(x))dt. \tag{7.3}$$

Next, let us define

$$v_k(x) = \int_0^\infty \chi_{\Omega_k \setminus \Omega_\ell} \circ \Phi_t^0(x)dt, \quad x \in K_0, \quad k \geqslant \ell. \tag{7.4}$$

Comparing (7.3) and (7.4), we get

$$(u_k \circ W_-(x) - u_k^0(x)) - (u_\ell \circ W_-(x) - u_\ell^0(x)) = v_k \circ S_E(x) - v_k(x), \quad x \in K_0. \tag{7.5}$$

From (7.2) it follows that $v_k \circ \Phi_t^0(x) = v_k(x)$ for all $x \in K_0$ and $|t| \leqslant T$. Let us define $\widetilde{v}_k : \widetilde{K}_0 \to \mathbb{R}$ such that $\widetilde{v}_k \circ \pi_0(x) = v_k(x)$, $x \in K_0$. Then from (7.5) it follows that

$$\begin{aligned} \int_{\widetilde{K}_0} \Big\{ (\widetilde{u}_k \circ \widetilde{W}_-(y) - \widetilde{u}_k^0(y)) - (\widetilde{u}_\ell \circ \widetilde{W}_-(y) - \widetilde{u}_\ell^0(y)) \Big\} \frac{\omega_0^{n-1}(y)}{(n-1)!} \\ = \int_{\widetilde{K}_0} (\widetilde{v}_k \circ \widetilde{S}_E(y) - \widetilde{v}_k(y)) \frac{\widetilde{\omega}_0^{n-1}(y)}{(n-1)!}. \end{aligned} \tag{7.6}$$

Since $\widetilde{S}_E : \widetilde{\Sigma}_E^0 \to \widetilde{\Sigma}_E^0$ is a symplectic diffeomorphism and $\widetilde{S}_E(x) = x$ for $x \notin \widetilde{K}_0$, we see that the r.h.s. of (7.6) vanishes. This proves that the r.h.s. of (2.17) is independent of $k \geqslant \ell$. Thus, the limit (2.15) exists.

2. Let us prove that the limit in (2.15) is independent of the choice of the sequence $\{\Omega_k\}$. First note that the limit (2.15) can be calculated over any subsequence of $\{\Omega_k\}$. Next, let $\{\Omega'_k\}$ be another sequence of sets with the same properties as $\{\Omega_k\}$. Then it is easy to construct sequences of indices $p_1 < p_2 < \cdots$ and $q_1 < q_2 < \cdots$ such that

$$\Omega_{p_1} \subset \Omega'_{q_1} \subset \Omega_{p_2} \subset \Omega'_{q_2} \subset \cdots \tag{7.7}$$

Then the sequence $\{\Omega_{p_k}\}$ is a subsequence of both the sequence (7.7) and the sequence $\{\Omega_k\}$. It follows that the limits (2.15) over the sequence (7.7) and over the sequence $\{\Omega_k\}$ coincide. In the same way, the limits (2.15) over the sequence (7.7) and over the sequence $\{\Omega'_k\}$ coincide.

3. Let us prove (2.16). Since $\operatorname{supp}(H - H_0) \cap \Sigma_E^0$ is compact, there exists a compact set $\Gamma_0 \subset \Gamma$ such that for all $z \in \Gamma \setminus \Gamma_0$ and all $t \in \mathbb{R}$, one has $\Phi_t(z) = \Phi_t^0(z)$ (for example, one can take $\Gamma_0 = \Gamma \cap K_0$). Then we have $\operatorname{supp} \tau_E \subset \Gamma_0$ and also

$$T_E = \int_{\Gamma_0} (u_k \circ W_-(z) - u_k^0(z)) \frac{\omega^{n-1}(z)}{(n-1)!},$$

for all sufficiently large k.

