A formula relating sojourn times to the time of arrival in Hamiltonian dynamics

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Abstract

We consider on a symplectic manifold $M$ with Poisson bracket $\{\cdot, \cdot\}$ an Hamiltonian $H$ with complete flow and a family $\Phi \equiv (\Phi_1, \ldots, \Phi_d)$ of abstract position observables satisfying the condition $\{\{\Phi_j, H\}, H\} = 0$ for each $j$. Under these assumptions, we prove a new formula relating sojourn times in dilated regions defined in terms of $\Phi$ to the time of arrival of classical orbits. The correspondence between this formula and a formula established recently in the framework of quantum mechanics is put into evidence.

Among other examples, our theory applies to Stark Hamiltonians, homogeneous Hamiltonians, purely kinetic Hamiltonians, the repulsive harmonic potential, the simple pendulum, central force systems, the Poincaré ball model, covering manifolds, the wave equation, the nonlinear Schrödinger equation, the Korteweg-de Vries equation and quantum Hamiltonians defined via expectation values.

2000 Mathematics Subject Classification: 37J05, 37K05, 37N05, 70H05, 70S05.
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1 Introduction and main results

The purpose of the present paper is to put into evidence a new formula in Hamiltonian dynamics, both simple and general, relating sojourn times in dilated regions defined in terms of abstract position observables to the time of arrival of classical orbits.

Our result is the following. Let $M$ be a (finite or infinite-dimensional) symplectic manifold with symplectic 2-form $\omega$ and Poisson bracket $\{\cdot, \cdot\}$. Let $H \in C^\infty(M)$ be an Hamiltonian on $M$ with complete flow $\{\varphi_t\}_{t \in \mathbb{R}}$. Let $\Phi \equiv (\Phi_1, \ldots, \Phi_d) \in C^\infty(M; \mathbb{R}^d)$ be a family of observables satisfying the condition

$$\{\{\Phi_j, H\}, H\} = 0$$

for each $j \in \{1, \ldots, d\}$. Then we have (see Theorem 3.3, Corollary 3.4 and Lemma 3.7 for a precise statement):

**Theorem 1.1.** Let $H$ and $\Phi$ be as above. Let $f : \mathbb{R}^d \to \mathbb{C}$ be such that $f = 1$ on a neighbourhood of $0$, $f = 0$ at infinity, and $f(x) = f(-x)$ for each $x \in \mathbb{R}^d$. Then there exist a closed subset $\text{Crit}(H, \Phi) \subset M$ and an observable $T_f \in C^\infty\left(M \setminus \text{Crit}(H, \Phi)\right)$ satisfying $\{T_f, H\} = 1$ on $M \setminus \text{Crit}(H, \Phi)$ such that

$$\lim_{r \to \infty} \frac{1}{2} \int_0^\infty dt \left[ (f(\Phi/r) \circ \varphi_t)(m) - (f(\Phi/r) \circ \varphi_t)(m) \right] = T_f(m)$$

for each $m \in M \setminus \text{Crit}(H, \Phi)$.

The observable $T_f$ admits a very simple expression given in terms of the Poisson brackets $\partial_j H := \{\Phi_j, H\}$ and the vector $\nabla H := (\partial_1 H, \ldots, \partial_d H)$, namely,

$$T_f := -\Phi \cdot (\nabla R_f)(\nabla H),$$

where $\nabla R_f : \mathbb{R}^d \to \mathbb{C}^d$ is some explicit function (see Section 2).

In order to give an interpretation of Formula (1.2), consider for a moment the situation where $M := T^*\mathbb{R}^n \simeq \mathbb{R}^{2n}$ is the standard symplectic manifold with canonical coordinates $(q, p)$ and 2-form $\omega := \sum_{j=1}^n dq_j \wedge dp_j$. Furthermore, let $H(q, p) := h(p)$ be a purely kinetic energy Hamiltonian, let $\Phi(q, p) := q$ be the standard family of position observables and let $f = \chi_1$ be the characteristic function for the unit ball $B_1$ in $\mathbb{R}^d$. In such a case, the condition (1.1) is readily verified, the vector $\nabla H$ reduces to the usual velocity observable $\nabla h$ associated to $H$, and the l.h.s. of Formula (1.2) has the following meaning: For $r > 0$ and $m \in M \setminus \text{Crit}(H, \Phi)$ fixed, it is equal to the distance of times spent by the classical orbit $\{\varphi_t(m)\}_{t \in \mathbb{R}}$ in the past (first term) and in the future (second term) within the ball $B_r$ of radius $r$ in $\mathbb{R}^d$. Moreover, the number $-T(q, p)$ reduces to $-q \cdot \frac{\nabla h(p)}{\|\nabla h(p)\|}$ and is equal to the time at which a particle in $\mathbb{R}^d$ with initial position $q$ and velocity $\nabla h(p)$ intersects the hyperplane (containing the origin) orthogonal to the unit vector $\frac{\nabla h(p)}{\|\nabla h(p)\|}$ (in the case where $H(q, p) := \frac{1}{2} p^2$ is the usual kinetic energy, this time is known as the arrival time of the free particle, see e.g. [35, Sec. II.E]). Therefore, Formula (1.2) provides a new relation between sojourn times in dilated regions to the time of arrival of classical orbits. Evidently, this interpretation remains valid in the general case provided that we consider the observables $\Phi_j$ as the components of an abstract position observable $\Phi$ (see Remark 3.6).

Our interest in this issue has been aroused by the three recent papers [10, 33, 34]. In [33], the authors establish a similar formula in the framework of quantum (Hilbertian) theory, and then use it in [34] to prove the existence of quantum time delay for general two-Hilbert spaces scattering systems. On another hand, the authors of [10] have recently put into evidence a relation linking the Calabi invariant of Poincaré scattering map to the classical time delay on fixed energy hypersurfaces (see Section 3.2 of [10]). Therefore, our purpose in this paper and its companion [18], is first to prove the classical counterparts of the results of [33, 34] and then to relate these results on time-dependent classical scattering theory to the result on the Calabi invariant obtained in [10] (see respectively [14, Sec. 4.1], [35, Sec. II], [38, Sec. 3.4] and [28, Sec. 10.3] for more informations on classical time delay and Calabi invariant).

We note that in [33], $H$ is a selfadjoint operator in a Hilbert space $\mathcal{H}$, $\Phi \equiv (\Phi_1, \ldots, \Phi_d)$ is a family of mutually commuting selfadjoint operators in $\mathcal{H}$, (1.1) is a suitable version of the commutation relation
2.1. The function $[\Phi, [H, H]] = 0$, and $T_f$ is a time operator for $H$ (i.e., a symmetric operator satisfying the canonical commutation relation $[T_f, H] = i$). So, apart from its intrinsic interest, the present paper provides also a new example of result valid both in quantum and classical mechanics. Points of the symplectic manifold correspond to vectors of the Hilbert space, complete Hamiltonian flows correspond to one-parameter unitary groups, Poisson brackets correspond to commutators of operators, etc. (see [1, Sec. 5.4] and [25] for the interconnections between classical and quantum mechanics). Accordingly, we try to put into light throughout all of the paper the relation between both theories. For instance, we link in Remark 3.5 the confinement (resp. the non-periodicity) of the classical orbits $\{\varphi(t, m)\}_{t \in \mathbb{R}}, m \in M$, to the belonging of the corresponding quantum orbits $\{e^{itH} \psi\}_{t \in \mathbb{R}}, \psi \in \mathcal{H}$, to the singular (resp. absolutely continuous) subspace of $\mathcal{H}$. Moreover, we show in Section 4.5.2 that the Hilbertian space theory of [33] can be recast into the present framework of symplectic geometry by using expectation values.

Let us now describe more precisely the content of this paper. In Section 2 we recall some definitions in relation with the function $f$ that appear in Theorem 1.1. The function $R_f$ is introduced and some of its properties are presented. Then we prove various versions of Formula (1.2) in the particular case where the functions $\Phi : M \to \mathbb{R}^d$ are fixed vectors $x \pm ty, x, y \in \mathbb{R}^d$ (see Proposition 2.3, Lemma 2.4 and Corollary 2.6).

In Section 3.1, we introduce the Hamiltonian system $(M, \omega, H)$ and the abstract position observable $\Phi$. Then we define the (closed) set of critical points $\text{Crit}(H, \Phi)$ associated to $H$ and $\Phi$ as (see [33, Def. 2.5] for the quantum analogue):

$$\text{Crit}(H, \Phi) := \{ m \in M \mid (\nabla H)(m) = 0 \}.$$ 

When $H(q, p) = h(p)$ and $\Phi(q, p) := q$ on $M = \mathbb{R}^{2n}$, $\text{Crit}(H, \Phi)$ coincides with the usual set $\text{Crit}(H)$ of critical points of the Hamiltonian vector field $X_H$, i.e.

$$\text{Crit}(H) \equiv \{ m \in M \mid X_H(m) = 0 \} = \{ (q, p) \in \mathbb{R}^{2n} \mid (\nabla h)(p) = 0 \} = \text{Crit}(H, \Phi).$$

But, in general, we simply have the inclusion $\text{Crit}(H) \subset \text{Crit}(H, \Phi)$.

In Section 3.2, we prove the main results of this paper. Namely, we show Formula (1.2) when the localisation function $f$ is regular (Theorem 3.3) or equal to a characteristic function (Corollary 3.4). We also establish in Theorem 3.8 a discrete-time version of Formula (1.2). The interpretation of these results is discussed in Remarks 3.5 and 3.6.

In Section 4, we show that our results apply to many Hamiltonian systems $(M, \omega, H)$ appearing in literature. In the case of finite-dimensional manifolds, we treat, among other examples, Stark Hamiltonians, homogeneous Hamiltonians, purely kinetic Hamiltonians, the repulsive harmonic potential, the simple pendulum, central force systems, the Poincaré ball model and covering manifolds. In the case of infinite-dimensional manifolds, we discuss separately classical and quantum Hamiltonian systems. In the classical case, we treat the wave equation, the nonlinear Schrödinger equation and the Korteweg-de Vries equation. In the quantum case, we explain how to recast into our framework the (Hilbertian) examples of [33, Sec. 7], and we also treat an example of Laplacian on trees and complete Fock spaces. In all these cases, we are able to exhibit a family of position observables $\Phi$ satisfying our assumptions. The diversity of the examples covered by our theory, together with the existence of a quantum analogue [33], makes us strongly believe that Formula (1.2) is of natural character. Moreover, it also suggests that the existence of time delay is a very common feature of classical scattering theory.

## 2 Integral formula

In this section, we prove an integral formula and a summation formula for functions on $\mathbb{R}^d$. For this, we start by recalling some properties of a class of averaged localisation functions which appears naturally when dealing with quantum scattering theory. These functions, which are denoted $R_f$, are constructed in terms of functions $f \in L^\infty(\mathbb{R}^d)$ of localisation around the origin $0 \in \mathbb{R}^d$. They were already used, in one form or another, in [17, 33, 34, 40, 41]. We use the notation $\langle x \rangle := \sqrt{1 + |x|^2}$ for any $x \in \mathbb{R}^d$.

### Assumption 2.1

The function $f \in L^\infty(\mathbb{R}^d)$ satisfies the following conditions:
(i) There exists \( \rho > 0 \) such that \( \| f(x) \| \leq \text{Const.} \langle x \rangle^{-\rho} \) for almost every \( x \in \mathbb{R}^d \).

(ii) \( f = 1 \) on a neighbourhood of \( 0 \).

It is clear that \( \lim_{r \to \infty} f(x/r) = 1 \) for each \( x \in \mathbb{R}^d \) if \( f \) satisfies Assumption 2.1. Furthermore, one has for each \( x \in \mathbb{R}^d \setminus \{0\} \)

\[
\left| \int_0^\infty \frac{d\mu}{\mu} \left( f(\mu x) - \chi_{[0,1]}(\mu) \right) \right| \leq \int_0^1 \frac{d\mu}{\mu} |f(\mu x) - 1| + \text{Const.} \int_1^\infty d\mu \mu^{-(1+\rho)} < \infty,
\]

where \( \chi_{[0,1]} \) denotes the characteristic function for the interval \([0, 1]\). Therefore the function \( R_f : \mathbb{R}^d \setminus \{0\} \to \mathbb{C} \) given by

\[
R_f(x) := \int_0^\infty \frac{d\mu}{\mu} \left[ f(\mu x) - \chi_{[0,1]}(\mu) \right]
\]

is well-defined.

