A symplectic approach to Schrödinger equations in the infinite-dimensional setting

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Abstract

By using the theory of analytic vectors and manifolds modelled on normed spaces, we provide a rigorous symplectic differential geometric approach to non-autonomous Schrödinger equations on separable (possibly infinite-dimensional) Hilbert spaces determined by unbounded time-dependent self-adjoint Hamiltonians satisfying a technical condition. As an application, the Marsden–Weinstein reduction procedure is employed to map above-mentioned non-autonomous Schrödinger equations onto projective spaces associated with Hilbert spaces.

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Contents

1 Introduction

The study of finite-dimensional symplectic manifolds has proven to be very fruitful in the description of mathematical and physical theories [1, 3, 8, 32]. Among its applications, one finds the analysis of problems appearing in classical and quantum mechanics (see [3, 10, 32] and references therein).

Nowadays, the analysis of symplectic manifolds modelled on (possibly infinite-dimensional) Banach spaces, the hereafter called *Banach symplectic manifolds*, is an interesting topic of research [2, 11, 19, 20, 31, 44, 42, 48, 58]. Banach symplectic manifolds appear in relevant physical topics such as Schrödinger equations [31, 44], non-linear Schrödinger equations [19, 20, 25], and fluid mechanics [44].

The theory of Banach symplectic manifolds emerges as a generalisation of finite-dimensional symplectic geometry obtained by addressing appropriate topological and analytical issues due to the infinite-dimensional nature of general Banach spaces. Banach symplectic manifolds differ significantly from their finite-dimensional counterparts, e.g. there exists no immediate analogue of the Darboux theorem [42]. Relevantly, quantum and classical problems related to infinite-dimensional Banach symplectic manifolds frequently require the study of non-smooth functions [39, 44].

Schrödinger quantum mechanics represents a relevant field of application of symplectic geometry [9, 10, 11, 12, 13, 15]. Despite that, just a bunch of works study rigorously the differential geometric properties of time-dependent Schrödinger equations on infinite-dimensional Hilbert manifolds (see [4, 31, 44] and references therein). Most geometric works in the literature only deal with such Schrödinger equations on finite-dimensional Hilbert spaces [9, 10, 11, 12] or on infinite-dimensional ones provided they are determined by a time-dependent bounded Hamiltonian operator, or other additional simplifications are used [4, 18, 19, 20, 31]. This is, in part, due to the lack of smoothness of the structures used to describe unbounded operators (cf. [44]). Moreover, most works do not provide a detailed explanation of the geometric constructions they use. As far as we know, there is no differential geometric work dealing with unbounded operators as the problems arising are not differentiable.

This work applies infinite-dimensional geometric and functional analysis techniques to the rigorous geometrical study of time-dependent Schrödinger equations determined by (possibly unbounded) self-adjoint Hamiltonian operators on separable Hilbert spaces. Separable Hilbert spaces occur in many physical problems, and separability ensures the existence of a countable set of coordinates [33]. As a new contribution, we have applied the theory of analytic vectors [17, 27, 29, 47] to improve the standard geometric approach given in [44] to deal with unbounded Hamiltonian operators. In particular, we restrict ourselves to time-dependent self-adjoint Hamiltonian operators taking values in a Lie algebra of operators with an appropriate common domain of analytic vectors. In short, although problems we are dealing with are not smooth, we will restrict ourselves to subspaces where problems are smooth enough to apply differential geometry.

Our approach seems to be general enough to provide a rigorous theory while studying interesting physical systems, but it requires using functional analysis techniques [44]. In particular, self-adjoint operators and their mean values are described as objects on manifolds modelled on normed spaces steaming from the manifold structure of Hilbert spaces. Due to the fact that functional analysis is not well-known for most researchers working on differential geometric methods in physics, this work provides a brief introduction to the results on functional analysis and infinite-dimensional manifolds to be used.

As an application of our techniques, the above-mentioned Schrödinger equations are projected onto (possibly infinite-dimensional) projective spaces using a Marsden–Weinstein reduction. Our methods represent an appropriate framework for the generalisation of the standard differential geometric works by G. Marmo and collaborators on quantum mechanics (see e.g. [10, 12, 14, 31]) to the analysis of quantum mechanical problems on infinite-dimensional Hilbert spaces not determined by bounded operators.

