A formula relating localisation observables to the variation of energy 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 observables satisfying the condition $\{\{\Phi_j, H\}, H\} = 0$ for each j. Under these assumptions, we prove a new formula relating the time evolution of localisation observables defined in terms of Φ to the variation of energy along 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.

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Contents

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 the time evolution of localisation observables to the variation of energy along classical orbits.

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

$$\big\{\{\Phi_j, H\}, H\big\} = 0 \tag{1.1}$$

for each $j \in \{1, \ldots, d\}$. Then we have (see Theorem 3.3, Corollary 3.4 and Lemma 3.6 for a precise statement):

Theorem 1.1. *Let H and Φ 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 $\mathsf{Crit}(H,\Phi) \subset M$ and an observable $T_f \in \mathsf{C}^\infty\big(M \setminus \mathsf{Crit}(H,\Phi)\big)$ satisfying $\{T_f, H\} = 1$ on $M \setminus \mathsf{Crit}(H,\Phi)$ such that*

$$\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t\, \big[\big(f(\Phi/r) \circ \varphi_{-t}\big)(m) - \big(f(\Phi/r) \circ \varphi_t\big)(m)\big] = T_f(m) \tag{1.2}$$

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

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,

$$T_f := -\Phi \cdot (\nabla R_f)(\nabla H), \tag{1.3}$$

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 $\omega := \sum_{j=1}^n \mathrm{d}q^j \wedge \mathrm{d}p_j$. Furthermore, let $H(q,p) := h(p)$ be a purely kinetic energy Hamiltonian and let $\Phi(q,p) := q$ be the standard family of position observables. In such a case, the condition (1.1) is readily verified, the vector ∇H reduces to the usual velocity observable ∇h associated to H, and the l.h.s. of Formula (1.2) has the following meaning: For $r > 0$ and $m \in M \setminus \mathsf{Crit}(H,\Phi)$ fixed, it is equal to 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 $\Sigma_r := \mathrm{supp}[f(\Phi/r)] \subset M$ defined by the localisation observable $f(\Phi/r)$. Moreover, if we interpret the map $\frac{\mathrm{d}}{\mathrm{d}H} := \{T_f, \,\cdot\,\}$ as a derivation on $\mathsf{C}^\infty\big(M \setminus \mathsf{Crit}(H,\Phi)\big)$, then T_f on the r.h.s. of (1.2) can be seen as an observable "derivative with respect to the energy H" on $M \setminus \mathsf{Crit}(H,\Phi)$, since $\frac{\mathrm{d}}{\mathrm{d}H}(H) = \{T_f, H\} = 1$ on $M \setminus \mathsf{Crit}(H,\Phi)$. Therefore, Formula (1.2) provides a new relation between sojourn times and variation of energy along classical orbits. Evidently, this interpretation remains valid in the general case provided that we consider the observables Φ_j as the components of an abstract position observable Φ (see Remark 3.7).

Our interest in this issue has been aroused by a recent paper [31], where the authors establish a similar formula in the framework of quantum (Hilbertian) theory. In that reference, 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 $\big[[\Phi_j, H], H\big] = 0$, 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 [24] for the interconnections between classical and quantum mechanics). Accordingly, we try 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 affiliation of the corresponding quantum orbits $\{\mathrm{e}^{itH}\,\psi\}_{t\in\mathbb{R}}$, $\psi \in \mathcal{H}$, to the singular (resp. absolutely continuous) subspace of $\mathcal{H}$. Moreover, we show in Section 4.5.2 that the Hilbertian space theory of [31] can be recast into the present framework of symplectic geometry by using expectation values.

We also mention that Formula (1.2), with r.h.s. defined by (1.3), provides a crucial preliminary step for the proof of the existence of classical time delay for abstract scattering pairs $\{H, H+V\}$ (see [10], [14, Sec. 4.1], and [35, Sec. 3.4] for an account on classical time delay). If V is an appropriate perturbation of H and S is the associated scattering map, then the classical time delay $\tau(m)$ for $m \in M$ defined in terms of the localisation operators $f(\Phi/r)$ should be reexpressed as follows: it is equal to the l.h.s. of (1.2) minus the same quantity with m replaced by $S(m)$. Therefore, if m and $S(m)$ are elements of $M \setminus \mathsf{Crit}(H,\Phi)$, then the classical time delay for the scattering pair $\{H, H+V\}$ should satisfy the equation

$$\tau(m) = (T_f - T_f \circ S)(m).$$

Now, the property $\{T_f, H\}(m) = 1$ implies that $T_f(m) = (T_f \circ \varphi_t)(m) - t$ for each $t \in \mathbb{R}$. Since S commutes with φ_t, this would imply that

$$\tau(m) = \big[(T_f - T_f \circ S) \circ \varphi_t\big](m)$$

for all $t \in \mathbb{R}$, meaning that the classical time delay is a first integral of the free motion. This property corresponds in the quantum case to the fact that the time delay operator is decomposable in the spectral representation of the free Hamiltonian (see [32, Rem. 4.4]).

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 $\Phi \circ \varphi_{\pm t} : M \to \mathbb{R}^d$ 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, ω, H) and the abstract position observable Φ. Then we define the (closed) set of critical points $\mathsf{Crit}(H,\Phi)$ associated to H and Φ as (see [31, Def. 2.5] for the quantum analogue):

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

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

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

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

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 3.7.

In Section 4, we show that our results apply to many Hamiltonian systems (M, ω, 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 Hamiltonians 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 [31, 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 Φ satisfying our assumptions. The diversity of the examples covered by our theory, together with the existence of a quantum analogue [31], make 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 $f \in \mathsf{L}^\infty(\mathbb{R}^d)$ of localisation around the origin $0 \in \mathbb{R}^d$. They were already used, in one form or another, in [17, 31, 32, 37, 38]. We use the notation $\langle x \rangle := \sqrt{1+|x|^2}$ for any $x \in \mathbb{R}^d$.

Assumption 2.1. *The function $f \in \mathsf{L}^\infty(\mathbb{R}^d)$ satisfies the following conditions:*

(i) There exists $\rho > 0$ such that $|f(x)| \le \mathrm{Const.}\,\langle x \rangle^{-\rho}$ 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 $x \in \mathbb{R}^d \setminus \{0\}$

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

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

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

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 [38, Sec. 2] for proofs and details. The symbol $\mathscr{S}(\mathbb{R}^d)$ 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 $j \in \{1, \dots, d\}$ and $x \in \mathbb{R}^d$, and suppose that there exists some $\rho > 0$ such that $\left|\frac{\partial f}{\partial x_j}(x)\right| \le \mathrm{Const.}\,\langle x \rangle^{-(1+\rho)}$ for each $x \in \mathbb{R}^d$. Then R_f is differentiable on $\mathbb{R}^d \setminus \{0\}$, and its gradient is given by

$$(\nabla R_f)(x) = \int_0^\infty \mathrm{d}\mu \, (\nabla f)(\mu x).$$

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

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

$$\begin{aligned} x \cdot (\nabla R_f)(x) &= -1, \\ t^{|\alpha|} (\partial^\alpha R_f)(tx) &= (\partial^\alpha R_f)(x), \end{aligned} \tag{2.1}$$

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

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

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 $y \in \mathbb{R}^d \setminus \{0\}$*

$$\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t \left[f\Big(\frac{x - ty}{r}\Big) - f\Big(\frac{x + ty}{r}\Big) \right] = -x \cdot (\nabla R_f)(y). \tag{2.2}$$

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

$$\begin{aligned}
&\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t \left[f\left(\tfrac{x-ty}{r}\right) - f\left(\tfrac{x+ty}{r}\right)\right] \\
&= \lim_{\nu\searrow 0} \tfrac{1}{2} \int_0^\infty \frac{\mathrm{d}\mu}{\nu} \left[f(\nu x - \mu y) - f(\nu x + \mu y)\right] \\
&= \lim_{\nu\searrow 0} \tfrac{1}{2} \int_0^\infty \mathrm{d}\mu \left\{\tfrac{1}{\nu}\left[f(\nu x - \mu y) - f(-\mu y)\right] - \tfrac{1}{\nu}\left[f(\nu x + \mu y) - f(\mu y)\right]\right\}. \qquad (2.3)
\end{aligned}$$

By using the mean value theorem and the assumptions of Lemma 2.2.(a), one obtains that

$$\tfrac{1}{\nu}\left|f(\nu x \pm \mu y) - f(\pm \mu y)\right| \leq \mathrm{Const.} \sup_{\xi\in[0,1]} \left\langle \xi\nu x \pm \mu y\right\rangle^{-(1+\rho)}$$

for some $\rho > 0$. Therefore, if μ is big enough, the integrant in (2.3) is bounded by

$$\mathrm{Const.} \left\langle \mu|y| - |x|\right\rangle^{-(1+\rho)}.$$

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 $\mathsf{L}^1\big([0,\infty), \mathrm{d}\mu\big)$. So, we can apply Lebesgue's dominated convergence theorem to interchange the limit on ν with the integration over μ in (2.3). This, together with the fact that $(\nabla f)(-x) = -(\nabla f)(x)$, leads to the desired result:

$$\begin{aligned}
\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t \left[f\left(\tfrac{x-ty}{r}\right) - f\left(\tfrac{x+ty}{r}\right)\right] &= \tfrac{1}{2} \int_0^\infty \mathrm{d}\mu \left[x \cdot (\nabla f)(-\mu y) - x \cdot (\nabla f)(\mu y)\right] \\
&= -\int_0^\infty \mathrm{d}\mu \, x \cdot (\nabla f)(\mu y) \\
&= -x \cdot (\nabla R_f)(y).
\end{aligned}$$