In the next lemma we recall some differentiability and homogeneity properties of \( R_f \). We also give the explicit form of \( R_f \) when \( f \) is a radial function. The reader is referred to [41, Sec. 2] for proofs and details. The symbol \( \mathcal{S}(\mathbb{R}^d) \) stands for the Schwartz space on \( \mathbb{R}^d \).

**Lemma 2.2.** Let \( f \) satisfy Assumption 2.1.

(a) Assume that \( \frac{\partial f}{\partial x_j}(x) \) exists for all \( j \in \{1, \ldots, d\} \) and \( x \in \mathbb{R}^d \), and suppose that there exists some \( \rho > 0 \) such that \( \left| \frac{\partial f}{\partial x_j}(x) \right| \leq \text{Const.} \langle x \rangle^{-(1+\rho)} \) for each \( x \in \mathbb{R}^d \). Then \( R_f \) is differentiable on \( \mathbb{R}^d \setminus \{0\} \), and its gradient is given by

\[
(\nabla R_f)(x) = \int_0^\infty d\mu \left( \nabla f \right)(\mu x).
\]

In particular, if \( f \in \mathcal{S}(\mathbb{R}^d) \) then \( R_f \) belongs to \( C^\infty(\mathbb{R}^d \setminus \{0\}) \).

(b) Assume that \( R_f \) belongs to \( C^m(\mathbb{R}^d \setminus \{0\}) \) for some \( m \geq 1 \). Then one has for each \( x \in \mathbb{R}^d \setminus \{0\} \) and \( t > 0 \) the homogeneity properties

\[
x \cdot (\nabla R_f)(x) = -1,
\]

\[
l^{(\alpha)}(\partial^\alpha R_f)(tx) = (\partial^\alpha R_f)(x),
\]

where \( \alpha \in \mathbb{N}^d \) is a multi-index with \( 1 \leq |\alpha| \leq m \).

(c) Assume that \( f \) is radial, i.e. there exists \( f_0 \in L^\infty(\mathbb{R}) \) such that \( f(x) = f_0(|x|) \) for almost every \( x \in \mathbb{R}^d \). Then \( R_f \) belongs to \( C^\infty(\mathbb{R}^d \setminus \{0\}) \), and \( (\nabla R_f)(x) = -x^{-2} \cdot x \).

In the sequel, we say that a function \( f : \mathbb{R}^d \to \mathbb{C} \) is even if \( f(x) = f(-x) \) for almost every \( x \in \mathbb{R}^d \).

**Proposition 2.3.** Let \( f : \mathbb{R}^d \to \mathbb{C} \) be an even function as in Lemma 2.2.(a). Then we have for each \( x \in \mathbb{R}^d \) and each \( y \in \mathbb{R}^d \setminus \{0\} \)

\[
\lim_{r \to \infty} \frac{1}{2} \int_0^\infty dt \left[ f \left( \frac{x - ty}{r} \right) - f \left( \frac{x + ty}{r} \right) \right] = -x \cdot (\nabla R_f)(y).
\]

In particular, if \( f \) is radial, the l.h.s. is independent of \( f \) and equal to \( (x \cdot y)/y^2 \).

**Proof.** The change of variables \( \mu := t/r, \nu := 1/r \), and the fact that \( f \) is even, gives

\[
\lim_{r \to \infty} \frac{1}{2} \int_0^\infty dt \left[ f \left( \frac{x - ty}{r} \right) - f \left( \frac{x + ty}{r} \right) \right] = \lim_{\nu \to 0} \frac{1}{2} \int_0^\infty \frac{d\mu}{\nu} \left[ f(\nu x - \mu y) - f(\nu x + \mu y) \right] = \lim_{\nu \to 0} \frac{1}{2} \int_0^\infty d\mu \left\{ \frac{1}{\nu} \left[ f(\nu x - \mu y) - f(-\mu y) \right] - \frac{1}{\nu} \left[ f(\nu x + \mu y) - f(\mu y) \right] \right\}.
\]
By using the mean value theorem and the assumptions of Lemma 2.2.(a), one obtains that
\[
\frac{1}{\rho} |f(\nu x \pm \mu y) - f(\pm \mu y)| \leq \text{Const.} \sup_{\xi \in [0,1]} |\xi \nu x \pm \mu y|^{-(1+\rho)}
\]
for some \( \rho > 0 \). Therefore, if \( \mu \) is big enough, the integrant in (2.3) is bounded by
\[
\text{Const.} \langle \mu |y - |x| \rangle^{-(1+\rho)},
\]
for all \( \nu \in (0, 1) \). This implies that the integrant in (2.3) is bounded uniformly in \( \nu \in (0, 1) \) by a function belonging to \( L^1([0, \infty), d\mu) \). So, we can apply Lebesgue’s dominated convergence theorem to interchange the limit on \( \nu \) with the integration over \( \mu \) in (2.3). This, together with the fact that \( (\nabla f)(-x) = -(\nabla f)(x) \), leads to the desired result:
\[
\lim_{r \to \infty} \frac{1}{2} \int_0^\infty dt \left[ f \left( \frac{x-tu}{r} \right) - f \left( \frac{x+tu}{r} \right) \right] = \frac{1}{2} \int_0^\infty d\mu \left[ x \cdot (\nabla f)(-\mu y) - x \cdot (\nabla f)(\mu y) \right] = - \int_0^\infty d\mu x \cdot (\nabla f)(\mu y) = -x \cdot (\nabla R_f)(y).
\]

The result of Proposition 2.3 can be extended to less regular functions \( f : \mathbb{R}^d \to \mathbb{C} \). The interested reader can check that the result holds for functions \( f \) admitting a weak derivative \( f' \) such that, for every real line \( L \subset \mathbb{R}^d \), \( f' \) is of class \( L^1 \) on \( L \) (see [44, Thm. 2.1.6]). We only present here the case (of particular interest for the theory of classical time delay) where \( f \) is the characteristic function \( \chi_1 \) for the unit ball \( B_1 := \{ x \in \mathbb{R}^d \mid |x| \leq 1 \} \).

**Lemma 2.4.** One has for each \( x \in \mathbb{R}^d \) and each \( y \in \mathbb{R}^d \setminus \{0\} \)
\[
\lim_{r \to \infty} \frac{1}{2} \int_0^\infty dt \left[ \chi_1 \left( \frac{x-ty}{r} \right) - \chi_1 \left( \frac{x+ty}{r} \right) \right] = \frac{x \cdot y}{y^2}.
\]

**Proof.** Direct calculations and the change of variables \( \mu := t/r, \nu := 1/r \), give
\[
\int_0^\infty dt \chi_1 \left( \frac{x+ty}{r} \right) = \int_0^\infty \frac{d\mu}{\nu} \chi_{[0,1]} \left( \nu x \pm |y|^2 \right) = \int_0^\infty d\mu \chi_{[0,|y|^2]} \left( \nu x \pm 2\nu y + \mu^2 \right) = \int_0^\infty \frac{d\mu}{\nu} \chi_{[0,|y|^2]} \left( \mu \pm \frac{\nu x y}{y^2} \right) = \int_0^\infty \frac{d\mu}{\nu} \chi_{[-a(\nu, x, y) \leq y^2 \leq a(\nu, x, y)]} \left( \mu \pm \frac{\nu x y}{y^2} \right),
\]
with \( a(\nu, x, y) := \frac{x^2}{y^2} \left(y^2 - (x \cdot y)^2\right) \). Now, \( a(\nu, x, y) \geq 0 \), and \( y^2 - a(\nu, x, y) \leq 0 \) if \( \nu > 0 \) is small enough. So, the last expression is equal to
\[
\int_0^\infty \frac{d\mu}{\nu} \chi_{[0, y^2 - a(\nu, x, y)]} \left( \mu \pm \frac{\nu x y}{y^2} \right) = \int_0^\infty \frac{d\mu}{\nu} \chi_{[\sqrt{y^2 - a(\nu, x, y)} \leq \frac{\nu x y}{y^2} \leq \sqrt{y^2 - a(\nu, x, y)} + \frac{\nu x y}{y^2}]}(\mu) = \frac{1}{\nu} \sqrt{y^2 - a(\nu, x, y) + \frac{\nu x y}{y^2}}.
\]
if \( \nu \) is small enough. This implies that
\[
\lim_{r \to \infty} \frac{1}{2} \int_0^\infty dt \left[ \chi_1 \left( \frac{x-tu}{r} \right) - \chi_1 \left( \frac{x+tu}{r} \right) \right] = \lim_{\nu \to 0} \frac{1}{2} \left( \frac{1}{\nu} \sqrt{y^2 - a(\nu, x, y) + \frac{\nu x y}{y^2}} - \frac{x \cdot y}{y^2} \right) = \frac{x \cdot y}{y^2}.
\]

For the next corollary, we need the following version of the Poisson summation formula (see [15, Thm. 5] or [42, Thm. 45]).

**Lemma 2.5.** Let \( g : (0, \infty) \to \mathbb{C} \) be a continuous function of bounded variation in \((0, \infty)\). Suppose that \( \lim_{t \to \infty} g(t) = 0 \) and that the improper Riemann integral \( \int_0^\infty dt \, g(t) \) exists. Then we have the identity
\[
\frac{1}{2} g(0) + \sum_{n \geq 1} g(n) = \int_0^\infty dt \, g(t) + 2 \sum_{n \geq 1} \int_0^\infty dt \, \cos(2\pi nt) g(t).
\]

**Corollary 2.6.** Let \( f : \mathbb{R}^d \to \mathbb{C} \) be an even function such that

(i) \( f = 1 \) on a neighbourhood of 0.

(ii) For each \( \alpha \in \mathbb{N}^d \) with \( |\alpha| \leq 2 \), the derivative \( \partial^\alpha f \) exists and satisfies \( |(\partial^\alpha f)(x)| \leq \text{Const.} \langle x \rangle^{-(1+\rho)} \) for some \( \rho > 0 \) and all \( x \in \mathbb{R}^d \).

Then we have for each \( x \in \mathbb{R}^d \) and each \( y \in \mathbb{R}^d \setminus \{0\} \)
\[
\lim_{r \to \infty} \frac{1}{2} \sum_{n \geq 1} \left[ f\left(\frac{x-ny}{r}\right) - f\left(\frac{x+ny}{r}\right) \right] = -x \cdot (\nabla R_f)(y). \tag{2.4}
\]

In particular, if \( f \) is radial, the l.h.s. is independent of \( f \) and equal to \( (x \cdot y)/y^2 \).