Let ℓ be sufficiently large so that (7.2) holds true and also assume (by increasing ℓ if necessary) that for all $k \geqslant \ell$ and all $z \in \Gamma_0$, one has $\Phi_t^0(z) \in \Omega_k$ for $|t| \leqslant |\tau(z)|$. Using (7.3) and the representation (2.12) for the scattering map, we get for all $z \in \Gamma_0$:

$$(7.8) \quad u_k \circ W_-(z) - u_k^0(z) = \int_0^\infty \{\chi_{\Omega_k} \circ \Phi_t^0 \circ \Phi_{-\tau(z)}^0 \circ \widetilde{s}_E(z) - \chi_{\Omega_k} \circ \Phi_t^0(z)\} dt$$
$$= \int_0^\infty \{\chi_{\Omega_k} \circ \Phi_t^0 \circ \widetilde{s}_E(z) - \chi_{\Omega_k} \circ \Phi_t^0(z)\} dt + \int_{-\tau(z)}^0 \chi_{\Omega_k} \circ \Phi_t^0 \circ \widetilde{s}_E(z) dt$$
$$= \int_0^\infty \{\chi_{\Omega_k} \circ \Phi_t^0 \circ \widetilde{s}_E(z) - \chi_{\Omega_k} \circ \Phi_t^0(z)\} dt + \tau(z).$$

Next, since $\widetilde{s}_E : \Gamma \to \Gamma$ is a symplectic diffeomorphism, we get

$$(7.9) \qquad \int_{\Gamma_0} \chi_{\Omega_k} \circ \Phi_t^0 \circ \widetilde{s}_E(z) \omega^{n-1}(z) = \int_{\Gamma_0} \chi_{\Omega_k} \circ \Phi_t^0(z) \omega^{n-1}(z)$$

for all $t \in \mathbb{R}$. Finally, integrating (7.8) over Γ_0 with respect to the symplectic volume form $\frac{\omega^{n-1}}{(n-1)!}$ and using (7.9), we arrive at (2.16).

7.2. **Proof of Theorem 3.2.** 1. Let $\Omega_1 \subset \Omega_2 \subset \cdots \subset \mathcal{N}$ be a sequence of open pre-compact sets such that $\cup_{k=1}^\infty \Omega_k = \mathcal{N}$. Choose ℓ sufficiently large so that

$$G(E_1) \cap \operatorname{supp}(H - H_0) \subset \Omega_\ell \quad \text{and } G_0(E_1) \cap \operatorname{supp}(H - H_0) \subset \Omega_\ell.$$

Then for all $k \geqslant \ell$,

$$\frac{d\xi}{dE}(E) = \frac{d}{dE}\left\{\int_{G_0(E)\cap\Omega_k} \frac{\omega^n}{n!} - \int_{G(E)\cap\Omega_k} \frac{\omega^n}{n!}\right\}.$$

2. Let Y_0 be a vector field defined in a neighbourhood of $\Sigma_E^0 \cap \Omega_k$ such that $dH_0(Y_0)|_{\Sigma_E^0} = 1$. Similarly, let Y be a vector field defined in a neighbourhood of $\Sigma_E \cap \Omega_k$ such that $dH(Y)|_{\Sigma_E} = 1$. Then

$$\frac{d\xi}{dE}(E) = \frac{1}{n!}\int_{\Sigma_E^0\cap\Omega_k} i(Y_0)\omega^n - \frac{1}{n!}\int_{\Sigma_E\cap\Omega_k} i(Y)\omega^n$$
$$= \frac{1}{(n-1)!}\int_{\Sigma_E^0\cap\Omega_k} (i(Y_0)\omega) \wedge \omega^{n-1} - \frac{1}{(n-1)!}\int_{\Sigma_E\cap\Omega_k} (i(Y)\omega) \wedge \omega^{n-1}.$$

3. Let us apply Lemma 5.2 to the integrals in the r.h.s. of the last identity. We will take $\mu = i(Y_0)\omega$ for the first integral and $\mu = i(Y)\omega$ for the second integral. Note that $i(X)i(Y)\omega = i(Y)dH = 1$ by our choice of Y, and in the same way $i(X_0)i(Y_0)\omega = 1$. Application of Lemma 5.2 yields

$$\frac{d\xi}{dE}(E) = \int_{\widetilde{\Sigma}_E^0} \widetilde{u}_k^0(y)\frac{\widetilde{\omega}_0^{n-1}(y)}{(n-1)!} - \int_{\widetilde{\Sigma}_E} \widetilde{u}_k(y)\frac{\widetilde{\omega}^{n-1}(y)}{(n-1)!}$$

with $\widetilde{u}_k^0$, $\widetilde{u}_k$ as in Section 2.5. By (2.15), the r.h.s. is $(-T_E)$, as required.