□

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 [41, 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 χ_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 $y \in \mathbb{R}^d \setminus \{0\}$*

$$\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t \left[\chi_1\Big(\frac{x-ty}{r}\Big) - \chi_1\Big(\frac{x+ty}{r}\Big)\right] = \frac{x \cdot y}{y^2}.$$

Proof. Direct calculations and the change of variables $\mu := t/r$, $\nu := 1/r$, give

$$\begin{aligned}
\int_0^\infty \mathrm{d}t \, \chi_1\left(\tfrac{x\pm ty}{r}\right) = \textstyle\int_0^\infty \frac{\mathrm{d}\mu}{\nu} \, \chi_{[0,1]}\left(|\nu x \pm \mu y|^2\right) &= \int_0^\infty \mathrm{d}\mu \, \chi_{[0,y^{-2}]}\Big(\tfrac{\nu^2 x^2}{y^2} \pm \tfrac{2\nu\mu x\cdot y}{y^2} + \mu^2\Big) \\
&= \int_0^\infty \frac{\mathrm{d}\mu}{\nu} \, \chi_{[0,y^{-2}]}\Big(\big(\mu \pm \tfrac{\nu x\cdot y}{y^2}\big)^2 + \tfrac{\nu^2}{y^4}\big(x^2 y^2 - (x\cdot y)^2\big)\Big) \\
&= \int_0^\infty \frac{\mathrm{d}\mu}{\nu} \, \chi_{[-a(\nu,x,y),y^{-2}-a(\nu,x,y)]}\Big(\big(\mu \pm \tfrac{\nu x\cdot y}{y^2}\big)^2\Big),
\end{aligned}$$

with $a(\nu,x,y) := \frac{\nu^2}{y^4}\big(x^2y^2 - (x\cdot y)^2\big)$. Now, $a(\nu,x,y) \geq 0$, and $y^{-2} - a(\nu,x,y) \geq 0$ if $\nu > 0$ is small enough. So, the last expression is equal to

$$\begin{aligned}
\int_0^\infty \frac{\mathrm{d}\mu}{\nu} \, \chi_{[0,y^{-2}-a(\nu,x,y)]}\Big(\big(\mu \pm \tfrac{\nu x\cdot y}{y^2}\big)^2\Big) &= \int_0^\infty \frac{\mathrm{d}\mu}{\nu} \, \chi_{\left[-\sqrt{y^{-2}-a(\nu,x,y)} \mp \frac{\nu x\cdot y}{y^2}, \sqrt{y^{-2}-a(\nu,x,y)} \mp \frac{\nu x\cdot y}{y^2}\right]}(\mu) \\
&= \frac{1}{\nu}\sqrt{y^{-2} - a(\nu,x,y)} \mp \frac{x\cdot y}{y^2}
\end{aligned}$$

if ν is small enough. This implies that

$$\begin{aligned}
&\lim_{r\to\infty} \tfrac{1}{2}\int_0^\infty \mathrm{d}t\,\big[\chi_1\big(\tfrac{x-ty}{r}\big)-\chi_1\big(\tfrac{x+ty}{r}\big)\big]\\
&=\lim_{\nu\searrow 0}\frac{1}{2}\Big(\frac{1}{\nu}\sqrt{y^{-2}-a(\nu,x,y)}+\frac{x\cdot y}{y^2}-\frac{1}{\nu}\sqrt{y^{-2}-a(\nu,x,y)}+\frac{x\cdot y}{y^2}\Big)\\
&=\frac{x\cdot y}{y^2}.
\end{aligned}$$

□

For the next corollary, we need the following version of the Poisson summation formula (see [15, Thm. 5] or [39, 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 $\int_0^\infty \mathrm{d}t\, g(t)$ exists. Then we have the identity*

$$\tfrac{1}{2}g(0)+\sum_{n\geq 1} g(n)=\int_0^\infty \mathrm{d}t\, g(t)+2\sum_{n\geq 1}\int_0^\infty \mathrm{d}t\,\cos(2\pi nt)g(t).$$

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 $|(\partial^\alpha f)(x)|\leq \mathrm{Const.}\,\langle x\rangle^{-(1+\rho)}$ for some $\rho>0$ and all $x\in\mathbb{R}^d$.

Then we have for each $x\in\mathbb{R}^d$ and each $y\in\mathbb{R}^d\setminus\{0\}$

$$\lim_{r\to\infty}\tfrac{1}{2}\sum_{n\geq 1}\Big[f\Big(\frac{x-ny}{r}\Big)-f\Big(\frac{x+ny}{r}\Big)\Big]=-x\cdot(\nabla R_f)(y). \tag{2.4}$$

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

$$g_r:(0,\infty)\to\mathbb{C},\quad t\mapsto g_r(t):=f\big(\tfrac{x-ty}{r}\big)-f\big(\tfrac{x+ty}{r}\big),$$

satisfies all the hypotheses of Lemma 2.5. Thus

$$\lim_{r\to\infty}\tfrac{1}{2}\sum_{n\geq 1}\big[f\big(\tfrac{x-ny}{r}\big)-f\big(\tfrac{x+ny}{r}\big)\big]=\lim_{r\to\infty}\tfrac{1}{2}\int_0^\infty \mathrm{d}t\, g_r(t)+\lim_{r\to\infty}\sum_{n\geq 1}\int_0^\infty \mathrm{d}t\,\cos(2\pi nt)g_r(t).$$

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

$$\begin{aligned}
&\lim_{r\to\infty}\sum_{n\geq 1}\int_0^\infty \mathrm{d}t\,\cos(2\pi nt)g_r(t)\\
&=\lim_{\nu\searrow 0}\sum_{n\geq 1}\int_0^\infty\frac{\mathrm{d}\mu}{\nu}\,\cos(2\pi n\mu/\nu)\big[f(\nu x-\mu y)-f(\nu x+\mu y)\big]\\
&=\sum_j y_j\lim_{\nu\searrow 0}\sum_{n\geq 1}\int_0^\infty \mathrm{d}\mu\,\frac{\sin(2\pi n\mu/\nu)}{2\pi n}\Big(\frac{\partial f}{\partial x_j}(\nu x-\mu y)+\frac{\partial f}{\partial x_j}(\nu x+\mu y)\Big)\\
&=\sum_j y_j\lim_{\nu\searrow 0}\sum_{n\geq 1}\frac{2\nu}{(2\pi n)^2}\frac{\partial f}{\partial x_j}(\nu x)\\
&\quad-\sum_{j,k} y_jy_k\lim_{\nu\searrow 0}\sum_{n\geq 1}\int_0^\infty \mathrm{d}\mu\,\frac{\nu\cos(2\pi n\mu/\nu)}{(2\pi n)^2}\Big(\frac{\partial^2 f}{\partial x_k\partial x_j}(\nu x-\mu y)+\frac{\partial^2 f}{\partial x_k\partial x_j}(\nu x+\mu y)\Big).
\end{aligned}$$

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,

$$\lim_{r\to\infty} \tfrac{1}{2} \sum_{n\geq 1} \left[f\left(\tfrac{x-ny}{r}\right) - f\left(\tfrac{x+ny}{r}\right)\right] = -x \cdot (\nabla R_f)(y),$$

and the claim is proved. □

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

In the sequel, the function $H \in \mathsf{C}^\infty(M)$ 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:

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

and satisfies the usual evolution equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} f \circ \varphi_t = \{f, H\} \circ \varphi_t, \quad t \in \mathbb{R}. \tag{3.1}$$

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

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

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

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

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

is called the set of critical points associated to H and Φ.

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

$$\mathsf{Crit}(H) := \big\{m \in M \mid X_H(m) = 0\big\} \equiv \big\{m \in M \mid \mathrm{d}H_m = 0\big\}$$

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

Our main assumption is the following:

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

Assumption 3.2. *One has* $\big\{\{\Phi_j, H\}, H\big\} = 0$ *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 $g_j \in \mathsf{C}^\infty(\mathbb{R}^n; \mathbb{R})$. Using the properties of $\{\,\cdot\,, H\}$ as a derivation, one infers that $\big\{g_j(J_1, \ldots, J_k)^{-1}\Phi_j, H\big\} = 1$ outside $g_j(J_1, \ldots, J_k)^{-1}(\{0\})$. Thus, if k first integrals as $J_1, \ldots, J_k$ are known, finding functions Φ_j satisfying Assumption 3.2 is to some extent equivalent to finding functions Φ_0 solving $\{\Phi_0, H\} = 1$ (the equivalence is not complete because these functions Φ_0 are in general not C^∞ since $\{\,\cdot\,, H\}$ is necessarily 0 on $\mathsf{Crit}(H)$).

For further use, we define the C^∞-function $T_f : M \setminus \mathsf{Crit}(H, \Phi) \to \mathbb{R}$ 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 fact, the closed subset $T^{-1}(\{0\})$ of $M \setminus \mathsf{Crit}(H, \Phi)$ admits an interesting interpretation: If we consider the observables Φ_j as the components of an abstract position observable Φ, then ∇H can be seen as the velocity vector for the Hamiltonian H, and the condition

$$T(m) = 0 \iff \Phi(m) \cdot (\nabla H)(m) = 0 \tag{3.2}$$

means that the position and velocity vectors are orthogonal at $m \in T^{-1}(\{0\})$. Alternatively, one has $T(m) = 0$ if and only if the vector fields $X_{|\Phi|^2}$ and X_H are ω-orthogonal at m, that is, $\omega_m\big(X_{|\Phi|^2}(m), X_H(m)\big) = 0$. The simplest example illustrating the condition (3.2) is when $\Phi(q, p) := q$ and $H(q, p) := \frac{1}{2}|p|^2$ are the usual position and kinetic energy on $(M, \omega) := \big(\mathbb{R}^{2n}, \sum_{j=1}^n \mathrm{d}q^j \wedge \mathrm{d}p_j\big)$. In such a case, (3.2) reduces to $q \cdot p = 0$.