Let us detail the contents of this work. Section 2 is devoted to the basic functional analysis techniques and notations to be used hereafter. Differential geometry modelled on normed spaces [23, 28, 44] and Banach spaces [2, 41] are discussed in Section 3. In Section 4, the theory of Banach symplectic manifolds is briefly addressed. After studying weak and strong Banach symplectic manifolds, we survey their related Darboux theorems, the canonical one- and two-forms on cotangent bundles to Banach manifolds, and we finally introduce the Marsden–Weinstein reduction theorem. Section 5 provides a symplectic approach to infinite-dimensional separable Hilbert spaces. Section 6 focuses on vector fields induced by unbounded self-adjoint operators while Section 7 analyses Hamiltonian functions for quantum models. Section 8 studies a class of time-dependent Hamiltonian systems related to the non-autonomous Schrödinger equations appearing in this work. In Section 9, a Marsden–Weinstein reduction procedure is used to project the above-mentioned non-autonomous Schrödinger equations onto an infinite-dimensional projective space. We also consider non-autonomous Schrödinger equations related to unbounded time-dependent Hamiltonian operators as a special type of Hamiltonian systems on Hilbert manifolds.

2 Fundamentals on operators

Let us discuss several basic facts on functional analysis to be applied hereafter, e.g. in the mathematical formulation of Schrödinger quantum mechanics (see [2, 22, 23, 26, 33] for details).

We call *operator* a linear map A defined on a dense subspace $D(A)$ of a Banach space $\mathcal{X}_1$ taking values on a Banach space $\mathcal{X}_2$ of the form $A : D(A) \subset \mathcal{X}_1 \to \mathcal{X}_2$. Operators are sometimes called *unbounded operators* to highlight that they do not need to be continuous. It is worth stressing that defining an operator amounts to giving both its domain and its value on it. If two operators $A_i : D(A_i) \subset \mathcal{X}_1 \to \mathcal{X}_2$, with $i = 1, 2$, satisfy that $D(A_1) \subset D(A_2)$ and A_2 and A_1 take the same values in $D(A_1)$, then we say that A_2 is an *extension of* A_1. Two operators are equal, and we write $A_1 = A_2$, when A_1 and A_2 have the same domain and they take the same values on it.

To define the sum and composition of operators with possibly different domains, we proceed as follows. Let $A_i : D(A_i) \subset \mathcal{X}_1 \to \mathcal{X}_2$, with $i = 1, 2$, be two operators. If $D(A_1) \cap D(A_2)$ is dense in $\mathcal{X}_1$, then $A_1 + A_2$ is an operator on $D(A_1) \cap D(A_2)$ whose value at $\psi \in D(A_1) \cap D(A_2)$ is $A_1\psi + A_2\psi$. Similarly, given an operator $B : D(B) \subset \mathcal{X}_2 \to \mathcal{X}_3$ such that $D = A_1^{-1}(\mathrm{Im}(A_1) \cap D(B))$ is dense in $\mathcal{X}_1$, then we can define the composition $B \circ A_1 : D \subset \mathcal{X}_1 \to \mathcal{X}_3$.

Let $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ be an operator on a Hilbert space $\mathcal{H}$. Consider the associated operator $H_\psi : \phi \in D(H) \subset \mathcal{H} \mapsto \langle \psi | H\phi \rangle \in \mathbb{C}$. Whenever H_ψ is continuous on $D(H)$, the Riesz representation theorem [22] ensures that there exists $\psi_0 \in \mathcal{H}$ such that $H_\psi(\phi) = \langle \psi_0 | \phi \rangle$ for every $\phi \in D(H)$. If H_ψ is continuous for every ψ in a dense subset $D(H^\dagger)$ of $\mathcal{H}$, then one can define the *adjoint* of H, denoted by $H^\dagger$, as the operator $H^\dagger : \psi \in D(H^\dagger) \subset \mathcal{H} \mapsto \psi_0 \in \mathcal{H}$. In other words, $\langle \psi \mid H\phi\rangle = \langle H^\dagger \psi \mid \phi\rangle$ for every $\psi \in D(H^\dagger)$, $\phi \in \mathcal{H}$.

Let us now detail certain relevant types of unbounded operators.

Definition 2.1. An unbounded operator $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ is called:

a) *symmetric*: if $\langle\psi|H\phi\rangle = \langle H\psi|\phi\rangle$ for all $\phi, \psi \in D(H)$,

b) *skew-symmetric*: if $\langle\psi|H\phi\rangle = -\langle H\psi|\phi\rangle$ for all $\phi, \psi \in D(H)$,

c) *self-adjoint*: if $H^\dagger = H$,

d) *skew-self-adjoint*: if $H^\dagger = -H$,

e) *essentially self-adjoint*: if H admits a unique self-adjoint extension.