Appendix A: Key formulas in quantum scattering

Here we collect those definitions and formulas in quantum scattering theory which are relevant to the rest of the paper. We do not make any attempt at being rigourous or even precise about the required assumptions. Our cavalier approach will probably horrify experts in quantum scattering but this collection of formulas might be useful for the purposes of comparison of "classical" and "quantum" cases.

Let H_0 and H be self-adjoint operators in a Hilbert space $\mathcal{H}$. In order to simplify our discussion, let us assume that both H_0 and H have purely absolutely continuous spectrum (see e.g. [23, Section VII.2]). The wave operators $W_\pm : \mathcal{H} \to \mathcal{H}$ are defined by

$$W_\pm \psi = \lim_{t\to\pm\infty} e^{itH} e^{-itH_0}\psi, \quad \psi \in \mathcal{H},$$

whenever these limits exist. The wave operators are easily seen to be isometric and intertwine H and H_0: $W_\pm H_0 = H W_\pm$. Completeness of the wave operators is the relation

$$\operatorname{Ran} W_+ = \operatorname{Ran} W_- = \mathcal{H}. \tag{A.1}$$

If H has a non-empty pure point or singular continuous spectrum, then the definition of the wave operators has to be modified and $\mathcal{H}$ in the right hand side of the last relation has to be replaced by the absolutely continuous subspace of H. See [32, Sections 2.1, 2.3] for the details.

If the wave operators exist and are complete, one defines the scattering operator $S = W_+^{-1} W_-$. The scattering operator is unitary and commutes with H_0: $SH_0 = H_0 S$. It follows that S is diagonalised by the direct integral of the spectral decomposition of H_0:

$$\mathcal{H} = \int^{\oplus}_{\operatorname{Spec}(H_0)} \mathfrak{h}(E) dE, \quad (H_0 f)(E) = E f(E), \quad (Sf)(E) = S_E f(E). \tag{A.2}$$

Here S_E is a unitary operator in the fibre space $\mathfrak{h}(E)$; S_E is called the scattering matrix. See [32, Section 2.4] for the details.

Let $P^{(k)}$ be a family of operators in $\mathcal{H}$ such that $P^{(k)}\psi \to \psi$ as $k \to \infty$ for any $\psi \in \mathcal{H}$. Let $\mathcal{T}^{(k)}$ be the operator defined by

$$(\mathcal{T}^{(k)}\psi, \psi) = \int_{-\infty}^{\infty} \|P^{(k)} e^{-itH} W_- \psi\|^2 \, dt - \int_{-\infty}^{\infty} \|P^{(k)} e^{-itH_0}\psi\|^2 \, dt,$$

assuming that these integrals exist. Then $\mathcal{T}^{(k)}$ commutes with H_0 and therefore is diagonal with respect to the direct integral decomposition (A.2). Let $\mathcal{T}_E^{(k)} : \mathfrak{h}(E) \to \mathfrak{h}(E)$ be the corresponding fibre operator. Then the limit $\mathcal{T}_E = \lim_{k\to\infty} \mathcal{T}_E^{(k)}$, whenever it exists, is called the global time delay operator, and $T_E = \operatorname{Tr} \mathcal{T}_E$ is called the global time delay. See [25] for the details.

The spectral shift function $\xi(E)$ is defined by the relation

$$\xi(E) = \operatorname{Tr}(\chi_{(-\infty,E)}(H_0) - \chi_{(-\infty,E)}(H))$$

which has to be understood in a certain regularised sense; see [32, Section 8.2] for the details. The existence of the spectral shift function and the global time delay requires some trace class assumptions on H and H_0, such as $H-H_0 \in$ Trace class or $(H+aI)^{-m}-(H_0+aI)^{-m} \in$ Trace class for some appropriate a and m.