**Proof.** For \( r > 0 \) given, the function
\[
g_r : (0, \infty) \to \mathbb{C}, \quad t \mapsto g_r(t) := f\left(\frac{x-ty}{r}\right) - f\left(\frac{x+ty}{r}\right),
\]
satisfies all the hypotheses of Lemma 2.5. Thus
\[
\lim_{r \to \infty} \frac{1}{2} \sum_{n \geq 1} \left[ f\left(\frac{x-ny}{r}\right) - f\left(\frac{x+ny}{r}\right) \right] = \lim_{r \to \infty} \frac{1}{2} \int_0^\infty dt \, g_r(t) = \lim_{r \to \infty} \sum_{n \geq 1} \int_0^\infty dt \, \cos(2\pi nt) g_r(t).
\]
The first term is equal to \( -x \cdot (\nabla R_f)(y) \) due to Proposition 2.3. For the second term, the change of variables \( \mu := t/r, \nu := 1/r \), and two integrations by parts give
\[
\lim_{r \to \infty} \sum_{n \geq 1} \int_0^\infty dt \, \cos(2\pi nt) g_r(t)
\]
\[
= \lim_{r \to \infty} \sum_{n \geq 1} \int_0^\infty \frac{d\mu}{\nu} \cos(2\pi n\mu/\nu) \left[ f(\nu x - \mu y) - f(\nu x + \mu y) \right]
\]
\[
= \sum_j y_j \lim_{r \to \infty} \sum_{n \geq 1} \int_0^\infty \frac{d\mu}{\nu} \frac{\nu}{2\pi n} \left[ \frac{\partial f}{\partial x_j}(\nu x - \mu y) + \frac{\partial f}{\partial x_j}(\nu x + \mu y) \right]
\]
\[
= \sum_j y_j \lim_{r \to \infty} \sum_{n \geq 1} \frac{2\nu}{(2\pi n)^2} \frac{\partial f}{\partial x_j}(\nu x)
\]
\[
- \sum_{j,k} y_j y_k \lim_{r \to \infty} \sum_{n \geq 1} \int_0^\infty \frac{d\mu}{\nu} \frac{\nu}{2\pi n} \frac{\cos(2\pi n\mu/\nu)}{(2\pi n)^2} \left[ \frac{\partial^2 f}{\partial x_k \partial x_j}(\nu x - \mu y) + \frac{\partial^2 f}{\partial x_k \partial x_j}(\nu x + \mu y) \right].
\]

Since \( \sum_{n \geq 1} 1/n^2 < \infty \), one sees directly that the first term is equal to zero. Using the fact that \( \left| \frac{\partial^2 f}{\partial x_k \partial x_j}(x) \right| \leq \text{Const.} \langle x \rangle^{-(1+\rho)} \) for some \( \rho > 0 \) and all \( x \in \mathbb{R}^d \), one also obtains that the second term is equal to zero. Therefore,
\[
\lim_{r \to \infty} \frac{1}{2} \sum_{n \geq 1} \left[ f\left(\frac{x-ny}{r}\right) - f\left(\frac{x+ny}{r}\right) \right] = -x \cdot (\nabla R_f)(y),
\]
and the claim is proved. \( \square \)
3 Hamiltonian dynamics

In the sequel, we require the presence of a symplectic structure in order to speak of Hamiltonian dynamics. However our results still hold if one is only given a Poisson structure. A lack of examples and some complications in infinite dimension regarding the identification of vector fields with derivations have led us to restrict the discussion to the symplectic case for the sake of clarity.

3.1 Critical points

Let \( M \) be a symplectic manifold, \textit{i.e.} a smooth manifold endowed with a closed two-form \( \omega \) such that the morphism \( TM \ni X \mapsto \omega^\flat(X) := i_X \omega \) 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 \( \omega^n \) must be a volume form. The Poisson bracket is defined as follows: for each \( f, g \in C^\infty(M) \) we define the vector field \( X_f := (\omega^n)^{-1}(df) \), \textit{i.e.} \( df(\cdot) = \omega(X_f, \cdot) \), and set \( \{f, g\} := \omega(X_f, X_g) \) for each \( f, g \in C^\infty(M) \).

In the sequel, the function \( H \in C^\infty(M) \) is an Hamiltonian with complete vector field \( X_H \). So, the flow \( \{\varphi_t\} \) associated to \( H \) is defined for all \( t \in \mathbb{R} \), it preserves the Poisson bracket:

\[
\{f \circ \varphi_t, g \circ \varphi_t\} = \{f, g\} \circ \varphi_t, \quad t \in \mathbb{R},
\]

and satisfies the usual evolution equation:

\[
\frac{d}{dt} f \circ \varphi_t = \{f, H\} \circ \varphi_t, \quad t \in \mathbb{R}. \tag{3.1}
\]

In particular, the Hamiltonian \( H \) is preserved along its flow, \textit{i.e.} \( H \circ \varphi_t = H \) for all \( t \in \mathbb{R} \). We also consider an abstract family \( \Phi \equiv \{\Phi_1, \ldots, \Phi_d\} \in C^\infty(M; \mathbb{R}^d) \) of observables\(^1\), and define the associated functions

\[
\partial_j H := \{\Phi_j, H\} \in C^\infty(M) \quad \text{and} \quad \nabla H := (\partial_1 H, \ldots, \partial_d H) \in C^\infty(M; \mathbb{R}^d).
\]

Then, one can introduce a natural set of critical points:

**Definition 3.1 (Critical points).** The set

\[
\text{Crit}(H, \Phi) := (\nabla H)^{-1}(\{0\}) \subset M
\]

is called the set of critical points associated to \( H \) and \( \Phi \).

The set \( \text{Crit}(H, \Phi) \) is closed in \( M \) since \( \nabla H \) is continuous. Furthermore, since \( \{\Phi_j, H\} = d\Phi_j(X_H) \), the set

\[
\text{Crit}(H) := \{m \in M \mid X_H(m) = 0\} \equiv \{m \in M \mid dH_m = 0\}
\]

of usual critical points of \( H \) satisfies the inclusion \( \text{Crit}(H) \subset \text{Crit}(H, \Phi) \).

Our main assumption is the following:

**Assumption 3.2.** One has \( \{\Phi_j, H\}, H\} = 0 \) for each \( j \in \{1, \ldots, d\} \).

Assumption 3.2 imposes that all the brackets \( \{\Phi_j, H\} \) are first integrals of the motion given by \( H \). When \( M \) is a symplectic manifold of dimension \( 2n \), these first integrals are functions of \( k \in \{1, 2, \ldots, 2n - 1\} \) independent first integrals \( J_1 \equiv H, J_2, \ldots, J_k \) (\( J_1, \ldots, J_k \) are independent in the sense that their differential are linearly independent at each point of \( M \))\(^2\). So, one should have \( \{\Phi_j, H\} = g_j(J_1, \ldots, J_k) \) for some functions

\(^1\)If need be, the results of this article can be extended to the case where \( H \) and \( \Phi_j \) are functions of class \( C^1 \) with \( \{\Phi_j, H\} \) also \( C^1 \).

\(^2\)In the setup of Liouville’s theorem [5, Sec. 49], we have \( k = n \) and the first integrals are mutually in involution. Furthermore, on the connected components of submanifolds given by fixing the values of these \( n \) integrals in involution, the flow is conjugate to a translation flow on cylinders \( \mathbb{R}^{n-k} \times T^k \) (see [1, Thm. 5.2.24]).
$g_f \in C^\infty(\mathbb{R}^n; \mathbb{R})$. Using the properties of $\{ \cdot, H \}$ as a derivation, one infers that $\{ g_f(\Phi_1, \ldots, \Phi_k), H \} = 1$ outside $g_f(\Phi_1, \ldots, \Phi_k)^{-1}(\{0\})$. Thus, if $k$ first integrals as $\Phi_1, \ldots, \Phi_k$ are known, finding functions $\Phi_j$ satisfying Assumption 3.2 is to some extent equivalent to finding functions $\Phi_0$ solving $\{ \Phi_0, H \} = 1$ (the equivalence is not complete because these functions $\Phi_0$ are in general not $C^\infty$ since $\{\cdot, H\}$ is necessarily 0 on $\text{Crit}(H)$).

For further use, we define the $C^\infty$-function $T_f : M \setminus \text{Crit}(H, \Phi) \rightarrow \mathbb{R}$ by

$$T_f := -\Phi \cdot (\nabla R_f)(\nabla H).$$

When $f$ is radial, $T_f$ is independent of $f$ and equal to

$$T := \Phi \cdot \frac{\nabla H}{|\nabla H|^2},$$

due to Lemma 2.2.(c). In such a case, the number $\lim_{r \to \infty} \frac{1}{2} \int_0^r dt \left[ (f(\Phi/r) \circ \varphi_{-t}) - (f(\Phi/r) \circ \varphi_t) \right](m) = T_f(m).$ (3.2)

In particular, if $f$ is radial, the l.h.s. is independent of $f$ and equal to $\Phi(m) \cdot \frac{(\nabla H)(m)}{|(\nabla H)(m)|^2}.$

Proof. Equation (3.1) implies that

$$\frac{d}{dt} \Phi_j \circ \varphi_t = \{ \Phi_j, H \} \circ \varphi_t$$

for each $t \in \mathbb{R}$. Similarly, using Assumption 3.2, one gets that

$$\frac{d}{dt} \{ \Phi_j, H \} \circ \varphi_t = \{ \{ \Phi_j, H \}, H \} \circ \varphi_t = 0.$$

So, $\Phi_j$ varies linearly in $t$ along the flow of $X_H$, and one gets for any $m \in M$

$$(\Phi_j \circ \varphi_t)(m) = (\Phi_j \circ \varphi_0)(m) + t \left( \frac{d}{dt} (\Phi_j \circ \varphi_t)(m) \right)_{t=0} = \Phi_j(m) + t(\partial_j H)(m).$$

This, together with Formula (2.2), gives

$$\lim_{r \to \infty} \frac{1}{2} \int_0^r dt \left[ (f(\Phi/r) \circ \varphi_{-t}) - (f(\Phi/r) \circ \varphi_t) \right](m)$$

$$= \lim_{r \to \infty} \frac{1}{2} \int_0^r dt \left[ f\left(\frac{\Phi(m) - t(\nabla H)(m)}{r}\right) - f\left(\frac{\Phi(m) + t(\nabla H)(m)}{r}\right) \right]$$

$$= T_f(m). \hfill \Box$$

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Due to Lemma 2.4, the proof of Theorem 3.3 also works in the case \( f = \chi_1 \). So, we have the following corollary.

**Corollary 3.4.** Let \( H \) and \( \Phi \) satisfy Assumption 3.2. Then we have for each point \( m \in M \setminus \text{Crit}(H, \Phi) \)

\[
\lim_{r \to \infty} \frac{1}{2} \int_0^\infty dt \left[ (x_1(\Phi/r) \circ \varphi_t)(m) - (x_1(\Phi/r) \circ \varphi_t)(m) \right] = \Phi(m) \cdot \left( \frac{(\nabla H)(m)}{(\nabla H)(m)} \right)^\top.
\]

(3.3)

We know from the proof of Theorem 3.3 that

\[
(\Phi_j \circ \varphi_t)(m) = \Phi_j(m) + t(\partial J)(m) \quad \text{for all } j \in \{1, \ldots, d\}, t \in \mathbb{R} \text{ and } m \in M.
\]

(3.4)

Therefore, the l.h.s. of (3.2) and (3.3) are zero if \( m \in \text{Crit}(H, \Phi) \).

For the next remark, we recall that any selfadjoint operator \( A \) in a Hilbert space \( \mathcal{H} \), with spectral measure \( E^A(\cdot) \), is reduced by an orthogonal decomposition \([33, \text{Sec. 7.4}]\)

\[
\mathcal{H} = \mathcal{H}_{\text{ac}}(A) \oplus \mathcal{H}_{\text{p}}(A) \oplus \mathcal{H}_{\text{sc}}(A) \equiv \mathcal{H}_{\text{ac}}(A) \oplus \mathcal{H}_{\text{s}}(A),
\]

where \( \mathcal{H}_{\text{ac}}(A), \mathcal{H}_{\text{p}}(A), \mathcal{H}_{\text{sc}}(A) \) and \( \mathcal{H}_{\text{s}}(A) \) are respectively the absolutely continuous, the pure point, the singular continuous and the singular subspaces of \( A \). Furthermore, a vector \( \varphi \in \mathcal{H} \) is said to have spectral support with respect to \( A \) in a set \( J \subseteq \mathbb{R} \) if \( \varphi = E^A(J) \varphi \).

**Remark 3.5.** One has \( (\nabla H)(\varphi_t(m)) = (\nabla H)(m) \) for all \( t \in \mathbb{R} \) and \( m \in M \) due to Assumption 3.2. Therefore,

\[
\varphi_t(\text{Crit}(H, \Phi)) = \text{Crit}(H, \Phi) \quad \text{and} \quad \varphi_t(M \setminus \text{Crit}(H, \Phi)) = M \setminus \text{Crit}(H, \Phi)
\]

for all \( t \in \mathbb{R} \). Furthermore, if \( m \in M \setminus \text{Crit}(H, \Phi) \), then one must have \( \varphi_t(m) \neq m \) for all \( t \neq 0 \), due to Equation (3.4). So, under Assumption 3.2, each orbit \( \{\varphi_t(m)\}_{t \in \mathbb{R}} \) either stays in \( \text{Crit}(H, \Phi) \) if \( m \in \text{Crit}(H, \Phi) \), or stays outside \( \text{Crit}(H, \Phi) \) and is not periodic if \( m \notin \text{Crit}(H, \Phi) \).