Let us briefly comment several facts. If H is symmetric, then the equality $\langle\psi|H\phi\rangle = \langle H\psi|\phi\rangle$ for $\psi, \phi \in D(H)$ ensures that H_ψ is continuous for $\psi \in D(H)$ and $D(H^\dagger) \supset D(H)$. Hence, $D(H^\dagger)$ is dense in $\mathcal{H}$ and $H^\dagger$ is a well-defined operator. Moreover, $H^\dagger\big|_{D(H)} = H$, where $H^\dagger\big|_{D(H)}$ is the restriction of $H^\dagger$ to $D(H)$, and $H^\dagger$ is therefore an extension of H. On the other hand, if H is symmetric and $D(H^\dagger) = D(H)$, then $H^\dagger = H$ and vice versa. An analogue discussion can be applied to the case of H being a skew-symmetric operator.

Definition 2.2. Let $A : D(A) \subset \mathcal{X} \to \mathcal{Y}$ be an operator. We say that A is *closed* if its graph is closed in $\mathcal{X} \times \mathcal{Y}$ relative to the product topology.

Theorem 2.3. (Closed graph theorem [33]) *Let $A : \mathcal{X} \to \mathcal{Y}$ be an operator. The operator A is continuous if and only if its graph is closed in $\mathcal{X} \times \mathcal{Y}$.*

If $A : \mathcal{X} \to \mathcal{Y}$ is continuous, then the closed graph theorem yields that A is closed. Nevertheless, an operator defined on a non-closed domain may be non-continuous and closed simultaneously. For instance, the derivative $\partial : \mathscr{C}^1[0,1] \subset \mathscr{C}^0[0,1] \to \mathscr{C}^0[0,1]$, where $\mathscr{C}^1[0,1]$ and $\mathscr{C}^0[0,1]$ stand for the spaces of differentiable with continuous derivative and continuous functions respectively on $[0,1]$, is closed but not continuous (see [60]). More generally, every self-adjoint operator is closed [60]. Then, if H is a symmetric operator such that $D(H) = \mathcal{H}$, then H is bounded.

Theorem 2.4. (Open mapping theorem [26, Theorem 4.10]) *If $A : \mathcal{X} \to \mathcal{Y}$ is a surjective continuous operator, then A is an open map.*

3 Geometry on normed and Banach manifolds

Our geometric study of quantum models will entail the analysis of classes of normed spaces [28, 44]. Since the Banach fixed point theorem does not hold on normed spaces, first-order differential equations in normal form do not need to admit unique integral curves (cf. [34, 38]). There exist no straightforward analogues of the Implicit function and Inverse function theorems neither (see [28, 34] for details). This section recalls the main results on differential calculus on normed spaces to be used hereafter. For details, we refer to [21, 28, 34, 44, 46].

We hereafter assume that every normed vector space E over $\mathbb{K}$ admits an *unconditional Schauder basis*, namely a topological basis $\{e_i\}_{i\in\mathbb{N}}$ so that every $v \in E$ admits a unique decomposition $v = \sum_{i=1}^{\infty} \lambda^i e_i$ for certain unique constants $\{\lambda^i\}_{i\in\mathbb{N}} \subset \mathbb{K}$ such that the sum does not depend on the order of summation of its terms. Hereafter, all basis are considered to be unconditional Schauder bases.

Let E and F be normed spaces and let $B(E, F)$ denote the space of continuous linear maps from E to F. The space $B(E, F)$ admits a topology (for details see [28]). Similarly, $B^r(E, F)$ stands for the space of continuous r-linear maps on E taking values in F.