The Birman-Krein formula reads

$$\det S_E = e^{-2\pi i \xi(E)}, \tag{A.3}$$

for a.e. E in the absolutely continuous spectrum of H_0. This formula first appeared in [18, 8] for the one-dimensional Schrödinger operator and was established in [2] in the general case; see e.g. [4] for the details and historical references. In concrete applications this formula is sometimes stated in the form

$$\frac{d}{dE}\log\det S_E = \operatorname{Tr}(S_E^* \frac{dS_E}{dE}) = -2\pi i \frac{d\xi(E)}{dE};$$

see e.g. [7]. The Eisenbud-Wigner formula reads

$$\frac{d}{dE}\operatorname{Im}\,\log\det S_E = T_E; \tag{A.4}$$

see e.g. [25, 9] for the details and references.

Appendix B: Symplectic diffeomorphisms and the Calabi invariant

B.1. **Symplectomorphisms.** We recall some notation and preliminaries from symplectic topology; see e.g. [20] for the details.

Let $(\mathcal{M}, \omega)$ be a non-compact $2m$-dimensional symplectic manifold, possibly with boundary. We need the following notation:

$\operatorname{Symp}(\mathcal{M})$ is the group of all symplectomorphisms (=symplectic diffeomorphisms) on $\mathcal{M}$.

$\operatorname{Symp}^c(\mathcal{M})$ is the group of all symplectomorphisms of $\mathcal{M}$ with compact support, $\operatorname{supp}\psi = \operatorname{Clos}\{x \mid \psi(x) \neq x\}$.

$\operatorname{Symp}^c_0(\mathcal{M})$ is the path connected component of the identity map in $\operatorname{Symp}^c(\mathcal{M})$.

$\operatorname{Ham}^c(\mathcal{M})$ is the set of all compactly supported Hamiltonian symplectomorphisms of $\mathcal{M}$. This means that $\psi \in \operatorname{Ham}^c(\mathcal{M})$ can be constructed as a time one flow of a family of time-dependent compactly supported Hamiltonians. More precisely, $\psi \in \operatorname{Ham}^c(\mathcal{M})$ means that there exists a smooth family h_t, $t \in [0,1]$ of Hamiltonians on $\mathcal{M}$ such that $\cup_{t\in[0,1]} \operatorname{supp} h_t$ lies in a compact set and if ψ_t is the corresponding flow and X_t the corresponding vector field,

$$\frac{d}{dt}\psi_t = X_t \circ \psi_t, \quad i(X_t)\omega = -dh_t, \quad \psi_0 = id, \tag{B.1}$$

then $\psi = \psi_1$.

It is easy to see (cf. [20, Section 10]) that

$$\operatorname{Ham}^c(\mathcal{M}) \subset \operatorname{Symp}^c_0(\mathcal{M}) \subset \operatorname{Symp}^c(\mathcal{M}). \tag{B.2}$$

B.2. **The Calabi invariant.** Let us assume that $\mathcal{M}$ is exact, i.e. there is a 1-form α such that $\omega = d\alpha$. We recall the definition of the Calabi invariant CAL; for the details, see [20]. For our purposes we need to define CAL on a wider set of symplectomorphisms than it is usually done. Let $\mathrm{Dom}(\mathrm{CAL}, \mathcal{M})$ be the set of all $\psi \in \mathrm{Symp}^c(\mathcal{M})$ such that there exists a 1-form α and $f \in C_0^\infty(\mathcal{M})$ with $d\alpha = \omega$ and $\alpha - \psi^*\alpha = df$. In this case we will say that f is an α-generating function of ψ.

If $\psi \in \mathrm{Dom}(\mathrm{CAL}, \mathcal{M})$ and f is an α-generating function of ψ, let us define

$$\mathrm{CAL}(\psi) = \frac{1}{m+1} \int_{\mathcal{M}} f(x) \frac{\omega^m(x)}{m!}. \tag{B.3}$$

Note that our sign conventions and normalisation differ from those of [20].

Since the choice of α above is not unique, a symplectomorphism can have many generating functions. However, we have

Proposition B.1. *(i)* $\mathrm{CAL}(\psi)$ *is independent of the choice of* α.