In the corresponding Hilbertian framework \([33]\), the Hamiltonian \( H \) and the functions \( \Phi_j \) are selfadjoint operators in a Hilbert space \( \mathcal{H} \), and the critical set \( \kappa \) associated to \( H \) and \( \Phi \) is a closed subset of the spectrum of \( H \). Outside \( \kappa \), the spectrum of \( H \) is purely absolutely continuous \([33, \text{Thm. 3.6.(a)}]\). Therefore, vectors \( \psi \in \mathcal{H} \) having spectral support with respect to \( H \) in \( \kappa \) belong to the singular subspace \( \mathcal{H}_{\text{s}}(H) \) of \( H \), and thus lead to orbits \( \{e^{itH} \psi\}_{t \in \mathbb{R}} \) confined in \( \mathcal{H}_{\text{s}}(H) \) (for instance, \( e^{itH} \psi \) stays in a one-dimensional subspace of \( \mathcal{H} \) if \( \psi \) is an eigenvector of \( H \)). Conversely, vectors \( \psi \in \mathcal{H} \) having spectral support outside \( \kappa \) belong to the absolute continuous subspace \( \mathcal{H}_{\text{ac}}(H) \) of \( H \), and thus lead to orbits \( \{e^{itH} \psi\}_{t \in \mathbb{R}} \) contained in \( \mathcal{H}_{\text{ac}}(H) \) (see \([3, \text{Prop. 5.7}]\) for the escape properties of such orbits). These properties are the quantum counterparts of the confinement to \( \text{Crit}(H, \Phi) \) (when \( m \in \text{Crit}(H, \Phi) \)) and the non-periodicity outside \( \text{Crit}(H, \Phi) \) (when \( m \notin \text{Crit}(H, \Phi) \)) of the classical orbits \( \{\varphi_t(m)\}_{t \in \mathbb{R}} \).

**Remark 3.6.** Corollary 3.4 relates the sojourn times of classical orbits within expanding regions of \( M \) to the observable \( T \). If we consider the observables \( \Phi_j \) as the components of an abstract position observable \( \Phi \), then the l.h.s. of Formula (3.3) has the following meaning: For \( r > 0 \) and \( m \in M \setminus \text{Crit}(H, \Phi) \), it can be interpreted as the difference of times spent by the classical orbit \( \{\varphi_t(m)\}_{t \in \mathbb{R}} \) in the past (first term) and in the future (second term) within the region \( \Phi^{-1}(B_r) \) with \( B_r := \{x \in \mathbb{R}^d \mid |x| \leq r\} \). On the other hand, we know from the last observation of Section 3.1 that the r.h.s. of Formula (3.3) is equal to the time at which a particle in \( \mathbb{R}^d \) with initial position \( \Phi(m) \) and velocity \( (\nabla H)(m) \) intersects the hyperplane (containing the origin) orthogonal to the unit vector \( (\nabla H)(m) / (\nabla H)(m)) \). Thus, Formula (3.3) shows in a very general setting that the difference of sojourn times of classical orbits in the past and in the future within \( \Phi^{-1}(B_r) \) tends as \( r \to \infty \) to the arrival time \( -T(m) = -\Phi(m) \cdot (\nabla H)(m) / (\nabla H)(m)) \).

The next lemma provides an alternative interpretation for the observable \( T_f \).

**Lemma 3.7.** If \( H, \Phi \) and \( f \) satisfy the assumptions of Theorem 3.3, then we have

\[
\{T_f, H\} \circ \varphi_t = \frac{d}{dt} (T_f \circ \varphi_t) = 1
\]

(3.5)

on \( M \setminus \text{Crit}(H, \Phi) \). In particular, one has \( T_f \circ \varphi_t = T_f + t \) on \( M \setminus \text{Crit}(H, \Phi) \).
If we interpret the map \( \frac{d}{dt} := \{T_f, \cdot\} \) as a derivation on \( C^\infty(M \setminus \text{Crit}(H, \Phi)) \), this implies that \( T_f \) can be seen as an observable “derivative with respect to the energy \( H \)” on \( M \setminus \text{Crit}(H, \Phi) \), since

\[
\frac{d}{dt}(H) = \{T_f, H\} = 1
\]
on each orbit \( \{\varphi_t(m)\}_{t \in \mathbb{R}} \), with \( m \in M \setminus \text{Crit}(H, \Phi) \).

**Proof of Lemma 3.7.** The first equality in (3.5) follows from (3.1). For the second one, we use successively the fact that \( \varphi_t \) leaves invariant \( H \) and the Poisson bracket, Assumption 3.2, and Equation (2.1). Doing so, we get on \( M \setminus \text{Crit}(H, \Phi) \) the following equalities

\[
\frac{d}{dt}(T_f \circ \varphi_t) = - \frac{d}{dt} (\Phi \circ \varphi_t) \cdot (\nabla R_f)(\{\Phi \circ \varphi_t, H\}) = - \frac{d}{dt} (\Phi + t(\nabla H)) \cdot (\nabla R_f)(\{\Phi + t(\nabla H), H\})
\]

\[
= - \frac{d}{dt} (\Phi + t(\nabla H)) \cdot (\nabla R_f)(\nabla H)
\]

\[
= - (\nabla H) \cdot (\nabla R_f)(\nabla H)
\]

\[
= 1. \quad \square
\]

As a final result, we give a discrete-time counterpart of Theorem 3.3, which could be of some interest in the context of approximation of symplectomorphisms by time-1 maps of Hamiltonians flows (see e.g. [7], [19, Appendix B], [24] and references therein).

**Theorem 3.8.** Let \( H \) and \( \Phi \) satisfy Assumption 3.2. Let \( f : \mathbb{R}^d \to \mathbb{C} \) be an even function such that

(i) \( f = 1 \) on a neighbourhood of 0.

(ii) For each \( \alpha \in \mathbb{N}^d \) with \( |\alpha| \leq 2 \), the derivative \( \partial^\alpha f \) exists and satisfies \( |(\partial^\alpha f)(x)| \leq \text{Const.} \langle x \rangle^{-(1+\rho)} \) for some \( \rho > 0 \) and all \( x \in \mathbb{R}^d \).

Then we have for each point \( m \in M \setminus \text{Crit}(H, \Phi) \)

\[
\lim_{r \to \infty} \frac{1}{2} \sum_{n \geq 1} [(f(\Phi/r) \circ \varphi_{-n})(m) - (f(\Phi/r) \circ \varphi_n)(m)] = T_f(m).
\]

In particular, if \( f \) is radial, the l.h.s. is independent of \( f \) and equal to \( \Phi(m) \cdot \frac{(\nabla H)(m)}{(\nabla H)(m)^2} \).

**Proof.** Let \( m \in M \setminus \text{Crit}(H, \Phi) \). Then we have by Equation (3.4)

\[
\lim_{r \to \infty} \frac{1}{2} \sum_{n \geq 1} [(f(\Phi/r) \circ \varphi_{-n})(m) - (f(\Phi/r) \circ \varphi_n)(m)]
\]

\[
= \lim_{n \to 0} \frac{1}{2} \sum_{n \geq 1} \left[ f\left(\Phi(m) - n(\nabla H)(m)\right) - f\left(\Phi(m) + n(\nabla H)(m)\right)\right],
\]

and the claim follows by Formula (2.4). \( \square \)

### 4 Examples

In this section we show that Assumption 3.2 is satisfied in various situations. In these situations all the results of Section 3 such as Theorem 3.3 or Formula (3.5) hold. Some of the examples presented here are the classical counterparts of examples discussed in [33, Sec. 7] in the context of Hilbertian theory.

The configuration space of the system under consideration will sometimes be \( \mathbb{R}^n \), and the corresponding symplectic manifold \( M = T^* \mathbb{R}^n \cong \mathbb{R}^{2n} \). In that case, we use the notation \((q, p)\), with \( q \equiv (q^1, \ldots, q^n) \) and \( p \equiv (p_1, \ldots, p_n) \), for the canonical coordinates on \( M \), and set \( \omega := \sum_{j=1}^n dq^j \wedge dp_j \) for the canonical symplectic form. We always assume that \( f = \chi_1 \) or that \( f \) satisfies the hypotheses of Theorem 3.3.
4.1 $\nabla H = g(H)$

Suppose that there exists a function $g \equiv (g_1, \ldots, g_d) \in C^\infty(\mathbb{R}; \mathbb{R}^d)$ such that $\nabla H = g(H)$. Then $H$ and $\Phi$ satisfy Assumption 3.2 since $\{g_j(H), H\} = 0$ for each $j$. Furthermore, one has $\text{Crit}(H, \Phi) = (g \circ H)^{-1}(\{0\})$, and $T_f = -\Phi \cdot (\nabla R_f)(g(H))$ on $M \setminus \text{Crit}(H, \Phi)$. We distinguish various cases:

(A) Suppose that $g$ is constant, i.e. $g = v \in \mathbb{R}^d \setminus \{0\}$. Then $\text{Crit}(H) = \text{Crit}(H, \Phi) = \emptyset$, and we have the equality $T_f = -\Phi \cdot (\nabla R_f)(v)$ on the whole of $M$.

Typical examples of functions $H$ and $\Phi$ fitting into this construction are Friedrichs-type Hamiltonian and position functions. For illustration, we mention the case (with $d = n$) of $H(q, p) := v \cdot p + V(q)$ and $\Phi(q, p) := q$ on $M := \mathbb{R}^{2n}$, with $v \in \mathbb{R}^n \setminus \{0\}$ and $V \in C^\infty([0, \infty); \mathbb{R})$. In such a case, one has $\nabla H = v$ and

$$\varphi_t(q, p) = (vt + q, p - \int_0^t ds (\nabla V)(vs + q)).$$

Stark-type Hamiltonians and momentum functions also fit into the construction, i.e. $H(q, p) := h(p) + V(q)$ and $\Phi(q, p) := p$ on $M := \mathbb{R}^{2n}$, with $v \in \mathbb{R}^n \setminus \{0\}$ and $h \in C^\infty([0, \infty); \mathbb{R})$. In such a case, one has $\nabla H = -v$ and

$$\varphi_t(q, p) = (q + \int_0^t ds (\nabla h)(p - vs), p - vt).$$

Note that these two examples are interesting since the Hamiltonians $H$ contain not only a kinetic part, but also a potential perturbation.

(B) Suppose that $\Phi$ has only one component ($d = 1$), and assume that $g(\lambda) = \lambda$ for all $\lambda \in \mathbb{R}$ (in the Hilbertian framework, one says in such a case that $H$ is $\Phi$-homogeneous [9]). Then $\text{Crit}(H, \Phi) = H^{-1}(\{0\})$ and we have the equality $T_f = -\Phi(\nabla R_f)(H)$ on $M \setminus H^{-1}(\{0\})$. We present a general class of pairs $(H, \Phi)$ satisfying these assumptions:

The Hamiltonian flow of the function $D(q, p) := q \cdot p$ on $\mathbb{R}^{2n}$ is given by $\varphi_t^D(q, p) = (e^{t \Phi} q, e^{-t \Phi} p)$. So, $D$ is the generator of a dilations group on $\mathbb{R}^{2n}$ (in the Hilbertian framework, the corresponding operator is the usual generator of dilations on $L^2(\mathbb{R}^n)$, see e.g. [4, Sec. 1.2]). Therefore, the relation $\{D, H\} = 0$ holds for a large class of homogeneous functions $H$ on $\mathbb{R}^{2n}$, due to Euler’s homogeneous function theorem. Let us consider an explicit situation. Take $\alpha > 0$ and let $M$ be some open subset of $(\mathbb{R}^n \setminus \{0\}) \times \mathbb{R}^n$. Define on $M$ the function $\Phi := \frac{1}{\alpha}D$ and the Hamiltonian $H(q, p) := h(p) + V(q)$, where $h \in C^\infty([0, \infty); \mathbb{R})$ is positive homogeneous of degree $\alpha$ and $V \in C^\infty([0, \infty) \setminus \{0\}; \mathbb{R})$ is positive homogeneous of degree $-\alpha$.