3.2 Sojourn times of classical orbits

Next Theorem is our main result. We refer to Remark 3.7 below for its interpretation.

Theorem 3.3. *Let H and Φ satisfy Assumption 3.2. Let $f : \mathbb{R}^d \to \mathbb{C}$ be an even function as in Lemma 2.2.(a). Then we have for each point $m \in M \setminus \mathsf{Crit}(H, \Phi)$*

$$\lim_{r\to\infty} \tfrac{1}{2} \int_0^\infty \mathrm{d}t \,\big[\big(f(\Phi/r) \circ \varphi_{-t}\big)(m) - \big(f(\Phi/r) \circ \varphi_t\big)(m)\big] = T_f(m). \tag{3.3}$$

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

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\, \{\Phi_j, H\} \circ \varphi_t = \big\{\{\Phi_j, H\}, H\big\} \circ \varphi_t = 0.$$

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

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

[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 $\mathbb{R}^{n-\ell} \times \mathbb{T}^\ell$ (see [1, Thm. 5.2.24]).

This, together with Formula (2.2), gives

$$
\begin{aligned}
&\lim_{r\to\infty}\tfrac12\int_0^\infty \mathrm{d}t\,\big[\big(f(\Phi/r)\circ\varphi_{-t}\big)(m)-\big(f(\Phi/r)\circ\varphi_t\big)(m)\big]\\
&=\lim_{r\to\infty}\tfrac12\int_0^\infty \mathrm{d}t\,\Big[f\Big(\tfrac{\Phi(m)-t(\nabla H)(m)}{r}\Big)-f\Big(\tfrac{\Phi(m)+t(\nabla H)(m)}{r}\Big)\Big]\\
&=T_f(m).
\end{aligned}
$$

□

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 Φ satisfy Assumption 3.2. Then we have for each point $m\in M\setminus\mathsf{Crit}(H,\Phi)$*

$$
\lim_{r\to\infty}\tfrac12\int_0^\infty \mathrm{d}t\,\big[\big(\chi_1(\Phi/r)\circ\varphi_{-t}\big)(m)-\big(\chi_1(\Phi/r)\circ\varphi_t\big)(m)\big]=\Phi(m)\cdot\tfrac{(\nabla H)(m)}{(\nabla H)(m)^2}\,. \tag{3.4}
$$

We know from the proof of Theorem 3.3 that

$$
(\Phi_j\circ\varphi_t)(m)=\Phi_j(m)+t(\partial_jH)(m)\quad\text{for all } t\in\mathbb{R}\text{ and all } m\in M. \tag{3.5}
$$

Therefore, the l.h.s. of (3.3) and (3.4) are zero if $m\in\mathsf{Crit}(H,\Phi)$.

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 [40, Sec. 7.4]

$$
\mathcal{H}=\mathcal{H}_{\rm ac}(A)\oplus\mathcal{H}_{\rm p}(A)\oplus\mathcal{H}_{\rm sc}(A)\equiv\mathcal{H}_{\rm ac}(A)\oplus\mathcal{H}_{\rm s}(A),
$$

where $\mathcal{H}_{\rm ac}(A),\mathcal{H}_{\rm p}(A),\mathcal{H}_{\rm sc}(A)$ and $\mathcal{H}_{\rm s}(A)$ 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 $J\subset\mathbb{R}$ if $\varphi=E^A(J)\varphi$.

Remark 3.5. *If $m\in\mathsf{Crit}(H,\Phi)$, then one must have $\varphi_t(m)\in\mathsf{Crit}(H,\Phi)$ for all $t\in\mathbb{R}$, since* (3.5) *implies $(\partial_jH)(\varphi_t(m))=(\partial_jH)(m)$ for all $t\in\mathbb{R}$. Conversely, if $m\in M\setminus\mathsf{Crit}(H,\Phi)$, then one must have $\varphi_t(m)\neq m$ for all $t\neq0$, since Φ cannot take two different values at a same point. So, under Assumption 3.2, each orbit $\{\varphi_t(m)\}_{t\in\mathbb{R}}$ either stays in $\mathsf{Crit}(H,\Phi)$ if $m\in\mathsf{Crit}(H,\Phi)$, or stays outside $\mathsf{Crit}(H,\Phi)$ and is not periodic if $m\notin\mathsf{Crit}(H,\Phi)$.*

In the corresponding Hilbertian framework [31], the Hamiltonian H and the functions Φ_j are selfadjoint operators in a Hilbert space $\mathcal{H}$, and the critical set κ associated to H and Φ is a closed subset of the spectrum of H. Outside κ, the spectrum of H is purely absolutely continuous [31, Thm. 3.6.(a)]. Therefore, vectors $\psi\in\mathcal{H}$ having spectral support with respect to H in κ belong to the singular subspace $\mathcal{H}_{\rm s}(H)$ of H, and thus lead to orbits $\{\mathrm{e}^{itH}\,\psi\}_{t\in\mathbb{R}}$ confined in $\mathcal{H}_{\rm s}(H)$ (for instance, $\mathrm{e}^{itH}\,\psi$ stays in a one-dimensional subspace of $\mathcal{H}$ if ψ is an eigenvector of H). Conversely, vectors $\psi\in\mathcal{H}$ having spectral support outside κ belong to the absolute continuous subspace $\mathcal{H}_{\rm ac}(H)$ of H, and thus lead to orbits $\{\mathrm{e}^{itH}\,\psi\}_{t\in\mathbb{R}}$ contained in $\mathcal{H}_{\rm ac}(H)$ (see [3, Prop. 5.7] for the escape properties of such orbits). These properties are the quantum counterparts of the confinement to $\mathsf{Crit}(H,\Phi)$ (when $m\in\mathsf{Crit}(H,\Phi)$) and the non-periodicity outside $\mathsf{Crit}(H,\Phi)$ (when $m\notin\mathsf{Crit}(H,\Phi)$) of the classical orbits $\{\varphi_t(m)\}_{t\in\mathbb{R}}$.

Lemma 3.6. *If H, Φ and f satisfy the assumptions of Theorem 3.3, then we have*

$$
\{T_f,H\}\circ\varphi_t\equiv\frac{\mathrm{d}}{\mathrm{d}t}(T_f\circ\varphi_t)=1 \tag{3.6}
$$

on $M\setminus\mathsf{Crit}(H,\Phi)$. In particular, one has $T_f\circ\varphi_t=T_f+t$ on $M\setminus\mathsf{Crit}(H,\Phi)$.

If we interpret the map $\frac{\mathrm{d}}{\mathrm{d}H}:=\{T_f,\,\cdot\,\}$ as a derivation on $\mathsf{C}^\infty\big(M\setminus\mathsf{Crit}(H,\Phi)\big)$, this implies that T_f can be seen as an observable "derivative with respect to the energy H" on $M\setminus\mathsf{Crit}(H,\Phi)$, since

$$
\tfrac{\mathrm{d}}{\mathrm{d}H}(H)=\{T_f,H\}=1
$$

on each orbit $\{\varphi_t(m)\}_{t\in\mathbb{R}}$, with $m\in M\setminus\mathsf{Crit}(H,\Phi)$.

Proof of Lemma 3.6. The first equality in (3.6) follows from (3.1). For the second one, we use successively the fact that φ_t leaves invariant H and the Poisson bracket, Assumption 3.2, and Equation (2.1). Doing so, we get on $M \setminus \mathsf{Crit}(H, \Phi)$ the following equalities

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(T_f \circ \varphi_t) = -\frac{\mathrm{d}}{\mathrm{d}t}(\Phi \circ \varphi_t) \cdot (\nabla R_f)\big(\{\Phi \circ \varphi_t, H\}\big) &= -\frac{\mathrm{d}}{\mathrm{d}t}\big(\Phi + t(\nabla H)\big) \cdot (\nabla R_f)\big(\{\Phi + t(\nabla H), H\}\big) \\ &= -\frac{\mathrm{d}}{\mathrm{d}t}\big(\Phi + t(\nabla H)\big) \cdot (\nabla R_f)(\nabla H) \\ &= -(\nabla H) \cdot (\nabla R_f)(\nabla H) \\ &= 1. \end{aligned}$$

□

Remark 3.7. *Theorem 3.3 relates the sojourn times of classical orbits within expanding regions of M to the observable T_f. If we consider the observables Φ_j as the components of an abstract position observable Φ, then the l.h.s. of Formula* (3.3) *has the following meaning: For $r > 0$ and $m \in M \setminus \mathsf{Crit}(H, \Phi)$ fixed, 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 $\Sigma_r := \operatorname{supp}[f(\Phi/r)] \subset M$ defined by the localisation observable $f(\Phi/r)$. Thus, Formula* (3.3) *shows that this difference of times tends as $r \to \infty$ to the value of the observable T_f at m. Since T_f can be interpreted as an observable derivative with respect to the energy H, Formula* (3.3) *provides a new relation between sojourn times and variation of energy along classical orbits.*

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], [18, Appendix B], [23] and references therein).