Partial derivatives on normed vector spaces can be defined using the *Gâteaux differential*. In particular, a function $f : U \subset E \to \mathbb{R}$ on an open U of the normed space E admits a *Gâteaux differential* at $u \in U$ in the direction $v \in E$ if the limit

$$(\mathfrak{D}_v f)(u) := \lim_{t\to 0} \frac{f(u+tv) - f(u)}{t}$$

exists. We call the function $u \mapsto (\mathfrak{D}_v f)(u)$ the *partial derivative* of f in the direction $v \in E$. If $\mathfrak{D}_v f(u)$ exists for every $v \in E$ at $u \in U$, we say that f is *Gâteaux differentiable* at u and we define $(\mathrm{d}f)_u : v \in E \mapsto \mathfrak{D}_v f(u) \in \mathbb{R}$. This function satisfies that $(\mathrm{d}f)_u(\lambda v) = \lambda(\mathrm{d}f)_u(v)$ for every $v \in E$ and $\lambda \in \mathbb{K}$. Despite that, $(\mathrm{d}f)_u$ does not need to be linear and, even if it is linear, it does not need to be continuous. If $(\mathrm{d}f)_u$ is linear and continuous, then we say that f is *Fréchet differentiable* at u. The function $f : U \subset E \to \mathbb{R}$ is said to be of class $\mathscr{C}^r$, for $r \in \bar{\mathbb{N}} := \{0\} \cup \mathbb{N}$, if it has well-defined partial derivatives up to order r and they are all continuous [21]. We say that f is *smooth* or of class $\mathscr{C}^\infty$ if it is of class $\mathscr{C}^r$ for every $r \in \bar{\mathbb{N}}$.

The composite mapping theorem and the Leibniz rule hold on sufficiently differentiable functions on normed spaces [44]. Although there is no *mean value theorem* in normed spaces, if $(\mathrm{d}f)_u = 0$ for every $u \in U$ and U is connected, then f is constant on U (see [44]). This result will be employed for studying the existence of Hamiltonian functions related to self-adjoint operators in quantum mechanics (see Section 6).

Once that a notion of differentiability has been stated on normed vector spaces, the definition of a manifold modelled on a normed vector space is similar to the one on a standard manifold modelled on a finite-dimensional vector space (see [21, 22, 28, 40, 44]).

If not otherwise stated, manifolds are assumed to be smooth and modelled on a separable Banach space $\mathcal{X}$, i.e. the manifold P admits a smooth differentiable structure whose charts take values in $\mathcal{X}$. Exceptions to this general rule appear in our description of quantum mechanical problems related to unbounded operators, which require the use of smooth manifolds modelled on normed spaces.

It can be proved that exists a natural one-to-one correspondence between the space T_uP of *tangent vectors* at $u \in P$, which are understood as equivalence classes of curves $\gamma : t \in \mathbb{R} \mapsto \gamma(t) \in P$ passing through u at $t = 0$ and having the same, well-defined, Gâteaux differential at $t = 0$ in the direction $1 \in \mathbb{R}$ [40], and the space $\mathcal{D}_uP$ of derivations $\mathfrak{D}_u : \mathscr{C}^\infty_u(P) \to \mathbb{R}$, where $\mathscr{C}^\infty_u(P)$ is the space of *germs* at $u \in P$ of functions on P, of the form $\mathfrak{D}_u f = \frac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}(f \circ \gamma)$ for a curve γ with $\gamma(0) = u$. Let us prove the analogue of this result on normed spaces. The case for general manifolds modelled on normed spaces follows then by using local charts and their compatibility relations.

Let $(E, \|\cdot\|)$ be a normed space over the reals. By our general assumption on normed spaces, E admits an unconditional Schauder basis $\{\psi_n\}_{n\in\mathbb{N}}$. We define the dual basis $\{f^n\}_{n\in\mathbb{N}}$ of E^*. Thus, if $\psi \in E$, then there exist unique real numbers c_n, with $n \in \mathbb{N}$, such that

$$\psi = \sum_{n\in\mathbb{N}} c_n\psi_n \quad \Rightarrow \quad f_n(\psi) = c_n\,, \qquad \forall n \in \mathbb{N}\,.$$

Every equivalence class of curves passing through $\psi_0 \in E$ is determined by the Gâteaux differential of the curves at $t = 0$ in the direction $1 \in \mathbb{R}$ and vice versa. Then, there is a one-to-one correspondence between $\mathrm{T}_{\psi_0}E$ and E, we may write $\mathrm{T}_{\psi_0}E \simeq E$.

In turn, $\psi \in E$ determines a derivative

$$\dot\psi_{\psi_0} f = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} [f(\psi_0 + t\psi)]\,, \qquad \forall f \in \mathscr{C}^\infty(E)\,. \tag{1}$$

Obviously $\dot\psi_{\psi_0} \in \mathcal{D}_{\psi_0}E$. The subindex ψ_0 will be omitted if it is clear from context or irrelevant to simplify the notation.