Then one has $\nabla H \equiv \{\Phi, H\} = H$ on $M$, and

$$\text{Crit}(H) = \{(q, p) \in M \mid (\nabla h)(p) = (\nabla V)(q) = 0\} \subset \{(q, p) \in M \mid p \cdot (\nabla h)(p) = q \cdot (\nabla V)(q) = 0\} = \{(q, p) \in M \mid H(q, p) = 0\} = \text{Crit}(H, \Phi).$$

Furthermore, if the functions $h$ and $V$ and the subset $M$ are well chosen, the Hamiltonian vector field $X_H$ of $H$ is complete. For instance,

(i) If $V \equiv 0$, then one can take $M = \mathbb{R}^{2n}$, and one has $\varphi_t(q, p) = (q + t(\nabla h)(p), p)$ and

$$\text{Crit}(H) = \{(q, p) \in M \mid (\nabla h)(p) = 0\} \subset \{(q, p) \in M \mid p \cdot (\nabla h)(p) = 0\} = \text{Crit}(H, \Phi)$$

(where $h(p) = \frac{1}{2}|p|^2$ is the classical kinetic energy, one has $\text{Crit}(H) = \text{Crit}(H, \Phi) = \mathbb{R}^n \times \{0\}$).

(ii) Let $K > 0$. Then the Hamiltonian given by $H(q, p) := \frac{1}{2}(|p|^2 + K|q|^2)$ on $M := \mathbb{R}^n \setminus \{0\} \times \mathbb{R}^n$ has a complete Hamiltonian vector field $X_H$. To see it, we use the push-forward of $X_H$ by the diffeomorphism $\iota : \mathbb{R}^n \setminus \{0\} \times \mathbb{R}^n \to \mathbb{R}^n \setminus \{0\} \times \mathbb{R}^n$, $(q, p) \mapsto (q|q|^{-2}, p)$, namely,

$$[\iota_*(X_H)](r, p) = \sum \left( (|r|^2 p_j - 2(p \cdot r) r_j) \frac{\partial}{\partial r_j} \bigg|_{(r, p)} + Kr^2 |r|^2 \frac{\partial}{\partial p_j} \bigg|_{(r, p)} \right).$$

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Consider on $M$. For instance, consider $H(q,p) := q^2/p^4$ and $\Phi(q,p) := p^2q^2 + 2q^4$ on $M := (\mathbb{R}^2 \setminus \{0\}) \times \mathbb{R}^2$. Then one has $\nabla H = H^2 - 4$, $\varphi_t(q,p) = (q + t\nabla h)(p), \nabla H = \nabla h$, and Assumption 3.2 is satisfied:

$$\{\{\Phi_j, H\}, H\} = \{\{\partial_j h)(p), h(p)\} = 0.\$$

In this example, we have $\text{Crit}(H) = \text{Crit}(H, \Phi) = \mathbb{R}^n \times (\nabla h)^{-1}(\{0\})$.

4.2 $H = h(p)$

Consider on $M := \mathbb{R}^{2n}$ a purely kinetic Hamiltonian $H(q,p) := h(p)$ with $h \in C^\infty(\mathbb{R}^n; \mathbb{R})$, and take the usual position functions $\Phi(q,p) := q$ with $d = n$. Then $\varphi_t(q,p) = (q + t(\nabla h)(p)), \nabla H = \nabla h$, and Assumption 3.2 is satisfied:

$$\{\{\Phi_j, H\}, H\} = \{\{\partial_j h)(p), h(p)\} = 0.\$$

As observed in Section 3.1, this is essentially equivalent (when $k$ independent first integrals $J_1 \equiv H, J_2, \ldots, J_k$ are known) to finding the solutions for $\Phi_0$ the second-order linear equation

$$\{\{\Phi_0, H\}, H\} = \left(\sum_{i=1}^n (H_{p_i} \partial_{q^i} - H_{q^i} \partial_{p_i})\right)^2 \Phi_0 = 0.\$$

The case $q = 1$ is sufficient, though trying to solve $\{\Phi_0, H\} = 1$ can at best provide solutions which are $C^\infty$ outside the set $\text{Crit}(H)$. A way to remove these singularities could be to multiply the solutions by a function $g(H)$ that vanishes and is infinitely flat on $\text{Crit}(H)$. For instance, if $H(\text{Crit}(H))$ consists of a finite number of values $c_1, \ldots, c_s \in \mathbb{R}$, one could take $g(H) = \prod_{i=1}^s e^{-2(H-c_i)^{-2}}$. Another possibility is to restrict the study to a submanifold $M'$ of $M$ (typically an open subset of the same dimension). However, problems can arise as the same (induced) symplectic structure (or Poisson bracket) must be used for the dynamic to remain unchanged; in particular, it must checked that the Hamiltonian flow preserves $M'$.

4.3 The assumption $\{\{\Phi_j, H\}, H\} = 0$ as a differential equation

Consider on $M := \mathbb{R}^{2n}$ an Hamiltonian function $H$ with partial derivatives $H_{p_k} := \partial H/\partial p_k$ and $H_{q^k} := \partial H/\partial q^k$. Then, finding the functions $\Phi_j$ of Assumption 3.2 amounts to solving for $\Phi_0$ the second-order linear equation

$$\{\{\Phi_0, H\}, H\} = \left(\sum_{i=1}^n (H_{p_i} \partial_{q^i} - H_{q^i} \partial_{p_i})\right)^2 \Phi_0 = 0.\$$

The case $q = 1$ is sufficient, though trying to solve $\{\Phi_0, H\} = 1$ can at best provide solutions which are $C^\infty$ outside the set $\text{Crit}(H)$. A way to remove these singularities could be to multiply the solutions by a function $g(H)$ that vanishes and is infinitely flat on $\text{Crit}(H)$. For instance, if $H(\text{Crit}(H))$ consists of a finite number of values $c_1, \ldots, c_s \in \mathbb{R}$, one could take $g(H) = \prod_{i=1}^s e^{-2(H-c_i)^{-2}}$. Another possibility is to restrict the study to a submanifold $M'$ of $M$ (typically an open subset of the same dimension). However, problems can arise as the same (induced) symplectic structure (or Poisson bracket) must be used for the dynamic to remain unchanged; in particular, it must checked that the Hamiltonian flow preserves $M'$.

(A) Repulsive harmonic potential. In this example we first solve the equation $\{\Phi_0, H\} = 1$, and then correct the functions $\Phi_0$ to make them $C^\infty$. So, let us consider for $K \neq 0$ the Hamiltonian $H(q,p) := \frac{1}{2}(|p|^2 - K^2|q|^2)$ on $M := \mathbb{R}^{2n}$. One can check that $\text{Crit}(H) = \{0\}$ and that

$$\varphi_t(q,p) = \left(\frac{K+2}{4K} e^{Kt} + \frac{K-2}{4K} e^{-Kt}, \frac{K+2}{4K} e^{Kt} - \frac{K-2}{4K} e^{-Kt}\right).\$$

For $j \in \{1, \ldots, n\}$, take $\Phi_j(q,p) := \frac{1}{K} \tanh^{-1}(Kq^j/p_j)$, where $\tanh^{-1}(z) = \frac{1}{2} \ln \left|\frac{1+z}{1-z}\right|$ is $C^\infty$ on $\mathbb{R} \setminus \{\pm 1\}$. Whenever $p_j = \pm Kq^j$, the $\Phi_j$ are not well-defined, but outside these regions, they satisfy $\{\Phi_j, H\} = 1$. It is possible in this case to get rid of the singular regions. Indeed, the functions $H_j(q,p) := \frac{1}{2}(p_j^2 - K^2(q^j)^2)$ are first integrals of the motion and the singular regions correspond to the level sets $H_j^{-1}(\{0\})$. Therefore, the functions $\Phi_j := e^{-H_j^{-2}} \Phi_j$ are well-defined and satisfy Assumption 3.2:

$$\{\{\Phi_j, H\}, H\} = \{e^{-H_j^{-2}}, H\} = 0.\$$

In this example, one has $\{0\} = \text{Crit}(H) \subseteq \text{Crit}(H, \Phi') = \bigcap_j H_j^{-1}(\{0\})$. 

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(B) Simple pendulum. In this example we first consider the dynamics on a manifold and then restrict it to an appropriate submanifold. For $K > 0$, take $H(q, p) := \frac{1}{2}(p^2 + K(1 - \cos q))$ on $M := \mathbb{R}^2$. One has $\text{Crit}(H) = \pi\mathbb{Z} \times \{0\}$ (the values $q \in 2\pi\mathbb{Z}$ correspond to minima, while $q \in 2\pi\mathbb{Z} + \pi$ correspond to inflexion points). Then, consider the open subset $M'$ of $M$ defined by the relation $H > K$, i.e. $M' := \{(q, p) \in \mathbb{R}^2 \mid p^2/2 - K \cos^2(q/2) > 0\}$. One verifies easily that $M'$ is preserved by the Hamiltonian flow, that $M' \cap \text{Crit}(H) = \emptyset$ and that $M'$ corresponds to the region where the values of $q$ along an orbit cover all of $\mathbb{R}$. Define also

$$\Phi(q, p) := \sqrt{\frac{2}{H(q, p)}} F(q/2|\sqrt{K/H(q, p)}) \equiv \sqrt{2} \int_0^{q/2} \frac{d\theta}{\sqrt{H(q, p) - K \sin^2(\theta)}}$$

where $F(\cdot | \cdot)$ denotes the incomplete elliptic integral of the first kind. Then one verifies that the function $\Phi$ is well-defined on $M'$ and a direct calculation gives $\{\Phi, H\}(q, p) = p/|p|$ for each $(q, p) \in M'$. Now, $p/|p| = 1$ on one connected component of $M'$ and $p/|p| = -1$ on the other one. Thus Assumption 3.2 is verified on $M'$ and $\text{Crit}(H, \Phi) = \emptyset$.

(C) Unbounded trajectories of central force systems. Once again, we first consider the dynamics on a manifold and then restrict it to an appropriate submanifold. For $K \in \mathbb{R} \setminus \{0\}$, take $H(q, p) := \frac{1}{2}(p^2 - K|q|^{-1})$ on $M := (\mathbb{R}^n \setminus \{0\}) \times \mathbb{R}^n$, with $n > 1$ if $K > 0$ and $n \geq 1$ if $K < 0$. One has $\text{Crit}(H) = \emptyset$.

When $K > 0$ (and $n > 1$), we must restrict our attention to the case where the Hamiltonian function $H$ is positive (to avoid periodic orbits), and where at least one of the two-dimensional angular momenta $L_{ij}(q, p) := q^i p_j - q^j p_i$ is nonzero (to avoid collisions, i.e. orbits whose flow is not defined for all $t \in \mathbb{R}$, see [31]). Therefore, the open set $M' := \{(q, p) \in M | H(p, q) > 0, \sum_{i,j=1}^n |L_{ij}(q, p)|^2 \neq 0\}$ is an appropriate submanifold of $M$ when $K > 0$.

Consider now the real valued functions on $M$ (resp. $M'$) when $K < 0$ (resp. $K > 0$ and $n > 1$) given by

$$\Phi_\pm(q, p) := \frac{p \cdot q}{2H(q, p)} \mp \frac{K}{2(2H(q, p))^{3/2}} \ln \left( \frac{|q|(2H(q, p) + |p|^2) \mp 2\sqrt{2H(q, p)} p \cdot q}{|q|} \right).$$

Since $|p|^2 < 2H(q, p)$ (resp. $|p|^2 > 2H(q, p)$), then

$$\left(\sqrt{2H(q, p) - |p|^2}\right)^2 > 0 \implies 2H(q, p)|p|^2 \mp 2\sqrt{2H(q, p)} p \cdot q > 0$$

$$\iff |q|(2H(q, p) + |p|^2) \mp 2\sqrt{2H(q, p)} p \cdot q > 0.$$  

So, $\Phi_\pm$ are well-defined, and further calculations show that $\{\Phi_\pm, H\} = 1$ on $M$ (resp. $M'$). As before, $\text{Crit}(H) = \text{Crit}(H, \Phi_\pm) = \emptyset$. Note that $\Phi_\pm(q, p) = p \cdot q/|p|^2$ when $K = 0$, which is coherent with the canonical function $\Phi$ for the purely kinetic Hamiltonian $H(q, p) = \frac{1}{2}|p|^2$.