Theorem 3.8. *Let H and Φ 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 $|(\partial^\alpha f)(x)| \leq \mathrm{Const.}\, \langle x \rangle^{-(1+\rho)}$ *for some $\rho > 0$ and all $x \in \mathbb{R}^d$.*

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

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

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 $m \in M \setminus \mathsf{Crit}(H, \Phi)$. Then we have by Equation (3.5)

$$\begin{aligned}&\lim_{r\to\infty} \tfrac{1}{2} \sum_{n\geq 1} \big[\big(f(\Phi/r) \circ \varphi_{-n}\big)(m) - \big(f(\Phi/r) \circ \varphi_n\big)(m)\big] \\ &= \lim_{\nu\searrow 0} \tfrac{1}{2} \sum_{n\geq 1} \Big[f\Big(\tfrac{\Phi(m)-n(\nabla H)(m)}{r}\Big) - f\Big(\tfrac{\Phi(m)+n(\nabla H)(m)}{r}\Big)\Big],\end{aligned}$$

and the claim follows by Formula (2.4). □

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 (3.6) hold. Some of the examples presented here are the classical counterparts of examples discussed in [31, 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 $M = T^*\mathbb{R}^n \simeq \mathbb{R}^{2n}$. 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 $\omega := \sum_{j=1}^n \mathrm{d}q^j \wedge \mathrm{d}p_j$ 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 Φ satisfy Assumption 3.2 since $\{g_j(H), H\} = 0$ for each j. Furthermore, one has $\mathsf{Crit}(H,\Phi) = (g \circ H)^{-1}(\{0\})$, and $T_f = -\Phi \cdot (\nabla R_f)\big(g(H)\big)$ on $M \setminus \mathsf{Crit}(H,\Phi)$. We distinguish various cases:

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

Typical examples of functions H and Φ fitting into this construction are Friedrichs-type Hamiltonians 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 $V \in \mathsf{C}^\infty(\mathbb{R}^n;\mathbb{R})$. In such a case, one has $\nabla H = v$ and
$$\varphi_t(q,p) = \big(vt + q, p - \textstyle\int_0^t \mathrm{d}s\, (\nabla V)(vs + q)\big).$$
Stark-type Hamiltonians and momentum functions also fit into the construction, *i.e.* $H(q,p) := h(p) + v \cdot q$ and $\Phi(q,p) := p$ on $M := \mathbb{R}^{2n}$, with $v \in \mathbb{R}^n \setminus \{0\}$ and $h \in \mathsf{C}^\infty(\mathbb{R}^n;\mathbb{R})$. In such a case, one has $\nabla H = -v$ and
$$\varphi_t(q,p) = \big(q + \textstyle\int_0^t \mathrm{d}s\, (\nabla h)(p - vs), p - vt\big).$$
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 Φ 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 Φ-homogeneous [9]). Then $\mathsf{Crit}(H,\Phi) = H^{-1}(\{0\})$ 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,Φ) satisfying these assumptions:

The Hamiltonian flow of the function $D(q,p) := q \cdot p$ on $\mathbb{R}^{2n}$ is given by $\varphi_t^D(q,p) = (\mathrm{e}^t\, q, \mathrm{e}^{-t}\, p)$. 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 $\mathsf{L}^2(\mathbb{R}^n)$, see *e.g.* [4, Sec. 1.2]). Therefore, the relation $\{D, H\} \propto H$ 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 $h \in \mathsf{C}^\infty(\mathbb{R}^n;\mathbb{R})$ is positive homogeneous of degree α and $V \in \mathsf{C}^\infty(\mathbb{R}^n \setminus \{0\};\mathbb{R})$ is positive homogeneous of degree $-\alpha$. Then one has $\nabla H \equiv \{\Phi, H\} = H$ on M, and
$$\begin{aligned}
\mathsf{Crit}(H) &= \big\{(q,p) \in M \mid (\nabla h)(p) = (\nabla V)(q) = 0\big\} \\
&\subset \big\{(q,p) \in M \mid p \cdot (\nabla h)(p) = q \cdot (\nabla V)(q) = 0\big\} \\
&= \big\{(q,p) \in M \mid H(q,p) = 0\big\} \\
&= \mathsf{Crit}(H,\Phi).
\end{aligned}$$
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 $\varphi_t(q,p) = \big(q + t(\nabla h)(p), p\big)$ and
$$\mathsf{Crit}(H) = \big\{(q,p) \in M \mid (\nabla h)(p) = 0\big\} \subset \big\{(q,p) \in M \mid p \cdot (\nabla h)(p) = 0\big\} = \mathsf{Crit}(H,\Phi)$$
(when $h(p) = \frac{1}{2}|p|^2$ is the classical kinetic energy, one has $\mathsf{Crit}(H) = \mathsf{Crit}(H,\Phi) = \mathbb{R}^n \times \{0\}$).

(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 $\iota : \mathbb{R}^n \setminus \{0\} \times \mathbb{R}^n \to \mathbb{R}^n \setminus \{0\} \times \mathbb{R}^n$, $(q,p) \mapsto \big(q|q|^{-2}, p\big) \equiv (r,p)$, namely,
$$[\iota_*(X_H)](r,p) = \sum_j \left(\big(|r|^2 p_j - 2(p \cdot r) r^j\big) \frac{\partial}{\partial r^j}\Big|_{(r,p)} + K r^j |r|^2 \frac{\partial}{\partial p_j}\Big|_{(r,p)}\right).$$

Then, we obtain that $\iota_*(X_H)$ is complete by using the criterion [1, Prop. 2.1.20] with the proper function $g : \mathbb{R}^n \setminus \{0\} \times \mathbb{R}^n \to [0, \infty)$ given by $g(r,p) := |p|^2 + K|r|^2$. Since ι is a diffeomorphism, this implies that X_H is also complete (see [19, Lemma 1.6.4]).

(C) Many other examples with $\nabla H = g(H)$ can be obtained using homogeneous Hamiltonians functions. For instance, consider $H(q,p) := q^2/q^1 + q^1/q^2$ and $\Phi(q,p) := p_1 q^2 + p_2 q^1$ on $M := (\mathbb{R}^2 \setminus \{0\}) \times \mathbb{R}^2$. Then one has $\nabla H = H^2 - 4$, $\varphi_t(q,p) = \big(q, p - t\frac{\partial H}{\partial q}(q,p)\big)$ and

$$\mathsf{Crit}(H) = \mathsf{Crit}(H,\Phi) = \big\{q \in \mathbb{R}^2 \setminus \{0\} \mid q^1 = \pm q^2\big\} \times \mathbb{R}^2.$$

4.2 $H = h(p)$

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

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

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

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 Φ_j of Assumption 3.2 amounts to solving for Φ_0 the second-order linear equation

$$\big\{\{\Phi_0, H\}, H\big\} \equiv \bigg(\sum_{\ell=1}^n \big(H_{p_\ell}\partial_{q^\ell} - H_{q^\ell}\partial_{p_\ell}\big)\bigg)^2 \Phi_0 = 0.$$

As observed in Section 3.1, this is essentially equivalent (when k independent first integrals $J_1 \equiv H, J_2, \dots, J_k$ are known) to find the solutions Φ_0 to

$$\{\Phi_0, H\} = \sum_{\ell=1}^n \big(H_{p_\ell}\partial_{q^\ell} - H_{q^\ell}\partial_{p_\ell}\big)\Phi_0 = g(J_1, \dots, J_k). \tag{4.1}$$

The case $g \equiv 1$ is sufficient, though trying to solve $\{\Phi_0, H\} = 1$ can at best provide solutions which are C^∞ outside the set $\mathsf{Crit}(H)$. A way to remove these singularities could be to multiply the solutions by a function $g(H)$ that vanishes and is infinitely flat on $\mathsf{Crit}(H)$. For instance, if $H\big(\mathsf{Crit}(H)\big)$ consists of a finite number of values $c_1, \dots, c_s \in \mathbb{R}$, one could take $g(H) = \prod_{j=1}^s \mathrm{e}^{-(H-c_j)^{-2}}$. 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 Φ_0 to make them C^∞. So, let us consider for $K \neq 0$ the Hamiltonian $H(q,p) := \frac{1}{2}\big(|p|^2 - K^2|q|^2\big)$ on $M := \mathbb{R}^{2n}$. One can check that $\mathsf{Crit}(H) = \{0\}$ and that

$$\varphi_t(q,p) = \big(\tfrac{Kq+p}{2K}\,\mathrm{e}^{Kt} + \tfrac{Kq-p}{2K}\,\mathrm{e}^{-Kt}, \tfrac{Kq+p}{2}\,\mathrm{e}^{Kt} - \tfrac{Kq-p}{2}\,\mathrm{e}^{-Kt}\big).$$

For $j \in \{1, \dots, n\}$, take $\Phi_j(q,p) := \frac{1}{K}\tanh^{-1}(Kq^j/p_j)$, where $\tanh^{-1}(z) \equiv \frac{1}{2}\ln\left|\frac{1+z}{1-z}\right|$ is C^∞ on $\mathbb{R} \setminus \{\pm 1\}$. Whenever $p_j = \pm Kq^j$, the Φ_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 $H_j(q,p) := \frac{1}{2}\big(p_j^2 - K^2(q^j)^2\big)$ are first integrals of the motion and the singular regions correspond to the level sets $H_j^{-1}(\{0\})$. Therefore, the functions $\Phi'_j := \mathrm{e}^{-H_j^{-2}}\,\Phi_j$ are well-defined and satisfy Assumption 3.2:

$$\big\{\{\Phi'_j, H\}, H\big\} = \big\{\,\mathrm{e}^{-H_j^{-2}}, H\big\} = 0.$$

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

(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 $H(q,p) := \frac{1}{2}\big(p^2 + K(1-\cos q)\big)$ on $M := \mathbb{R}^2$. One has $\mathsf{Crit}(H) = \pi\mathbb{Z} \times \{0\}$ (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.* $M' := \big\{(q,p) \in \mathbb{R}^2 \mid p^2/2 - K\cos^2(q/2) > 0\big\}$. One verifies easily that M' is preserved by the Hamiltonian flow, that $M' \cap \mathsf{Crit}(H) = \varnothing$ and that M' corresponds to the region where the values of q along an orbit cover all of $\mathbb{R}$. Define also

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

where $F(\,\cdot\,|\,\cdot\,)$ denotes the incomplete elliptic integral of the first kind. Then one verifies that the function Φ 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 $\mathsf{Crit}(H,\Phi) = \varnothing$.