(ii) If f *is an* α*-generating function of* ψ*, then* $\mathrm{CAL}(\psi)$ *can be calculated as*

$$\mathrm{CAL}(\psi) = \frac{1}{(m+1)!} \int_{\mathcal{M}} (\psi^*\alpha) \wedge \alpha \wedge \omega^{m-1}. \tag{B.4}$$

(iii) Suppose $\psi \in \mathrm{Ham}^c(\mathcal{M})$ *is generated by a family of Hamiltonians* $\{h_t\}$*, see* (B.1). *Then* $\psi \in \mathrm{Dom}(\mathrm{CAL}, \mathcal{M})$ *and*

$$\mathrm{CAL}(\psi) = \int_0^1 dt \int_{\mathcal{M}} h_t(x) \frac{\omega^m(x)}{m!}.$$

Proof. (i) This is a well known calculation, see e.g. [20, Lemma 10.27]. Suppose that $\alpha_j - \psi^*\alpha_j = df_j$, $f_j \in C_0^\infty(\mathcal{M})$, $d\alpha_j = \omega$, $j = 1, 2$. Denote $\beta = \alpha_2 - \alpha_1$, $g = f_2 - f_1$; then we have $d\beta = 0$, $\beta - \psi^*\beta = dg$. We need to prove that $\int_{\mathcal{M}} g\omega^m = 0$.

As in [20, Lemma 10.27], we have

$$\begin{aligned}\int_{\mathcal{M}} g\omega^m &= \int_{\mathcal{M}} g\, d\alpha_1 \wedge \omega^{m-1} = \int_{\mathcal{M}} (d(g\alpha_1) - (dg) \wedge \alpha_1) \wedge \omega^{m-1} = -\int_{\mathcal{M}} (dg) \wedge \alpha_1 \wedge \omega^{m-1} \\ &= \int_{\mathcal{M}} (\psi^*\beta - \beta) \wedge \alpha_1 \wedge \omega^{m-1} = \int_{\mathcal{M}} (\psi^*\beta) \wedge \alpha_1 \wedge \omega^{m-1} - \int_{\mathcal{M}} \psi^*(\beta \wedge \alpha_1 \wedge \omega^{m-1}) \\ &= \int_{\mathcal{M}} \psi^*\beta \wedge (\alpha_1 - \psi^*\alpha_1) \wedge \omega^{m-1} = \int_{\mathcal{M}} \psi^*\beta \wedge df_1 \wedge \omega^{m-1} = -\int_{\mathcal{M}} d(f_1 \psi^*\beta \wedge \omega^{m-1}) = 0,\end{aligned}$$

as required.

(ii) Similarly to the previous calculation, using Stokes formula, we have

$$\begin{aligned}(m+1)!\, \mathrm{CAL}(\psi) &= \int_{\mathcal{M}} f(d\alpha) \wedge \omega^{m-1} = \int_{\mathcal{M}} f d(\alpha \wedge \omega^{m-1}) = -\int_{\mathcal{M}} df \wedge \alpha \wedge \omega^{m-1} \\ &= \int_{\mathcal{M}} (\psi^*\alpha - \alpha) \wedge \alpha \wedge \omega^{m-1} = \int_{\mathcal{M}} \psi^*\alpha \wedge \alpha \wedge \omega^{m-1},\end{aligned}$$

since $\alpha \wedge \alpha = 0$.

(iii) Is well known; see [20, Lemma 10.27]. ∎

Remark B.2. The Calabi invariant is usually defined as a map $\mathrm{Ham}^c(\mathcal{M}) \to \mathbb{R}$, in which case it is a homomorphism; see [20]. On the domain $\mathrm{Dom}(\mathrm{CAL}, \mathcal{M})$ this is in general not the case: it is not difficult to show that $\mathrm{Dom}(\mathrm{CAL}, \mathcal{M})$ is, in general, not a subgroup of $\mathrm{Symp}^c(\mathcal{M})$. Example B.3 below shows that in general neither of the two sets $\mathrm{Symp}^c_0(\mathcal{M})$, $\mathrm{Dom}(\mathrm{CAL}, \mathcal{M})$ is a subset of the other one.