One can construct a more intuitive function $\Phi_0$ in terms of $\Phi_\pm$, namely,

$$\Phi_0(q, p) := \frac{1}{2}(\Phi_+ + \Phi_-)(q, p) = \frac{p \cdot q}{2H(q, p)} - \frac{K}{2(2H(q, p))^{3/2}} \tanh^{-1} \left( \frac{2\sqrt{2H(q, p)} p \cdot q}{|q|(2H(q, p) + |p|^2)} \right),$$

which also satisfies $\{\Phi_0, H\} = 1$. Since the functions satisfying Assumption 3.2 are linear in $t$, one can regard them as inverse functions for the flow. The appearance of the inverse hyperbolic function $\tanh^{-1}$ in $\Phi_0$ is related to the fact that unbounded trajectories of the central force system given by $H > 0$ are hyperbolas.

(D) Poincaré ball model. Consider $B_1 := \{q \in \mathbb{R}^n \mid |q| < 1\}$ endowed with the Riemannian metric $g$ given by

$$g_q(X_q, Y_q) := \frac{4}{(1 - |q|^2)^2} (X_q \cdot Y_q), \quad q \in B_1, \ X_q, Y_q \in T_qB_1 \simeq \mathbb{R}^n.$$
Let \( M := T^*B_1 \simeq \{(q, p) \in B_1 \times \mathbb{R}^n\} \) be the cotangent bundle on \( B_1 \) with symplectic form \( \omega := \sum_{j=1}^n dq_j \wedge dp_j \), and let

\[
H : M \to \mathbb{R}, \quad (q, p) \mapsto \frac{1}{2} \sum_{j,k=1}^n g^{jk}(q)p_jp_k = \frac{1}{8} |p|^2 (1 - |q|^2)^2
\]

be the kinetic energy Hamiltonian. It is known that the integral curves of the vector field \( X_H \) correspond to the geodesics curves of \( (B_1, g) \) (see [20, Thm. 1.6.3] or [11, Sec. 6.4]). Since, \( (B_1, g) \) is geodesically complete (see Proposition 3.5 and Exercise 6.5 of [26]), this implies that \( X_H \) is complete. There remains only to find a function \( \Phi \) satisfying Assumption 3.2 in order to apply the theory.

Some calculations using spherical-type coordinates suggest the function

\[
\Phi : M \to \mathbb{R}, \quad (q, p) \mapsto e^{-1/H(q,p)} \tanh^{-1} \left( \frac{(p \cdot q)(1 - |q|^2)}{\sqrt{2H(q,p)}(1 + |q|^2)} \right).
\]

Indeed, since

\[
\left| \frac{(p \cdot q)(1 - |q|^2)}{\sqrt{2H(q,p)}(1 + |q|^2)} \right| = \frac{2|p \cdot q|}{|p|(1 + |q|^2)} \leq \frac{2|q|}{1 + |q|^2} < 1,
\]

the function \( \Phi \) is well-defined. Furthermore, direct calculations show that \( \Phi \) is \( C^\infty \) and that \( \{\Phi, H\} = e^{-1/H} \sqrt{2H} \). Therefore, Assumption 3.2 is verified and one has \( \text{Crit}(H) = \text{Crit}(H, \Phi) = B_1 \setminus \{0\} \).

In one dimension, \( q(t) := \tanh(t) \) is (up to speed and direction) the only geodesic curve, and

\[
\Phi(q, p) = e^{-1/H(q,p)} \tanh^{-1} \left( \frac{2pq}{|p|(1 + q^2)} \right) = 2 e^{-1/H(q,p)} \frac{p}{|p|} \tan^{-1}(q).
\]

So, apart from the smoothing factor \( 2 e^{-1/H} \), our \( \Phi \) coincides in one dimension with the inverse function of the flow.

### 4.4 Passing to a covering manifold

In this subsection we briefly discuss a way of avoiding the obstruction of periodic orbits: Given \( M \) a symplectic manifold with symplectic form \( \omega \) and Hamiltonian \( H \), we let \( \pi : \tilde{M} \to M \setminus \text{Crit}(H) \) be \( C^\infty \)-covering manifold. In order to preserve the dynamics, we endow the manifold \( \tilde{M} \) with the pullback \( \tilde{\omega} := \pi^* \omega \) of the symplectic form \( \omega \) and with the pullback \( \tilde{H} := \pi^* H \) of the Hamiltonian \( H \).

Here are two simple examples of finite-dimensional symplectic covering manifolds.

(A) Consider on the sphere \( M := S^2 \) (as seen in \( \mathbb{R}^3 \)) and with its standard symplectic structure) the Hamiltonian \( \tilde{H} \) given by the projection onto the \( z \)-coordinate. Outside the 2 polar critical points, all the orbits are periodic: the flow corresponds to rotations around the \( z \)-axis. In this case, one can use the covering of \( S^2 \setminus \{(0, 0, \pm 1)\} \) given by \( \tilde{M} := \{ (\vartheta, z) \mid \vartheta \in \mathbb{R}, \ z \in (-1, 1) \} \) and the covering map

\[
\pi : \tilde{M} \to M \setminus \text{Crit}(H) \equiv S^2 \setminus \{(0, 0, \pm 1)\}, \quad (\vartheta, z) \mapsto (\sqrt{1 - z^2} \cos(\vartheta), \sqrt{1 - z^2} \sin(\vartheta), z).
\]

Consequently, \( \tilde{H} : \tilde{M} \to (-1, 1) \) is the projection onto the \( z \)-coordinate and \( \tilde{\omega} = d\vartheta \wedge dz \). One can also check that \( \varphi_t(\vartheta, z) := (\vartheta + t, z) \) is the flow of \( \tilde{H} \) and that \( \{\tilde{\Phi}, \tilde{H}\} = 1 \) for \( \tilde{\Phi}(\vartheta, z) := \vartheta \). So, Assumption 3.2 is verified on \( \tilde{M} \) and \( \text{Crit}(\tilde{H}) = \text{Crit}(H, \tilde{\Phi}) = \emptyset \).

---

3If one wants to consider only a Poisson manifold \( \tilde{M} \), a Poisson structure can also be defined on \( \tilde{M} \) given that \( \pi \) is \( C^\infty \). Indeed, for \( U \subset M \setminus \text{Crit}(H) \) a sufficiently small open set (i.e. such that \( \pi^{-1}(U) \) is disjoint union of diffeomorphic copies), connected components of \( \pi^{-1}(U) \) are diffeomorphic to \( U \) and the Poisson structure can be induced by this diffeomorphism.
(B) Harmonic oscillator. Consider on \( M := \mathbb{R}^{2n} \) (with its standard symplectic structure) the Hamiltonian given by \( H(q,p) = \frac{1}{2}(|p|^2 + K^2|q|^2) \), where \( K \in \mathbb{R} \setminus \{0\} \). Define \( \tilde{M} := \{(r, \vartheta) \mid r \in (0, \infty)^n, \vartheta \in \mathbb{R}^n \} \) and \( \pi : \tilde{M} \to M \setminus \text{Crit}(H) \equiv \mathbb{R}^{2n} \setminus \{0\} \), with
\[
\pi(r, \vartheta) := (K^{-1} r_1 \cos(\vartheta_1), \ldots, K^{-1} r_n \cos(\vartheta_n), r_1 \sin(\vartheta_1), \ldots, r_n \sin(\vartheta_n)).
\]
Then \( \tilde{H}(r, \vartheta) = \frac{1}{2}|r|^2 \), \( \omega = K^{-1} \sum_{j=1}^{n} r_j \, dr_j \wedge d\vartheta_j \), and \( \varphi_t(r, \vartheta) = (r, \vartheta - Kt) \) is the flow of \( \tilde{H} \).

Furthermore, one has \( \tilde{\Phi}_j, \tilde{H} \rangle = -K \) for each function \( \tilde{\Phi}_j(r, \vartheta) := \vartheta_j \). Therefore, Assumption 3.2 is verified on \( M \) with \( \Phi \equiv (\tilde{\Phi}_1, \ldots, \tilde{\Phi}_n) \) and \( \text{Crit}(H) = \text{Crit}(\tilde{H}, \Phi) = \emptyset \).

4.5 Infinite dimensional Hamiltonian systems

4.5.1 Classical systems

In the following examples, the infinite dimensional manifold \( M \) is either \( L^2(\mathbb{R}) \) or \( L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \) (equivalence classes of real valued square integrable functions). The atlas of \( M \) consists in only one chart, the tangent space \( T_uM \) at a point \( u \in M \) is isomorphic to \( M \), and the Riemannian metric on \( M \) is flat (i.e. independent of the base point in \( M \)) and given by the usual scalar product \( \langle \cdot, \cdot \rangle \) on \( L^2(\mathbb{R}) \) or \( L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \).

To define the symplectic form on \( M \) in terms of the metric \( \langle \cdot, \cdot \rangle \) we let \( H^s, s \in \mathbb{R} \), denote the real Sobolev space \( \mathcal{H}^s(\mathbb{R}) \) or \( \mathcal{H}^s(\mathbb{R}) \oplus \mathcal{H}^s(\mathbb{R}) \) (see [4, Sec. 4.1] for the definition in the complex case) and we let \( \mathcal{S} \) denote the real Schwartz space \( \mathcal{S}(\mathbb{R}) \) or \( \mathcal{S}(\mathbb{R}) \oplus \mathcal{S}(\mathbb{R}) \). Then we consider an operator \( J : \mathcal{S} \to \mathcal{S} \) (which can be interpreted by continuity as an endomorphism of the tangent spaces \( T_uM \subset M \) satisfying the following:

(i) There exists a number \( d_j \geq 0 \), called the order of \( J \), such that for each \( s \in \mathbb{R} \) the operator \( J \) extends to an isomorphism \( \mathcal{H}^s \to \mathcal{H}^{s-d_j} \) (which we denote by the same symbol).

(ii) \( J \) is antisymmetric on \( \mathcal{S} \), i.e. \( \langle Jf, g \rangle = -\langle f, Jg \rangle \) for all \( f, g \in \mathcal{S} \).

It is known [23, Lemma 1.1] that the operator \( \bar{J} := -J^{-1} : M \to \mathcal{H}^{d_j} \) (of order \( -d_j \)) is bounded and anti-selfadjoint in \( M \). In consequence, for each \( s \geq 0 \) the map \( \omega : \mathcal{H}^s \times \mathcal{H}^s \to \mathbb{R} \) given by
\[
\omega(f, g) := -\langle Jf, g \rangle
\]
defines a symplectic form on \( \mathcal{H}^s \).

The functions on the phase space (such as \( H \) or \( \Phi_j \)) are infinitely Fréchet differentiable mappings from \( O_{su} \) (a subset of \( \mathcal{H}^{s_H} \) for some \( s_H \geq 0 \)) to \( \mathcal{S} \), i.e. elements of \( C^\infty(O_{su}; \mathbb{R}) \). The Hamiltonian function \( H \in C^\infty(O_{su}; \mathbb{R}) \) is defined as follows: for some \( h \in C^\infty(\mathbb{R}^{k+1}; \mathbb{R}) \) (or \( h \in C^\infty(\mathbb{R}^{2k+1}; \mathbb{R}) \) if \( M = L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \)), one has for each \( u \in O_{su} \)
\[
H(u) := \int_\mathbb{R} dx \, h(u_0, u_1, \ldots, u_{su}),
\]
where \( u_j := \frac{d^j u}{dx^j} \). Since \( H \in C^\infty(O_{su}; \mathbb{R}) \), the differential of \( H \) at \( u \in O_{su} \) on a tangent vector \( f \in \mathcal{S} \subset M \simeq T_uM \) is given by
\[
dH(u)(f) = \lim_{t \to 0} \frac{1}{t} [H(u + tf) - H(u)] = \int_\mathbb{R} dx \sum_{j=0}^{su} \frac{\partial h}{\partial u_j} \frac{d^j f}{dx^j} = \sum_{j=0}^{su} \int_\mathbb{R} dx (-1)^j f \frac{d^j h}{dx^j} \frac{\partial h}{\partial u_j},
\]
where the second equality is obtained using integrations by parts (with vanishing boundary contributions).