If $\dot\psi_{\psi_0} = \dot\phi_{\psi_0}$, then it follows from (1) that $f^n(\psi) = f^n(\phi)$ for all $n \in \mathbb{N}$ and $\psi = \phi$. Then, every element of $\mathcal{D}_{\psi_0}E$ determines a unique element of E, which defines a unique tangent vector at ψ_0.

Then, we can identify $\mathrm{T}_{\psi_0}E$ and $\mathcal{D}_{\psi_0}E$ and to write $\mathrm{T}_{\psi_0}E := \{\dot{\psi}_{\psi_0} \mid \psi \in E\}$. Moreover, each $\psi \in E$ is associated with a derivation $\dot{\psi} \in \mathrm{T}_{\psi_0}E$ via the isomorphism $\lambda_{\psi_0} : E \to \mathrm{T}_{\psi_0}E;\ \ \psi \mapsto \dot{\psi}_{\psi_0}$.

The previous construction allows for building the tangent and cotangent bundles of a Banach manifold P and other geometric structures, e.g. generalised tangent bundles [41], following the same ideas as in the finite-dimensional case. In particular, a *vector field* is a section of the tangent bundle $\mathrm{T}P$, more precisely, a map $X : P \to \mathrm{T}P$ such that $\tau \circ X = \mathrm{Id}_P$, where $\tau : \mathrm{T}P \to P$ is the projection onto the base space P and Id_P is the identity map on P. [44]. Similarly, a *differential k-form* is a section of the bundle $\bigwedge^k \mathrm{T}^*P \to P$, where $(\bigwedge^k \mathrm{T}^*P)_u$ is the space of continuous $\mathbb{R}$-valued k-linear skew-symmetric mappings on T_uP. We hereafter write $\Omega^k(P)$ for the space of differential k-forms on P and we denote by $\mathscr{C}^\infty(P)$ the space of smooth functions on P. Similarly to the finite-dimensional manifold case, one can define the *exterior derivative* $\mathrm{d} : \Omega^k(P) \to \Omega^{k+1}(P)$ which exists on an appropriate subset of $\Omega^k(P)$.

If P is not modelled on a Banach space, then a vector field on P may not have certain integral curves [38]. Then, additional conditions must be required to ensure their existence. Moreover, our study of quantum mechanical problems will demand the definition of vector fields with a domain.

Definition 3.1. A *vector field on a domain $D \subset P$* is a map $X : D \subset P \to \mathrm{T}P$ such that D is a manifold modelled on a normed space that, as a subset of P, is dense in P, the inclusion $\jmath : D \to P$ is smooth, and $\tau \circ X = \mathrm{Id}_D$. Moreover, X called *smooth* if $X : D \to \mathrm{T}P$ is smooth.

Example 3.2. Let us provide an example of a vector field on a domain that will be generalised and studied in detail in Section 6. Consider the complex Hilbert space $L^2(\mathbb{R})$ of equivalence classes of square integrable complex functions on $\mathbb{R}$ which coincide almost everywhere. This space is naturally a real manifold modelled on a real Hilbert space given by the differential structure induced by the atlas $\jmath : L^2(\mathbb{R}) \to L^2_{\mathbb{R}}(\mathbb{R})$, where $L^2_{\mathbb{R}}(\mathbb{R})$ is $L^2(\mathbb{R})$ considered, in the natural way, as a real Hilbert space. The isomorphisms $\lambda_\psi : L^2(\mathbb{R}) \to \mathrm{T}_\psi L^2(\mathbb{R})$, for every $\psi \in L^2(\mathbb{R})$, allow us to write $\mathrm{T}L^2(\mathbb{R}) \simeq L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$ and to consider every skew-symmetric operator $A : D(A) \subset L^2(\mathbb{R}) \to L^2(\mathbb{R})$, as a map $X_A : \psi \in D(A) \subset L^2(\mathbb{R}) \mapsto (\psi, A\psi) \in \mathrm{T}_\psi L^2(\mathbb{R})$.