(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 $H(q,p) := \frac{1}{2}\big(|p|^2 - K|q|^{-1}\big)$ 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 $\mathsf{Crit}(H) = \varnothing$.

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 [29]). Therefore, the open set $M' := \big\{(q,p) \in M | H(p,q) > 0,\ \sum_{i,j=1}^n |L_{ij}(q,p)|^2 \neq 0\big\}$ 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

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

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

$$\begin{aligned}\big(\sqrt{2H(q,p)} - |p|\big)^2 > 0 &\Longrightarrow 2H(q,p)|p|^2 \pm 2\sqrt{2H(q,p)}\,p \cdot \frac{q}{|q|} > 0\\ &\Longleftrightarrow\ |q|\big(2H(q,p) + |p|^2\big) \pm 2\sqrt{2H(q,p)}\,p \cdot q > 0.\end{aligned}$$

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

One can construct a more intuitive function Φ_0 in terms of $\Phi_\pm$, namely,

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

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 Φ_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 $B_1 := \big\{q \in \mathbb{R}^n \mid |q| < 1\big\}$ endowed with the Riemannian metric g given by

$$g_q(X_q, Y_q) := \frac{4}{(1-|q|^2)^2}\,(X_q \cdot Y_q), \quad q \in B_1,\ X_q, Y_q \in T_q B_1 \simeq \mathbb{R}^n.$$

Let $M := T^*B_1 \simeq \big\{(q,p) \in B_1 \times \mathbb{R}^n\big\}$ be the cotangent bundle on B_1 with symplectic form $\omega := \sum_{j=1}^n \mathrm{d}q^j \wedge \mathrm{d}p_j$, and let

$$H : M \to \mathbb{R}, \quad (q,p) \mapsto \tfrac{1}{2} \sum_{j,k=1}^n g^{jk}(q) p_j p_k = \tfrac{1}{8}|p|^2\big(1-|q|^2\big)^2$$

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 [19, Thm. 1.6.3] or [11, Sec. 6.4]). Since, (B_1, g) is geodesically complete (see Proposition 3.5 and Exercice 6.5 of [25]), this implies that X_H is complete. There remains only to find a function Φ satisfying Assumption 3.2 in order to apply the theory.

Some calculations using spherical-type coordinates suggest the function

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

Indeed, since

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

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

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

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

So, apart from the smoothing factor $2\,\mathrm{e}^{-1/H}$, our Φ 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 ω and Hamiltonian H, we let $\pi : \widetilde{M} \to M \setminus \mathsf{Crit}(H)$ be C^∞-covering manifold. In order to preserve the dynamics, we endow the manifold $\widetilde{M}$ with the pullback $\widetilde{\omega} := \pi^*\omega$ of the symplectic form ω and with the pullback $\widetilde{H} := \pi^*H$ of the Hamiltonian H.[3]

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

(A) Consider on the sphere $M := \mathbb{S}^2$ (as seen in $\mathbb{R}^3$ and with its standard symplectic structure) the Hamiltonian 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 $\mathbb{S}^2 \setminus \{(0,0,\pm 1)\}$ given by $\widetilde{M} := \big\{(\vartheta, z) \mid \vartheta \in \mathbb{R},\ z \in (-1,1)\big\}$ and the covering map

$$\pi : \widetilde{M} \to M \setminus \mathsf{Crit}(H) \equiv \mathbb{S}^2 \setminus \{(0,0,\pm 1)\}, \quad (\vartheta, z) \mapsto \big(\sqrt{1-z^2}\cos(\vartheta), \sqrt{1-z^2}\sin(\vartheta), z\big).$$

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

[3] If one wants to consider only a Poisson manifold M, a Poisson structure can also be defined on $\widetilde{M}$ given that π is C^∞. Indeed, for $U \subset M \setminus \mathsf{Crit}(H)$ a sufficiently small open set (*i.e.* such that $\pi^{-1}(U)$ is a 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 $H(q,p) := \frac{1}{2}\big(|p|^2+K^2|q|^2\big)$, where $K \in \mathbb{R}\setminus\{0\}$. Define $\widetilde{M} := \big\{(r,\vartheta) \mid r \in (0,\infty)^n,\ \vartheta \in \mathbb{R}^n\big\}$ and $\pi : \widetilde{M} \to M \setminus \mathsf{Crit}(H) \equiv \mathbb{R}^{2n} \setminus \{0\}$, with

$$\pi(r,\vartheta) := \big(K^{-1}r_1\cos(\vartheta_1),\dots,K^{-1}r_n\cos(\vartheta_n), r_1\sin(\vartheta_1),\dots,r_n\sin(\vartheta_n)\big).$$

Then $\widetilde{H}(r,\vartheta) = \frac{1}{2}|r|^2$, $\widetilde{\omega} = K^{-1}\sum_{j=1}^n r_j\,\mathrm{d}r_j \wedge \mathrm{d}\theta_j$, and $\varphi_t(r,\vartheta) = (r,\vartheta - Kt)$ is the flow of $\widetilde{H}$. Furthermore, one has $\big\{\Phi_j,\widetilde{H}\big\} = -K$ for each function $\Phi_j(r,\vartheta) := \vartheta_j$. Therefore, Assumption 3.2 is verified on $\widetilde{M}$ with $\Phi \equiv (\Phi_1,\dots,\Phi_n)$ and $\mathsf{Crit}(\widetilde{H}) = \mathsf{Crit}(\widetilde{H},\Phi) = \varnothing$.

4.5 Infinite dimensional Hamiltonian systems

4.5.1 Classical systems

In the following examples, the infinite dimensional manifold M is either $\mathsf{L}^2(\mathbb{R})$ or $\mathsf{L}^2(\mathbb{R}) \oplus \mathsf{L}^2(\mathbb{R})$ (equivalence classes of real valued square integrable functions)[4]. 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 $\mathsf{L}^2(\mathbb{R})$ or $\mathsf{L}^2(\mathbb{R}) \oplus \mathsf{L}^2(\mathbb{R})$.

To define the symplectic form on M in terms of the metric $\langle\,\cdot\,,\,\cdot\,\rangle$ we let $\mathcal{H}^s$, $s \in \mathbb{R}$, 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 $\mathscr{S}$ denote the real Schwartz space $\mathscr{S}(\mathbb{R})$ or $\mathscr{S}(\mathbb{R}) \oplus \mathscr{S}(\mathbb{R})$. Then we consider an operator $J : \mathscr{S} \to \mathscr{S}$ (which can be interpreted by continuity as an endomorphism of the tangent spaces $T_uM \simeq M$) 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 $\mathscr{S}$, *i.e.* $\langle Jf,g\rangle = -\langle f,Jg\rangle$ for all $f,g \in \mathscr{S}$.

It is known [22, 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

$$\omega(f,g) := -\big\langle \bar{J}f,g\big\rangle$$

defines a symplectic form on $\mathcal{H}^s$.

The functions on the phase space (such as H or Φ_j) are infinitely Fréchet differentiable mappings from $\mathcal{O}_{s_H}$ (a subset of $\mathcal{H}^{s_H}$ for some $s_H \geq 0$) to $\mathbb{R}$, *i.e.* elements of $\mathsf{C}^\infty(\mathcal{O}_{s_H};\mathbb{R})$. The Hamiltonian function $H \in \mathsf{C}^\infty(\mathcal{O}_{s_H};\mathbb{R})$ is defined as follows: for some $h \in \mathsf{C}^\infty(\mathbb{R}^{k+1};\mathbb{R})$ (or $h \in \mathsf{C}^\infty(\mathbb{R}^{2(k+1)};\mathbb{R})$ if $M = \mathsf{L}^2(\mathbb{R}) \oplus \mathsf{L}^2(\mathbb{R})$), one has for each $u \in \mathcal{O}_{s_H}$

$$H(u) := \int_{\mathbb{R}} \mathrm{d}x\, h(u_0,u_1,\dots,u_{s_H}),$$

where $u_j := \frac{\mathrm{d}^j u}{\mathrm{d}x^j}$. Since $H \in \mathsf{C}^\infty(\mathcal{O}_{s_H};\mathbb{R})$, the differential of H at $u \in \mathcal{O}_{s_H}$ on a tangent vector $f \in \mathscr{S} \subset M \simeq T_uM$ is given by

$$\mathrm{d}H_u(f) = \lim_{t\to0}\frac{1}{t}\big[H(u+tf)-H(u)\big] = \int_{\mathbb{R}}\mathrm{d}x\sum_{j=0}^{s_H}\frac{\partial h}{\partial u_j}\frac{\mathrm{d}^j f}{\mathrm{d}x^j} = \sum_{j=0}^{s_H}\int_{\mathbb{R}}\mathrm{d}x\,(-1)^j f\,\frac{\mathrm{d}^j}{\mathrm{d}x^j}\frac{\partial h}{\partial u_j}\,,$$

where the second equality is obtained using integrations by parts (with vanishing boundary contributions). The (Riemannian) gradient vector field $\mathrm{grad}H$ associated to the linear functional $\mathrm{d}H$ satisfies by definition $\big\langle(\mathrm{grad}H)(u),f\big\rangle = \mathrm{d}H_u(f)$ for all $u \in \mathcal{O}_{s_H}$ and $f \in \mathscr{S}$ (here $(\mathrm{grad}H)(u)$ *a priori* only belongs to the