The (Riemannian) gradient vector field \( \text{grad} H \) associated to the linear functional \( \text{d}H \) satisfies by definition \( \langle (\text{grad} H)(u), f \rangle = \text{d}H_u(f) \) for all \( u \in O_{su} \) and \( f \in \mathcal{S} \) (here \( (\text{grad} H)(u) \) \textit{a priori} only belongs to the

\footnote{In the case of the wave and the Schrödinger equations below, one can easily extend the results to the situation where \( L^2(\mathbb{R}) \) is replaced by \( L^2(\mathbb{R}^n) \). We restrict ourselves to the case \( n = 1 \) for the sake of notational simplicity.}
topological dual $\mathcal{J}^*$ of $\mathcal{J}$, which means that $(\cdot, \cdot)$ denotes \textit{a priori} the duality map between $\mathcal{J}^*$ and $\mathcal{J}$. So, $(\text{grad}H)(u)$ is given by
\begin{equation}
(\text{grad}H)(u) = \sum_{j=0}^{\mathcal{S}_{\mathcal{H}}} (-1)^j \frac{\partial h}{\partial x^j} \partial u_j.
\end{equation}
Then, the Hamiltonian vector field $X_H$ is the map $\mathcal{O}_{s_{\mathcal{H}}} \to \mathcal{J}^*$ satisfying
\[ \langle \tilde{J} f, X_H(u) \rangle = -\omega(f, X_H(u)) = dH_u(f) = \langle f, (\text{grad}H)(u) \rangle \]
for all $u \in \mathcal{O}_{s_{\mathcal{H}}}$ and $f \in \mathcal{J}$. Since $J$ is anti-selfadjoint, this implies that $J X_H(u) = -(\text{grad}H)(u)$ in $\mathcal{J}^*$, which is equivalent to $X_H(u) = J(\text{grad}H)(u)$ in $\mathcal{J}^*$. So, the equation of motion with Hamiltonian $H$ has the form $\frac{d}{dt} u = J(\text{grad}H)(u)$, and $\{\Phi, H\} = d\Phi(X_H) = \langle \text{grad}\Phi, J(\text{grad}H) \rangle$ for all functions $\Phi, H \in C^\infty(\mathcal{O}_{s_{\mathcal{H}}}, \mathbb{R})$ with appropriate gradient.

Before passing to concrete examples, we refer to [21] for standard results on the local existence in time of Hamiltonian flows (global existence is specific to the system considered).

(A) The wave equation. We refer to [1, Ex. 5.5.1], [2, Ex. 8.1.12], [13, Sec. 2.1] and [32, Sec. X.13] for a description of the model. The existence of the flow for all times depends on the nonlinear term in the Hamiltonian function (see for instance [32, Thm. X.74] and the corollary that follows).

In this example, the scale $\{\mathcal{H}^s\}_{s \geq 0}$ is given by $\mathcal{H}^s := \mathcal{H}^s(\mathbb{R}) \oplus \mathcal{H}^s(\mathbb{R})$. The metric on $M := L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$ is given for each $(p, q), (\tilde{p}, \tilde{q}) \in M$ by $\langle (p, q), (\tilde{p}, \tilde{q}) \rangle := \int_\mathbb{R} dx (p \tilde{p} + q \tilde{q})$, and the operator $J$ is given by
\[ J : M \to M, \quad (p, q) \mapsto (-q, p). \]

It is an isomorphism of degree 0 with $\tilde{J} = J$. Given $m \geq 0$ and $F \in C^\infty(\mathbb{R}; \mathbb{R})$, one can find a subset $\mathcal{O}_1 \subset \mathcal{H}^1$ (depending on $F$) such that the Hamiltonian function
\[ H : \mathcal{O}_1 \to \mathbb{R}, \quad (p, q) \mapsto \int_\mathbb{R} dx \ h(p, q, \partial_x q) \equiv \frac{1}{2} \int_\mathbb{R} dx \ \{ p^2 + (\partial_x q)^2 + m^2 q^2 + 2F(q) \}, \]
is well-defined and $C^\infty$. In fact, we assume that $\mathcal{O}_1$ is chosen such that (i) all the functions on the phase space appearing below are elements of $C^\infty(\mathcal{O}_1; \mathbb{R})$, and (ii) integrations by parts involving these functions come vanishing boundary contributions. Then one checks that $(\text{grad}H)(p, q) = (p, m^2 q + F'(q) - \partial_x^2 q)$ due to (4.2), and that $X_H(p, q)$ is trivial if and only if $p = 0$ and $m^2 q + F'(q) - \partial_x^2 q = 0$. The constraint on $q$ depends on the choice of $F$. For example, when $F(q) = 0$, or $q^2$; the solution $q$ of the differential equation does not decay as $|x| \to \infty$. In consequence, the corresponding pairs $(p, q)$ cannot belong to $M$, and $\text{Crit}(H) = \{(0, 0)\}$. The equation of motion
\[ \frac{d}{dt} (p, q) = J(\text{grad}H)(p, q) \]
coincides with the usual wave equation since the combination of $\frac{d}{dt} p = \partial_x^2 q - m^2 q - F'(q)$ and $\frac{d}{dt} q = p$ gives
\[ \frac{d^2}{dt^2} q = \partial_x^2 q - m^2 q - F'(q). \]
When $m \neq 0$, this equation is called the Klein-Gordon equation, and $F$ is usually assumed to be a nonlinear term of the form $F(q) = q^\lambda$ for some $\lambda \in \mathbb{R}$. A first relevant observation is that the function $C_0 \in C^\infty(\mathcal{O}_1; \mathbb{R})$ given by $C_0(p, q) := \int_\mathbb{R} dx \ p(\partial_x q)$ is a first integral of the motion. Furthermore, the function $\Phi_0 \in C^\infty(\mathcal{O}_1; \mathbb{R})$ given by $\Phi_0(p, q) := \int_\mathbb{R} dx \ id_\mathbb{R} h(p, q, \partial_x q)$ has gradient $(\text{grad}\Phi_0)(p, q) = (id_\mathbb{R} p, id_\mathbb{R} m^2 q + id_\mathbb{R} F'(q) - \partial_x (id_\mathbb{R} \partial_x q))$. Therefore,
\[ \{\Phi_0, H\}(p, q) = \langle (\text{grad}\Phi_0)(p, q), J(\text{grad}H)(p, q) \rangle = \int_\mathbb{R} dx \ p \ \{ id_\mathbb{R} \partial_x^2 q - \partial_x (id_\mathbb{R} \partial_x q) \} = -C_0(p, q), \]
and $\Phi_0$ satisfies Assumption 3.2. Here, we clearly have

$$\text{Crit}(H, \Phi_0) = C_0^{-1}(\{0\}) = \{(p, q) \in O_1 \mid \int_\mathbb{R} p(\partial_x q) \, dx = 0\} \ni \{(0, 0)\} = \text{Crit}(H).$$

If we assume further that $F \equiv 0$, then the equation of motion (4.3) is linear. Therefore any pair $(\partial_x p, \partial_x q)$, $j \geq 1$, with $(p, q)$ a solution of (4.3), also satisfies (4.3). Consequently, if the subsets $O_j \subset \mathcal{H}^j$ have properties similar to the ones of $O_1$, then the functions $C_j \in C^\infty(O_{j+1}; \mathbb{R})$ and $H_j \in C^\infty(O_{j+1}; \mathbb{R})$ given by $C_j(p, q) := \int_\mathbb{R} dx (\partial_x p) (\partial_x^2 q)$ and $H_j(p, q) := \int_\mathbb{R} dx h(\partial_x p, \partial_x q, \partial_x^2 q)$ are first integrals of the motion. Accordingly, one deduces that the functions $\Phi_j \in C^\infty(O_{j+1}; \mathbb{R})$ given by $\Phi_j(p, q) := \int_\mathbb{R} dx \, id_{\mathbb{R}} h(\partial_x p, \partial_x q, \partial_x^2 q)$ satisfy $\{\Phi_j, H\} = -C_j$ on $O_{j+1}$. So, if $F \equiv 0$, there is an infinite family of functions $\Phi_j$ satisfying Assumption 3.2, and one has again $\text{Crit}(H, \Phi_j) \supsetneq \text{Crit}(H)$, with $\partial_x^j : \text{Crit}(H, \Phi_j) \rightarrow \text{Crit}(H, \Phi_0)$ an isomorphism.

Finally, when $F \equiv 0$ and $m = 0$ one can check that the function $\tilde{\Phi}_0 \in C^\infty(O_1; \mathbb{R})$ given by $\tilde{\Phi}_0(p, q) := \int_\mathbb{R} dx \, \partial_x p(\partial_x q)$ has gradient $(\partial_x p)(p, q) = (\partial_x^2 p, -\partial_x p - p)$. Then,

$$\{\tilde{\Phi}_0, H\}(p, q) = \int_\mathbb{R} dx \, (\partial_x p(\partial_x q)) - \partial_x^2 p \partial_x q - p^2 = -\frac{1}{2} \int_\mathbb{R} dx \, (\partial_x q)^2 + p^2 = -H(p, q),$$

where the third equality is obtained using integrations by parts (with vanishing boundary contributions). Thus $\tilde{\Phi}_0$ satisfies Assumption 3.2. Furthermore, since $\{\tilde{\Phi}_0, H\}(p, q) = 0$ implies $\int_\mathbb{R} dx \, \{(\partial_x q)^2 + p^2\} = 0$, one has $\text{Crit}(H, \tilde{\Phi}_0) = \text{Crit}(H) = \{(0, 0)\}$. As before, any derivative of a solution of the equation of motion is still a solution of the equation of motion. So, it can be checked that the functions $\Phi_j \in C^\infty(O_{j+1}; \mathbb{R})$ given by $\Phi_j(p, q) := \int_\mathbb{R} dx \, \partial_x^2 p(\partial_x^2 q)$ satisfy $\{\Phi_j, H\} = -H_j$ on $O_{j+1}$. Therefore, one has once again $\text{Crit}(H, \Phi_j) = \text{Crit}(H) = \{(0, 0)\}$ and the $\Phi_j$’s constitute a second infinite family of functions satisfying Assumption 3.2.

(B) The nonlinear Schrödinger equation. We refer to [23, Ex. 1.3, p. 3 & 5] for a description of the model. The existence of the flow for all times depends on the nonlinear term in the Hamiltonian (see for instance [8, Sec. 1.2] and [36, Sec. 3.2.2-3.2.3]).

The setting is the same as that of the previous example, except that the Hamiltonian function $H \in C^\infty(O_1; \mathbb{R})$ is given by

$$H(p, q) := \frac{1}{2} \int_\mathbb{R} dx \, \{(\partial_x p)^2 + (\partial_x q)^2 + V \cdot (p^2 + q^2) + F(p^2 + q^2)\},$$

where $V, F \in C^\infty(\mathbb{R}; \mathbb{R})$. Using (4.2), one checks that the gradient of $H$ at $(p, q) \in O_1$ is

$$(\text{grad} H)(p, q) = (\partial_x p V + p V' (p^2 + q^2), -\partial_x q V + q V' (p^2 + q^2)).$$

So, the equation of motion $\frac{d}{dt} (p, q) = J(\text{grad} H)(p, q)$ is equivalent to the nonlinear Schrödinger equation

$$\frac{d}{dt} u = i(-\partial_x^2 u + V u + u F'(|u|^2)),$$

with $u := p + iq$. Without additional assumptions on $F$ or $V$, it is hardly possible to determine the set $\text{Crit}(H)$ of functions $u$ for which the r.h.s. of (4.4) vanishes. However, it is known that in general $\text{Crit}(H)$ is not trivial, as in the case of elliptic stationary nonlinear Schrödinger equations (see Theorem 1.1 and Proposition 1.1 of [6]).