In particular, consider $\partial_x : D(\partial_x) \subset L^2(\mathbb{R}) \to L^2(\mathbb{R})$ whose $D(\partial_x)$ is considered to be spanned by the algebraic basis of orthogonal functions $H_n(x)e^{-x^2/2}$, with $n \in \bar{\mathbb{N}} = \mathbb{N} \cup \{0\}$ and $H_n(x)$ being the Hermite polynomial of order n. Then, $D(\partial_x)$ is dense in $L^2(\mathbb{R})$ (cf. [54]). Moreover, $D(\partial_x)$ is a normed vector space relative to the restriction of the topology of $L^2(\mathbb{R})$ to $D(\partial_x)$. The restriction of the global atlas of $L^2(\mathbb{R})$ to $D(\partial_x)$ induces a second one on $D(\partial_x)$ that is modelled only on a normed, not complete, space because $L^2(\mathbb{R}) = \overline{D(\partial_x)} \neq D(\partial_x)$. Hence, X_{∂_x} becomes a vector field on a domain. Since $\partial_x(D(\partial_x)) \subset D(\partial_x)$, we can write that $X_{\partial_x} : D(\partial_x) \to \mathrm{T}D(\partial_x)$. △

Example 3.2 can easily be generalised to vector fields on domains induced by self-adjoint operators, which will be the standard case in our study of quantum mechanics. This case will also turn out to be the general case in the literature [44].

Similarly to vector fields on a domain, one can define differential k-forms on a domain. We write $\Omega^k(D)$ for the space of differential k-forms on a domain D. Moreover, it is straightforward to define time-dependent vector fields on a domain [1].

Definition 3.3. A *(local) flow* for $X : D \subset P \to \mathrm{T}P$ is a map of the form $F : (t, u) \in (-\varepsilon, \varepsilon) \times U \mapsto F_t(u) := F(t, u) \in D$, where U is an open in P containing D and $\varepsilon > 0$, such that

$$X(F_t(u)) = \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=t} F_s(u)\,,$$

for all $u \in D$ and $t \in (-\epsilon, \epsilon)$.

At first glance, it may seem strange that the flow of a time-dependent vector field X on a domain may be defined on an open set U strictly containing D, but this will be useful and natural in this work.

More precisely, skew-self-adjoint operators on a Hilbert space will give rise to vector fields on domains whose flows are defined on the full $\mathbb{R}\times\mathcal{H}$ but they are differentiable only on a subset of it.

Example 3.4. Recall again the vector field X_{∂_x} from Example 3.2. For an element $\psi\in D(\partial_x)$ and since $\partial_x\psi\in D(\partial_x)$, one has that $[\exp(t\partial_x)\psi](y)=\psi(y+t)$ and $\exp(t\partial_x)\psi$ does not need to belong to $D(\partial_x)$ (cf. [33]). Since $\mathrm{i}\partial_x$ admits a self-adjoint extension, the Stone–von Neumann theorem ensures that $\exp(t\partial_x)$ can be defined as a unitary map on $L^2(\mathbb{R})$ and X_{∂_x} admits a flow given by $F:(t;\psi)\in\mathbb{R}\times L^2(\mathbb{R})\mapsto\exp(t\partial_x)\psi\in L^2(\mathbb{R})$. For elements $\psi\in D(\partial_x)$ one observes that $\mathrm{d}/\mathrm{d}tF(t,\psi)=\partial_x\psi$, but F may not be differentiable for $\psi\notin D(\partial_x)$. In Section 6 we will show how $D(\partial_x)$ can be chosen so as to give rise to a flow F of X_{∂_x} on an appropriate domain invariant under the maps F_t for $t\in\mathbb{R}$. $\triangle$

Since the sum and composition of vector fields related to operators with different domains do not need to be defined commonly at a new domain, the Lie bracket of such vector fields may not be defined. In this work, conditions will be given to ensure that the Lie bracket of studied vector fields is defined on a dense subspace of P.

We write $C(D)$ for the space of functions on a subset D of P, where D admits a differential structure modelled on a normed space.

It is interesting to our purposes to consider the case when a subset D of a manifold P modelled on a Banach space is a manifold modelled on a normed space. In this case, the operator exterior differential d can be similarly defined on differential forms on D. Moreover, $\mathrm{T}_pD\subset\mathrm{T}_pP$ and one can consider whether a function $f:D\to\mathbb{R}$ is such that its differential, namely $\mathrm{d}f_u:\mathrm{T}_uD\to\mathbb{R}$, can be extended at points $u\in D$ to elements of $(\mathrm{d}f)_u\in\mathrm{T}^*_pP$. This will be important in our quantum mechanical applications and it becomes the main reason to provide the following definition.