Example B.3. Let $(\mathcal{M}, \omega)$ be $T^*\mathbb{S}^1$ with the canonical symplectic structure of the cotangent bundle (see e.g. [20, Section 3.1]). Let $(s, \theta) \in \mathbb{R} \times [0, 2\pi]$ be the coordinates in $T^*\mathbb{S}^1$. All possible one-forms α such that $d\alpha = \omega$ can be described as $\alpha = sd\theta + \gamma d\theta + dg$, where $\gamma \in \mathbb{R}$ and $g \in C^\infty(T^*\mathbb{S}^1)$. Consider the symplectic diffeomorphism ψ of $T^*\mathbb{S}^1$, defined by

$$\psi : (s, \theta) \mapsto (s, \theta + \phi(s)),$$

where $\phi \in C^\infty(\mathbb{R})$. Consider the following cases:

(i) Suppose $\phi(s) = 0$ for $s \leqslant -1$ and $\phi(s) = 2\pi$ for $s \geqslant 1$, and $\int_{\mathbb{R}} s\phi'(s)ds = 0$. Then ψ is not homotopic to identity, but $\psi^*(sd\theta) - sd\theta = s\phi'(s)ds$ and so $\psi \in \mathrm{Dom}(\mathrm{CAL}, T^*\mathbb{S}^1)$. Thus, $\mathrm{Dom}(\mathrm{CAL}, T^*\mathbb{S}^1)$ is not a subset of $\mathrm{Symp}^c_0(T^*\mathbb{S}^1)$.

(ii) Suppose $\phi \in C_0^\infty(\mathbb{R})$, and $\int_{\mathbb{R}} s\phi'(s)ds \neq 0$. Then it is easy to see that $\psi \in \mathrm{Symp}^c_0(T^*\mathbb{S}^1)$ but $\psi \notin \mathrm{Dom}(\mathrm{CAL}, T^*\mathbb{S}^1)$.

B.3. $\log\det$ **and** CAL**.** Here, without any attempt at being rigourous, we point out an analogy between the Calabi invariant of a symplectic map and the logarithm of the determinant of a unitary operator. This analogy helps to understand the relation between Theorems 3.1, 3.2 and their "quantum" counterparts (A.3), (A.4).

In order to make our discussion concrete, suppose $\mathcal{M} = \mathbb{R}^{2n}$ and let us use the Weyl quantisation procedure. That is, for a real valued function $h \in C_0^\infty(\mathbb{R}^{2n})$, let us define the self-adjoint operator

$$(Hu)(q) = \int_{\mathbb{R}^{2n}} e^{i\langle q-q',p\rangle} h(\tfrac{q+q'}{2}, p) u(q') d^n q' d^n p.$$

Then, clearly,

$$\mathrm{Tr}\, H = \int_{\mathbb{R}^{2n}} h(q,p)\; d^n q\; d^n p = \int_{\mathbb{R}^{2n}} h(x) \frac{\omega^n(x)}{n!}. \tag{B.5}$$

Further, let U be the unitary operator obtained from H by means of exponentiation: $U = \exp(-iH)$. U can be regarded as a time one map corresponding to the differential equation $i\frac{d}{dt}U(t) = HU(t)$. The "classical" analogue of this procedure is taking the time one map of the Hamiltonian flow Φ_t generated by h. We have

$$\det U = \exp(-i\,\mathrm{Tr}\, H) = \exp\left(-i \int h \frac{\omega^n}{n!}\right) = \exp(-i\,\mathrm{CAL}(\Phi_1)).$$

In other words, we have a diagram

$$\begin{array}{ccc}
h & \xrightarrow{\textit{Quantisation}} & H \\
{\scriptstyle \textit{classical dynamics}}\downarrow & & \downarrow{\scriptstyle \textit{quantum dynamics}} \\
\Phi_1 & & e^{-iH} \\
\downarrow & & \downarrow \\
\exp(-i\,\mathrm{CAL}(\Phi_1)) & = & \det e^{-iH}
\end{array}$$

This to some extent explains the analogy between $-\mathrm{Im}\,\log\det$ and CAL.

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