Now, assume that $V \equiv F \equiv 0$ and for each $j \geq 1$ let $O_j \subset \mathcal{H}^j$ be a subset having properties similar to the ones of $O_1$. Then the functions $H_j \in C^\infty(O_j; \mathbb{R})$ and $C_j \in C^\infty(O_{j+1}; \mathbb{R})$ given by $H_j(p, q) := \frac{1}{2} \int_\mathbb{R} dx \, \{(\partial_x p)^2 + (\partial_x q)^2\} = \int_\mathbb{R} dx h_j(p, q)$ and $C_j(p, q) := \int_\mathbb{R} dx \, \{(\partial_x p)(\partial_x^2 q) - (\partial_x^2 p)(\partial_x q)\} = \int_\mathbb{R} dx c_j(p, q)$ are first integrals of the motion. Furthermore, the functions $\Phi_j \in C^\infty(O_j; \mathbb{R})$ and $\Phi_j \in C^\infty(O_{j+1}; \mathbb{R})$ given by $\Phi_j(p, q) := \int_\mathbb{R} dx \, \partial_x h_j(p, q)$ and $\tilde{\Phi}_j(p, q) := \int_\mathbb{R} dx \, \partial_x c_j(p, q)$ satisfy $\{\Phi_j, H\} = \{(0, 0)\}$.
\[ C_j \text{ and } \{ \Phi_j, H \} = 4H_{j+1} \text{ on } O_{j+1}. \text{ So, the } \Phi_j's \text{ and the } \Phi_j's \text{ constitute two infinite families of functions satisfying Assumption 3.2. Note that the sets } \text{C} \{ \Phi_0, H \} = C_0 \text{ on } O_1 \text{ remains valid for all } V \text{ and } F. \text{ Furthermore, if } V = \text{Const}., \text{ then } \{ C_0, H \} = 0 \text{ on } O_1. \text{ Consequently, } \Phi_0 \text{ satisfies Assumption 3.2 for all } F \text{ and for } V = \text{Const}., \text{ and one has } \text{C} \{ \Phi_0, H \} \geq \text{C} \{ \Phi, H \}. \text{ This last example is interesting since it applies to a large class of nonlinear Schrödinger equations.}

\[ (C) \text{ The Korteweg-de Vries equation. Among many other possible references, we mention } [1, \text{Ex. } 5.5.7] \text{ and } [23, \text{Ex. } 1.4, \text{p. } 3 & 5]. \text{ For the global existence of the flow, we refer the reader to } [12, \text{Sec. } 1] \text{ and references therein.}

In this example, the set \( \{ H^* \} \) is given by \( H^* := H^*(\mathbb{R}) \) and the sets \( O_j, j \in \mathbb{N} \), are appropriate subsets of \( H^* \). The Hamiltonian function \( H \in C^\infty(\mathcal{O}_1; \mathbb{R}) \) is given by

\[ H(u) := \int_\mathbb{R} dx \left( \frac{1}{2}(\partial_x u)^2 + u^3 \right), \]

and the isomorphism \( J := \partial_x \) is of order 1.

The gradient of \( H \) at \( u \in \mathcal{O}_1 \) is \( -\partial_x^2 u + 3u^2 \). So, the elements of \( \text{C} \{ H \} \) are functions \( u \) satisfying \( -\partial_x^2 u + 3u^2 = 0 \); these are Weierstrass \( \wp \)-functions [22, Sec. 134.F], that is, functions with many singularities and no decay at infinity. Thus, \( \text{C} \{ H \} = \{0\} \). Furthermore, the equation of motion for \( \frac{d}{dt} u = J(\text{grad} H)(u) \) coincides with the KdV equation \( \frac{d}{dt} u = \partial_x \left( -\partial_x^2 u + 3u^2 \right) \).

There exists an infinite number of first integrals of the motion with polynomial density, that is, of the form \( H_j := \int \mathbb{R} dx \partial_{h_j} \), where \( h_j \) is a finite polynomial in \( u \) and its derivatives (see [29, Sec. 3]). For example, when \( h_1(u) = u, h_2(u) = u^2, h_3(u) = \frac{1}{2}(\partial_x u)^2 + u^3 \), or \( h_4(u) = (\partial_x^2 u)^2 + 10u(\partial_x u)^2 + 5u^4 \). So, let \( \Phi_0 \in C^\infty(\mathcal{O}_0; \mathbb{R}) \) be given by \( \Phi_0(u) := \int_\mathbb{R} dx \text{id}_\mathbb{R} u \). Then the gradient of \( \Phi_0 \) at \( u \) is \( \text{id}_\mathbb{R} \), and \( \{ \Phi_0, H \} = -3H_2 \) on \( \mathcal{O}_1 \). Since \( H_2 \) is a first integral of the motion, this implies that \( \Phi_0 \) satisfies Assumption 3.2. Furthermore, the fact that \( H_2(u) = ||u||_{L^2(\mathbb{R})} \) implies that \( \text{C} \{ \Phi, H \} = \{0\} \).

Looking for others \( \Phi \) of the form \( \Phi(u) = \int_\mathbb{R} dx g(x) G(u, \partial_x u, \ldots, \partial_x^k u) \), with \( G \) a polynomial and \( g \) a \( C^\infty \) function, is unnecessary. Indeed, both \( \{ \Phi, H \} \) and \( \text{crit}(\text{crit}(\text{crit}(\Phi, H))) \) are first integrals of the motion with density \( C^\infty \) in \( x \) and polynomial in \( u \) and its derivatives (and \( t \)-linear in the case of \( \text{crit} \)). Thus, we know from [37, Thm. 1 & Rem. 3] that they are completely characterised, up to the usual equivalence of conservation laws [30, Sec. 4.3]. Therefore, the functions \( \Phi \) are also completely characterised. Note however, that it is not excluded that functions \( \Phi \) with an integrand \( G \) involving fractional derivatives, an infinite number of derivatives, or of class \( C^\infty \) might work. Non-polynomial conserved densities are known to exist in the periodic case (see [29, Sec. 5]).

### 4.5.2 Quantum systems

Let \( \mathcal{H} \) be a complex Hilbert space, with scalar product \( \langle \cdot, \cdot \rangle \) antilinear in the left entry. Define on \( \mathcal{H} \) the usual quantum-mechanical symplectic form

\[ \omega : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{R}, \quad (\psi_1, \psi_2) \mapsto 2 \text{Im}\langle \psi_1, \psi_2 \rangle. \]

The pair \( (\mathcal{H}, \omega) \) has the structure of an (infinite-dimensional) symplectic vector space. Now, define for any bounded selfadjoint operator \( H_{op} \in \mathcal{B}(\mathcal{H}) \) the expectation value Hamiltonian function

\[ H : \mathcal{H} \rightarrow \mathbb{R}, \quad \psi \mapsto \langle H_{op} \rangle(\psi) := \langle \psi, H_{op} \psi \rangle. \]

Then, it is known [27, Cor. 2.5.2] that the vector field and the flow associated to \( H \) are \( X_H = -iH_{op} \) and \( \varphi_t(\psi) = e^{-itH_{op}} \psi \). Therefore, the Poisson bracket of two such Hamiltonian functions \( H, K \) satisfies for each \( \psi \in \mathcal{H} \)

\[ \{ K, H \}(\psi) = \omega(X_K(\psi), X_H(\psi)) = -\omega(K_{op} \psi, H_{op} \psi) = \langle \psi, i[K_{op}, H_{op}] \psi \rangle. \]
Then we know from [16, Sec. 3.1] that any polynomial in \( U \) and \( \Phi_j \) is well-defined and symmetric. In fact, it is shown that \( H \) is well-defined and symmetric. In fact, it is shown that \( H \) is well-defined. We do not present here the whole theory since much of it, examples included, is similar to that of [33]. We prefer to present a new example inspired by [16], where all the calculations can be easily justified.

Let \( U \) be an isometry in \( \mathcal{H} \) admitting a number operator, that is, a selfadjoint operator \( N \) such that \( U N U^* = N - 1 \). Define on \( \mathcal{H} \) the bounded selfadjoint operators

\[
\Delta := \text{Re}(U) \equiv \frac{1}{2}(U + U^*) \quad \text{and} \quad S := \text{Im}(U) \equiv \frac{1}{2i}(U - U^*).
\]

Then we know from [16, Sec. 3.1] that any polynomial in \( U \) and \( U^* \) leaves invariant the domain \( \mathcal{D}(N) \subset \mathcal{H} \) of \( N \). In particular, the operator

\[
A_0 := \frac{1}{2}(SN + NS), \quad \mathcal{D}(A_0) := \mathcal{D}(N),
\]

is well-defined and symmetric. In fact, it is shown that \( A_0 \) admits a selfadjoint extension \( A \) with domain \( \mathcal{D}(A) = \mathcal{D}(NS) \). Furthermore, one has on \( \mathcal{D}(N) \) the identity \( i[A, \Delta] = \Delta^2 - 1 \). So, if we define the Hamiltonian functions

\[
H : \mathcal{H} \to \mathbb{R}, \quad \psi \mapsto \langle \Delta \rangle(\psi) \quad \text{and} \quad \Phi : \mathcal{D}(N) \to \mathbb{R}, \quad \psi \mapsto \langle A \rangle(\psi),
\]

we obtain for each \( \psi \in \mathcal{D}(N) \)

\[
(\nabla H)(\psi) = \{\Phi, H\}(\psi) = \langle i[A, H] \rangle(\psi) = \langle \Delta^2 - 1 \rangle(\psi),
\]

and Assumption 3.2 is verified for each \( \psi \in \mathcal{D}(N) \):

\[
\{\{\Phi, H\}, H\}(\psi) = \omega(\chi_{\{\Delta^2 - 1\}}(\psi), X_{\{\Delta\}}(\psi)) = \langle i[\Delta^2 - 1, \Delta] \rangle(\psi) = 0.
\]

Now, since the spectrum of \( \Delta \) is \([-1, 1]\), the operator \( 1 - \Delta^2 \) is positive, so we have the equivalences

\[
\langle \Delta^2 - 1 \rangle(\psi) = 0 \iff \| (1 - \Delta^2)^{1/2} \psi \|^2 = 0 \iff \psi \in E^\Delta(\{\pm 1\}).
\]

Thus,

\[
\text{Crit}(H, \Phi) \equiv (\nabla H)^{-1}(\{0\}) = \{ \psi \in \mathcal{D}(N) \mid \langle \Delta^2 - 1 \rangle(\psi) = 0 \} = \mathcal{D}(N) \cap E^\Delta(\{\pm 1\}).
\]

On the other hand, the elements \( \psi \in \text{Crit}(H) \) satisfy the condition

\[
0 = X_H(\psi) = -i\Delta \psi \iff \psi \in E^\Delta(\{0\}).
\]

This implies that \( \text{Crit}(H) = \{0\} \), since the spectrum of \( \Delta \) is purely absolutely continuous outside the points \( \pm 1 \) [16, Prop. 3.2]. Finally, the function \( T_f \) is given by

\[
T_f = -\langle A \rangle \cdot \langle \nabla R_f \rangle(\langle \Delta^2 - 1 \rangle)
\]

on \( \mathcal{D}(N) \setminus \text{Crit}(H, \Phi) \).

Typical examples of operators \( \Delta \) and \( N \) of the preceding type are Laplacians and number operators on trees or complete Fock spaces (see [16] for details).

**Acknowledgements**

Part of this work was done while R.T.d.A was visiting the Max Planck Institute for Mathematics in Bonn. He would like to thank Professor Dr. Don Zagier for his kind hospitality. R.T.d.A also thanks Professor M. Musso for a useful conversation on the stationary nonlinear Schrödinger equation.
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