[4] In the case of the wave and the Schrödinger equations below, one can easily extend the results to the situation where $\mathsf{L}^2(\mathbb{R})$ is replaced by $\mathsf{L}^2(\mathbb{R}^n)$. We restrict ourselves to the case $n = 1$ for the sake of notational simplicity.

topological dual $\mathscr{S}^*$ of $\mathscr{S}$, which means that $\langle\,\cdot\,,\,\cdot\,\rangle$ denotes *a priori* the duality map between $\mathscr{S}^*$ and $\mathscr{S}$). So, $(\mathrm{grad}H)(u)$ is given by

$$(\mathrm{grad}H)(u)=\sum_{j=0}^{s_H}(-1)^j\,\frac{\mathrm{d}^j}{\mathrm{d}x^j}\frac{\partial h}{\partial u_j}\,. \tag{4.2}$$

Then, the Hamiltonian vector field X_H is the map $\mathcal{O}_{s_H}\to\mathscr{S}^*$ satisfying

$$\big\langle \bar J f, X_H(u)\big\rangle=-\omega\big(f,X_H(u)\big)=\mathrm{d}H_u(f)=\big\langle f,(\mathrm{grad}H)(u)\big\rangle$$

for all $u\in\mathcal{O}_{s_H}$ and $f\in\mathscr{S}$. Since $\bar J$ is anti-selfadjoint, this implies that $\bar J X_H(u)=-(\mathrm{grad}H)(u)$ in $\mathscr{S}^*$, which is equivalent to $X_H(u)=J(\mathrm{grad}H)(u)$ in $\mathscr{S}^*$. So, the equation of motion with Hamiltonian H has the form $\frac{\mathrm{d}}{\mathrm{d}t}\,u=J(\mathrm{grad}H)(u)$, and $\{\Phi,H\}=\mathrm{d}\Phi(X_H)=\big\langle\mathrm{grad}\Phi,J(\mathrm{grad}H)\big\rangle$ for all functions $\Phi,H\in\mathsf{C}^\infty(\mathcal{O}_{s_H};\mathbb{R})$ with appropriate gradient.

Before passing to concrete examples, we refer to [20] 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 [30, 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 (see for instance [30, Thm. X.74] and the corollary that follows).

In this example, the scale $\{\mathcal{H}^s\}_{s\ge 0}$ is given by $\mathcal{H}^s:=\mathcal{H}^s(\mathbb{R})\oplus\mathcal{H}^s(\mathbb{R})$. The metric on $M:=\mathsf{L}^2(\mathbb{R})\oplus\mathsf{L}^2(\mathbb{R})$ is given for each $(p,q),(\widetilde p,\widetilde q)\in M$ by $\big\langle(p,q),(\widetilde p,\widetilde q)\big\rangle:=\int_{\mathbb{R}}\mathrm{d}x\,(p\widetilde p+q\widetilde q)$, 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 $\bar J=J$. Given $m\ge 0$ and $F\in\mathsf{C}^\infty(\mathbb{R};\mathbb{R})$, one can find a subset $\mathcal{O}_1\subset\mathcal{H}^1$ (depending on F) such that the Hamiltonian function

$$H:\mathcal{O}_1\to\mathbb{R},\quad (p,q)\mapsto\int_{\mathbb{R}}\mathrm{d}x\,h(p,q,\partial_x q)\equiv\tfrac12\int_{\mathbb{R}}\mathrm{d}x\,\big\{p^2+(\partial_x q)^2+m^2q^2+2F(q)\big\},$$

is well-defined and C^∞. 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 $\mathsf{C}^\infty(\mathcal{O}_1;\mathbb{R})$, and (ii) integrations by parts involving these functions come vanishing boundary contributions. Then one checks that $(\mathrm{grad}H)(p,q)=\big(p,m^2q+F'(q)-\partial_x^2q\big)$ due to (4.2), and that $X_H(p,q)$ is trivial if and only if $p=0$ and $m^2q+F'(q)-\partial_x^2q=0$. The constraint on q depends on the choice of F. For example, when $F(q)=0,q$ 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 $\mathsf{Crit}(H)=\{(0,0)\}$. The equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\,(p,q)=J(\mathrm{grad}H)(p,q) \tag{4.3}$$

coincides with the usual the wave equation since the combination of $\frac{\mathrm{d}}{\mathrm{d}t}p=\partial_x^2q-m^2q-F'(q)$ and $\frac{\mathrm{d}}{\mathrm{d}t}q=p$ gives

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\,q=\partial_x^2q-m^2q-F'(q).$$

When $m\ne 0$, 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 $C_0\in\mathsf{C}^\infty(\mathcal{O}_1;\mathbb{R})$ given by $C_0(p,q):=\int_{\mathbb{R}}\mathrm{d}x\,p(\partial_x q)$ is a first integral of the motion. Furthermore, the function $\Phi_0\in\mathsf{C}^\infty(\mathcal{O}_1;\mathbb{R})$ given by $\Phi_0(p,q):=\int_{\mathbb{R}}\mathrm{d}x\,\mathrm{id}_{\mathbb{R}}\,h(p,q,\partial_x q)$ has gradient $(\mathrm{grad}\Phi_0)(p,q)=\big(\mathrm{id}_{\mathbb{R}}\,p,\mathrm{id}_{\mathbb{R}}\,m^2q+\mathrm{id}_{\mathbb{R}}\,F'(q)-\partial_x(\mathrm{id}_{\mathbb{R}}\,\partial_x q)\big)$. Therefore,

$$\{\Phi_0,H\}(p,q)=\big\langle(\mathrm{grad}\Phi_0)(p,q),J(\mathrm{grad}H)(p,q)\big\rangle=\int_{\mathbb{R}}\mathrm{d}x\,p\big\{\,\mathrm{id}_{\mathbb{R}}\,\partial_x^2q-\partial_x(\mathrm{id}_{\mathbb{R}}\,\partial_x q)\big\}=-C_0(p,q),$$

and Φ_0 satisfies Assumption 3.2. Here, we clearly have

$$\mathsf{Crit}(H,\Phi_0)=C_0^{-1}(\{0\})=\big\{(p,q)\in\mathcal{O}_1\mid \textstyle\int_{\mathbb{R}}p(\partial_x q)\,\mathrm{d}x=0\big\}\supsetneq\{(0,0)\}=\mathsf{Crit}(H).$$

If we assume further that $F\equiv 0$, then the equation of motion (4.3) is linear. Therefore any pair $(\partial_x^j p,\partial_x^j q)$, $j\geq 1$, with (p,q) a solution of (4.3), also satisfies (4.3). Consequently, if the subsets $\mathcal{O}_j\subset\mathcal{H}^j$ have properties similar to the ones of $\mathcal{O}_1$, then the functions $C_j\in\mathsf{C}^\infty(\mathcal{O}_{j+1};\mathbb{R})$ and $H_j\in\mathsf{C}^\infty(\mathcal{O}_{j+1};\mathbb{R})$ given by $C_j(p,q):=\int_{\mathbb{R}}\mathrm{d}x\,\big(\partial_x^j p\big)\big(\partial_x^{j+1}q\big)$ and $H_j(p,q):=\int_{\mathbb{R}}\mathrm{d}x\,h\big(\partial_x^j p,\partial_x^j q,\partial_x^{j+1}q\big)$ are first integrals of the motion. Accordingly, one deduces that the functions $\Phi_j\in\mathsf{C}^\infty(\mathcal{O}_{j+1};\mathbb{R})$ given by $\Phi_j(p,q):=\int_{\mathbb{R}}\mathrm{d}x\,\mathrm{id}_{\mathbb{R}}\,h\big(\partial_x^j p,\partial_x^j q,\partial_x^{j+1}q\big)$ satisfy $\{\Phi_j,H\}=-C_j$ on $\mathcal{O}_{j+1}$. So, if $F\equiv 0$, there is an infinite family of functions Φ_j satisfying Assumption 3.2, and one has again $\mathsf{Crit}(H,\Phi_j)\supsetneq\mathsf{Crit}(H)$, with $\partial_x^j:\mathsf{Crit}(H,\Phi_j)\to\mathsf{Crit}(H,\Phi_0)$ an isomorphism.

Finally, when $F\equiv 0$ and $m=0$ one can check that the function $\widetilde{\Phi}_0\in\mathsf{C}^\infty(\mathcal{O}_1;\mathbb{R})$ given by $\widetilde{\Phi}_0(p,q):=\int_{\mathbb{R}}\mathrm{d}x\,\mathrm{id}_{\mathbb{R}}\,p(\partial_x q)$ has gradient $\big(\mathrm{grad}\widetilde{\Phi}_0\big)(p,q)=(\mathrm{id}_{\mathbb{R}}\,\partial_x q,-\mathrm{id}_{\mathbb{R}}\,\partial_x p-p)$. Then,

$$\big\{\widetilde{\Phi}_0,H\big\}(p,q)=\int_{\mathbb{R}}\mathrm{d}x\,\big(\,\mathrm{id}_{\mathbb{R}}(\partial_x q)(\partial_x^2 q)-\mathrm{id}_{\mathbb{R}}\,p\,\partial_x p-p^2\big)=-\tfrac{1}{2}\int_{\mathbb{R}}\mathrm{d}x\,\big((\partial_x q)^2+p^2\big)=-H(p,q),$$

where the third equality is obtained using integrations by parts (with vanishing boundary contributions). Thus $\widetilde{\Phi}_0$ satisfies Assumption 3.2. Furthermore, since $\{\widetilde{\Phi}_0,H\}(p,q)=0$ implies $\int_{\mathbb{R}}\mathrm{d}x\,\big\{(\partial_x q)^2+p^2\big\}=0$, one has $\mathsf{Crit}(H,\widetilde{\Phi}_0)=\mathsf{Crit}(H)=\{(0,0)\}$. 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 $\widetilde{\Phi}_j\in\mathsf{C}^\infty(\mathcal{O}_{j+1};\mathbb{R})$ given by $\widetilde{\Phi}_j(p,q):=\int_{\mathbb{R}}\mathrm{d}x\,\mathrm{id}_{\mathbb{R}}\,\big(\partial_x^j p\big)\big(\partial_x^{j+1}q\big)$ satisfy $\{\widetilde{\Phi}_j,H\}=-H_j$ on $\mathcal{O}_{j+1}$. Therefore, one has once again $\mathsf{Crit}(H,\widetilde{\Phi}_j)=\mathsf{Crit}(H)=\{(0,0)\}$ and the $\widetilde{\Phi}_j$'s constitutes a second infinite family of functions satisfying Assumption 3.2.

(B) The nonlinear Schrödinger equation. We refer to [22, 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. I.2] and [33, Sec. 3.2.2-3.2.3]).

The setting is the same as that of the previous example, except that the Hamiltonian function $H\in\mathsf{C}^\infty(\mathcal{O}_1;\mathbb{R})$ is given by

$$H(p,q):=\tfrac{1}{2}\int_{\mathbb{R}}\mathrm{d}x\,\big\{(\partial_x p)^2+(\partial_x q)^2+V\cdot(p^2+q^2)+F(p^2+q^2)\big\},$$

where $V,F\in\mathsf{C}^\infty(\mathbb{R};\mathbb{R})$. Using (4.2), one checks that the gradient of H at $(p,q)\in\mathcal{O}_1$ is

$$(\mathrm{grad}H)(p,q)=\big(-\partial_x^2 p+Vp+pF'(p^2+q^2),-\partial_x^2 q+Vq+qF'(p^2+q^2)\big).$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}u=i\big(-\partial_x^2 u+Vu+uF'(|u|^2)\big),\tag{4.4}$$

with $u:=p+iq$. Without additional assumptions on F or V, it is hardly possible to determine the set $\mathsf{Crit}(H)$ of functions u for which the r.h.s. of (4.4) vanishes. However, it is known that in general $\mathsf{Crit}(H)$ 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 $\mathcal{O}_j\subset\mathcal{H}^j$ be a subset having properties similar to the ones of $\mathcal{O}_1$. Then the functions $H_j\in\mathsf{C}^\infty(\mathcal{O}_j;\mathbb{R})$ and $C_j\in\mathsf{C}^\infty(\mathcal{O}_{j+1};\mathbb{R})$ given by $H_j(p,q):=\frac{1}{2}\int_{\mathbb{R}}\mathrm{d}x\,\big\{(\partial_x^j q)^2+(\partial_x^j p)^2\big\}\equiv\int_{\mathbb{R}}\mathrm{d}x\,h_j(p,q)$ and $C_j(p,q):=\int_{\mathbb{R}}\mathrm{d}x\,\big\{(\partial_x^j q)(\partial_x^{j+1}p)-(\partial_x^{j+1}q)(\partial_x^j p)\big\}\equiv\int_{\mathbb{R}}\mathrm{d}x\,c_j(p,q)$ are first integrals of the motion. Furthermore, the functions $\Phi_j\in\mathsf{C}^\infty(\mathcal{O}_j;\mathbb{R})$ and $\widetilde{\Phi}_j\in\mathsf{C}^\infty(\mathcal{O}_{j+1};\mathbb{R})$ given by $\Phi_j(p,q):=\int_{\mathbb{R}}\mathrm{d}x\,\mathrm{id}_{\mathbb{R}}\,h_j(p,q)$ and $\widetilde{\Phi}_j(p,q):=\int_{\mathbb{R}}\mathrm{d}x\,\mathrm{id}_{\mathbb{R}}\,c_j(p,q)$ satisfy $\{\Phi_j,H\}=$

C_j and $\{\widetilde{\Phi}_j, H\} = 4H_{j+1}$ on $\mathcal{O}_{j+1}$. So, the Φ_j's and the $\widetilde{\Phi}_j$'s constitute two infinite families of functions satisfying Assumption 3.2. Note that the sets $\mathsf{Crit}(H, \Phi_j) = C_j^{-1}(\{0\}) = \big\{(p,q) \in \mathcal{O}_{j+1} \mid \int_{\mathbb{R}} \mathrm{d}x\, (\partial_x^j q)(\partial_x^{j+1} p) = 0\big\}$ (with isomorphisms $\partial_x^j : \mathsf{Crit}(H,\Phi_j) \to \mathsf{Crit}(H,\Phi_0)$) are rather large, whereas $\mathsf{Crit}(H, \widetilde{\Phi}_j) = \mathsf{Crit}(H) = \{(0,0)\}$.

Some of the above functions still work when V and F are not trivial. For instance, the identity $\{\Phi_0, H\} = C_0$ on $\mathcal{O}_1$ remains valid for all V and F. Furthermore, if $V = \mathrm{Const.}$, then $\{C_0, H\} = 0$ on $\mathcal{O}_1$. Consequently, Φ_0 satisfies Assumption 3.2 for all F and for $V = \mathrm{Const.}$, and one has $\mathsf{Crit}(H, \Phi_0) \supsetneq \mathsf{Crit}(H)$. This last example is interesting since it applies to a large class of nonlinear Schrödinger equations.

(C) The Korteweg-de Vries equation. Among many other possible references, we mention [1, Ex. 5.5.7] and [22, Ex. 1.4, p. 3 & 5]. For the global existence of the flow, we refer the reader to [12, Sec. 1] and references therein.

In this example, the scale $\{\mathcal{H}^s\}_{s\geq 0}$ is given by $\mathcal{H}^s := \mathcal{H}^s(\mathbb{R})$ and the sets $\mathcal{O}_j$, $j \in \mathbb{N}$, are appropriate subsets of $\mathcal{H}^j$. The Hamiltonian function $H \in \mathsf{C}^\infty(\mathcal{O}_1; \mathbb{R})$ is given by

$$H(u) := \int_{\mathbb{R}} \mathrm{d}x\, \big(\tfrac{1}{2}(\partial_x u)^2 + u^3\big),$$

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 $\mathsf{Crit}(H)$ are functions u satisfying $-\partial_x^2 u + 3u^2 = 0$; these are Weierstrass $\wp$-functions [21, Sec. 134.F], that is, functions with many singularities and no decay at infinity. Thus, $\mathsf{Crit}(H) = \{0\}$. Furthermore, the equation of motion $\frac{\mathrm{d}}{\mathrm{d}t} u = J(\mathrm{grad} H)(u)$ coincides with the KdV equation $\frac{\mathrm{d}}{\mathrm{d}t} u = \partial_x\big(-\partial_x^2 u + 3u^2\big)$.

There exists an infinite number of first integrals of the motion with polynomial density, that is, of the form $H_j := \int_{\mathbb{R}} \mathrm{d}x\, h_j$, where h_j is a finite polynomial in u and its derivatives (see [27, 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 $\Phi_0 \in \mathsf{C}^\infty(\mathcal{O}_0; \mathbb{R})$ be given by $\Phi_0(u) := \int_{\mathbb{R}} \mathrm{d}x\, \mathrm{id}_{\mathbb{R}}\, u$. Then the gradient of Φ_0 at u is $\mathrm{id}_{\mathbb{R}}$, and $\{\Phi_0, H\} = -3H_2$ on $\mathcal{O}_1$. Since H_2 is a first integral of the motion, this implies that Φ_0 satisfies Assumption 3.2. Furthermore, the fact that $H_2(u) = \|u\|_{\mathsf{L}^2(\mathbb{R})}$ implies that $\mathsf{Crit}(H, \Phi_0) = \{0\} = \mathsf{Crit}(H)$.

Looking for others Φ of the form $\Phi(u) = \int_{\mathbb{R}} \mathrm{d}x\, g(x)\, G(u, \partial_x u, \ldots, \partial_x^k u)$, with G a polynomial and g a C^∞ function, is unnecessay. Indeed, both $\{\Phi, H\}$ and $\Upsilon(t) := \Phi - t\{\Phi, H\}$ are first integrals of the motion with density C^∞ in x and polynomial in u and its derivatives (and t-linear in the case of Υ). Thus, we know from [34, Thm. 1 & Rem. 3] that they are completely characterised, up to the usual equivalence of conservation laws [28, Sec. 4.3]. Therefore, the functions Φ are also completely characterised. Note however, that it is not excluded that functions Φ with an integrand G involving fractional derivatives, an infinite number of derivatives, or of class C^∞ might work. Non-polynomial conserved densities are known to exist in the periodic case (see [27, 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

$$\omega : \mathcal{H} \times \mathcal{H} \to \mathbb{R}, \quad (\psi_1, \psi_2) \mapsto 2\,\mathsf{Im}\langle \psi_1, \psi_2 \rangle.$$

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

$$H : \mathcal{H} \to \mathbb{R}, \quad \psi \mapsto \langle H_{\mathrm{op}} \rangle(\psi) := \langle \psi, H_{\mathrm{op}} \psi \rangle.$$

Then, it is known [26, Cor. 2.5.2] that the vector field and the flow associated to H are $X_H = -iH_{\mathrm{op}}$ and $\varphi_t(\psi) = \mathrm{e}^{-itH_{\mathrm{op}}}\psi$. Therefore, the Poisson bracket of two such Hamiltonian functions H, K satisfies for each $\psi \in \mathcal{H}$

$$\{K, H\}(\psi) = \omega\big(X_K(\psi), X_H(\psi)\big) = -\omega(K_{\mathrm{op}}\psi, H_{\mathrm{op}}\psi) = \big\langle \psi, i[K_{\mathrm{op}}, H_{\mathrm{op}}]\psi \big\rangle.$$

So, in this framework, verifying Assumption 3.2 amounts to finding Hamiltonian functions $H \equiv \langle H_{\mathrm{op}} \rangle$ and $\Phi_j \equiv \langle (\Phi_j)_{\mathrm{op}} \rangle$ satisfying the commutation relation

$$\big[[(\Phi_j)_{\mathrm{op}}, H_{\mathrm{op}}], H_{\mathrm{op}}\big] = 0. \tag{4.5}$$

In concrete examples, the operators H_{op} and $(\Phi_j)_{\mathrm{op}}$ are usually unbounded. Therefore, the preceding calculations can only be justified (using the theory of sesquilinear forms) on subspaces of $\mathcal{H}$ where all the operators are well-defined. We do not present here the whole theory since much of it, examples included, is similar to that of [31]. 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 $UNU^* = N - 1$. Define on $\mathcal{H}$ the bounded selfadjoint operators

$$\Delta := \mathsf{Re}(U) \equiv \tfrac{1}{2}(U + U^*) \qquad \text{and} \qquad S := \mathsf{Im}(U) \equiv \tfrac{1}{2i}(U - U^*).$$

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

$$A_0 := \tfrac{1}{2}(SN + NS), \quad \mathcal{D}(A_0) := \mathcal{D}(N),$$

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

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

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 $\psi \in \mathcal{D}(N)$:

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

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

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

Thus,

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

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

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

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

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

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

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

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References

[1] R. Abraham and J. E. Marsden. *Foundations of mechanics*. Benjamin/Cummings Publishing Co. Inc. Advanced Book Program, Reading, Mass., 1978. Second edition, revised and enlarged, With the assistance of Tudor Raţiu and Richard Cushman.

[2] R. Abraham, J. E. Marsden and T. Raţiu. *Manifolds, tensor analysis, and applications*. Applied Mathematical Sciences, 75. Springer-Verlag, New York, 1988. Second edition.

[3] W. O. Amrein. *Hilbert space methods in quantum mechanics*. Fundamental Sciences. EPFL Press, Lausanne, 2009.

[4] W. O. Amrein, A. Boutet de Monvel, and V. Georgescu. *C_0-groups, commutator methods and spectral theory of N-body Hamiltonians*, volume 135 of *Progress in Math.* Birkhäuser, Basel, 1996.

[5] V. I. Arnold. *Mathematical methods of classical mechanics*, volume 60 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, second edition, 1989. Translated from the Russian by K. Vogtmann and A. Weinstein.

[6] A. Bahri and Y. Y. Li. On a min-max procedure for the existence of a positive solution for certain scalar field equations in $\mathbf{R}^N$. *Rev. Mat. Iberoamericana*, 6(1-2):1–15, 1990.

[7] G. Benettin and A. Giorgilli. On the Hamiltonian interpolation of near-to-the-identity symplectic mappings with application to symplectic integration algorithms. *J. Statist. Phys.*, 74(5-6):1117–1143, 1994.

[8] J. Bourgain. *Global solutions of nonlinear Schrödinger equations*, volume 46 of *American Mathematical Society Colloquium Publications*. American Mathematical Society, Providence, RI, 1999.

[9] A. Boutet de Monvel and V. Georgescu. The method of differential inequalities. In *Recent developments in quantum mechanics (Poiana Braşov, 1989)*, volume 12 of *Math. Phys. Stud.*, pages 279–298. Kluwer Acad. Publ., Dordrecht, 1991.

[10] V. Buslaev and A. Pushnitski. The scattering matrix and associated formulas in Hamiltonian mechanics. *Comm. Math. Phys.*, 293(2):563–588, 2010.

[11] O. Calin and D.-C. Chang. *Geometric mechanics on Riemannian manifolds*. Applied and Numerical Harmonic Analysis. Birkhäuser Boston Inc., Boston, MA, 2005. Applications to partial differential equations.

[12] J. Colliander, M. Keel, G. Staffilani, H. Takaoka and T. Tao Sharp global well-posedness for KdV and modified KdV on $\mathbb{R}$ and $\mathbb{T}$. J. Amer. Math. Soc. 16 (2003), no. 3, 705–749 (electronic).

[13] P. R. Chernoff and J. E. Marsden. *Properties of infinite dimensional Hamiltonian systems*, volume 425 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin-New York, 1974.

[14] C. A. A. de Carvalho and H. M. Nussenzveig. Time delay. *Phys. Rep.*, 364(2):83–174, 2002.

[15] L. Dixon and W. L. Ferrar. On the summation formulae of Voronoï and Poisson. *The Quarterly Journal of Mathematics*, 8(1):66–74, 1937.

[16] G. Georgescu and S. Golénia. Isometries, Fock spaces, and spectral analysis of Schrödinger operators on trees. *J. Funct. Anal.*, 227(2):389–429, 2005.

[17] C. Gérard and R. Tiedra de Aldecoa. Generalized definition of time delay in scattering theory. *J. Math. Phys.*, 48(12):122101, 15, 2007.

[18] À. Haro. The primitive function of an exact symplectomorphism. *Nonlinearity*, 13(5):1483–1500, 2000.

[19] J. Jost. *Riemannian geometry and geometric analysis*. Universitext. Springer-Verlag, Berlin, fourth edition, 2005.

[20] T. Kato. Quasi-linear equations of evolution, with applications to partial differential equations. *Spectral theory and differential equations*, pp. 25–70. Springer-Verlag, Lecture Notes in Mathematics 448, 1975.

[21] Kiyosi Itō, editor. *Encyclopedic dictionary of mathematics. Vol. I–IV*. MIT Press, Cambridge, MA, second edition, 1987. Translated from the Japanese.

[22] S. Kuksin. *Nearly integrable infinite-dimensional Hamiltonian systems.* Springer-Verlag, Lecture notes in mathematics 1556, 1993.

[23] S. Kuksin and J. Pöschel *On the inclusion of analytic symplectic maps in analytic Hamiltonian flows and its applications.* Seminar on Dynamical Systems (St. Petersburg, 1991), 96–116, Progr. Nonlinear Differential Equations Appl., 12, Birkhäuser, Basel, 1994.

[24] N. P. Landsman. *Mathematical topics between classical and quantum mechanics*. Springer Monographs in Mathematics. Springer-Verlag, New York, 1998.

[25] J. M. Lee. *Riemannian manifolds*, volume 176 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, 1997. An introduction to curvature.

[26] J. E. Marsden and T. S. Ratiu. *Introduction to mechanics and symmetry*, volume 17 of *Texts in Applied Mathematics*. Springer-Verlag, New York, second edition, 1999. A basic exposition of classical mechanical systems.

[27] R. M. Miura, C. S. Gardner, and M. D. Kruskal. Korteweg-de Vries equation and generalizations. II. Existence of conservation laws and constants of motion. *J. Mathematical Phys.*, 9:1204–1209, 1968.

[28] P. J. Olver. *Applications of Lie groups to differential equations*, volume 107 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, second edition, 1993.

[29] M. Önder and A. Verçin. Orbits of the n-dimensional Kepler-Coulomb problem and universality of the Kepler laws. *European J. Phys.*, 27(1):49–55, 2006.

[30] M. Reed and B. Simon. *Methods of modern mathematical physics. Volume II. Fourier analysis, self-adjointness.* Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1975.

[31] S. Richard and R. Tiedra de Aldecoa. A new formula relating localisation operators to time operators. preprint on `http://arxiv.org/abs/0908.2826`.

[32] S. Richard and R. Tiedra de Aldecoa. Time delay is a common feature of quantum scattering theory. preprint on `http://arxiv.org/abs/1008.3433`.

[33] C. Sulem and P.-L. Sulem. *The nonlinear Schrödinger equation*, volume 139 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1999. Self-focusing and wave collapse.

[34] J. A. Sanders and J. P. Wang. Classification of conservation laws for KdV-like equations. *Math. Comput. Simulation*, 44(5):471–481, 1997.

[35] W. Thirring. *Classical mathematical physics*. Springer-Verlag, New York, third edition, 1997. Dynamical systems and field theories, Translated from the German by Evans M. Harrell, II.

[36] R. Tiedra de Aldecoa. Time delay and short-range scattering in quantum waveguides. *Ann. Henri Poincaré*, 7(1):105–124, 2006.

[37] R. Tiedra de Aldecoa. Anisotropic Lavine's formula and symmetrised time delay in scattering theory. *Math. Phys. Anal. Geom.*, 11(2):155–173, 2008.

[38] R. Tiedra de Aldecoa. Time delay for dispersive systems in quantum scattering theory. *Rev. Math. Phys.*, 21(5):675–708, 2009.

[39] E. C. Titchmarsh. *Introduction to the theory of Fourier integrals*. Oxford University Press, London, second edition, 1948.

[40] J. Weidmann. *Linear operators in Hilbert spaces*, volume 68 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, 1980. Translated from the German by Joseph Szücs.

[41] W. P. Ziemer, *Weakly differentiable functions. Sobolev spaces and functions of bounded variation*. Graduate Texts in Mathematics, 120. Springer-Verlag, New York, 1989.