Definition 3.5. Let D be a subset of a manifold P that is, again, a manifold modelled on a normed space. We say that $f:D\to\mathbb{R}$ is *admissible* when $(\mathrm{d}f)_u:\mathrm{T}_uD\to\mathbb{R}$ can be extended continuously to T_uP.

For a vector field X on a domain $D_X\subset P$, which is assumed to be a manifold modelled on a normed space such that $X(D_X)\subset\mathrm{T}D_X$, the *interior product* $\iota_X:\Omega^k(P)\to\Omega^{k-1}(D_X)$ is defined by restricting the contraction with X of differential forms on points of P and its evaluation on vector fields on D_X.

Similarly, the *Lie derivative* $\mathscr{L}_X:\alpha\in\Omega^k(P)\mapsto\mathscr{L}_X\alpha\in\Omega^k(D_X)$ is defined by

$$(\mathscr{L}_X\alpha)(u)=(\iota_X\mathrm{d}\alpha+\mathrm{d}\iota_X\alpha)(u)\,,\qquad\forall u\in D_X\,.$$

Theorem 3.6. *Let X be a vector field on a domain $D_X\subset P$ and let $F:(-\epsilon,\epsilon)\times D_X\to D_X$ be the flow of X. Then*

$$[F_t^*(\mathscr{L}_X\alpha)]_u=\left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=t}(F_s^*\alpha)_u\,,$$

for any $\alpha\in\Omega^k(P)$, values $t,s\in(-\epsilon,\epsilon)$, and arbitrary $u\in D_X$.

For a diffeomorphism $\phi:P_1\to P_2$ and a vector field X on a domain $D_X\subseteq P_1$, the *push-forward* of X by ϕ, if it exists, has a domain $\phi(D_X)\subseteq P_2$ and is defined by $(\phi_*X)_u=\mathrm{T}_u\phi[X_{\phi^{-1}(u)}]$. If the flow of X is given by F_t, then ϕ_*X has the flow $\hat{F}_t:=\phi\circ F_t\circ\phi^{-1}$ for every $t\in(-\epsilon,\epsilon)$. In particular, one has to assume that $\phi(D_X)$ is dense in P_2 for the vector field ϕ_*X to exist.

Definition 3.7. A diffeomorphism $\phi:D\to D$ with a domain $D\subset P$ is said to be *admissible* if and only if for every $u\in D$, the map $\mathrm{T}_u\phi:\mathrm{T}_uD\to\mathrm{T}_{\phi(u)}D$ extends to a continuous linear map from T_uP into $\mathrm{T}_{\phi(u)}P$.

The following results are the generalisation to the infinite-dimensional context of the quotient manifold theorem [2] (see also [6, 7] for details).

Theorem 3.8. *Let $\Phi : G \times P \to P$ be a free and proper action on a Hilbert manifold. Then, P/G is a manifold and $\pi : P \to P/G$ is a submersion.*

Proposition 3.9. *If G is a compact Lie group, then every Lie group action $\Phi : G \times P \to P$ is proper.*

4 Symplectic geometry in the infinite-dimensional context

This section introduces and studies symplectic and related structures on Banach manifolds. As shown next, the fact that a symplectic form is defined on a Banach manifold yields several relevant differences with respect to the case of symplectic forms on finite-dimensional manifolds.

Definition 4.1. A *symplectic form* is a closed differential two-form ω on a manifold P that is *non-degenerate*, i.e. $\omega_u^\flat : v_u \in \mathrm{T}_uP \mapsto \omega_u(v_u, \cdot) \in \mathrm{T}_u^*P$ is injective for every $u \in P$. If $\omega_u^\flat$ is an isomorphism for every $u \in P$, then we call ω a *strong symplectic form*. A *(*resp. *strong) symplectic manifold* is a pair (P, ω), where ω is a (resp. strong) symplectic form on P.

Every strong symplectic form is always a symplectic form, whereas a symplectic form ω on P is strong provided $\omega_u^\flat$ is also surjective for every $u \in P$. The latter can be warranted, for instance, when P is finite-dimensional. If the symplectic form ω of a Banach symplectic manifold (P, ω) is known from context, then one will simply say that P is a Banach symplectic manifold.

The Darboux theorem is a well-known result from standard finite-dimensional symplectic geometry that states that every symplectic manifold admits a local coordinate system in which the associated symplectic form takes a canonical form [1, 41]. This result cannot be extended to symplectic forms on Banach manifolds, as shown by Marsden [44], which in turn leads to different generalisations of the Darboux Theorem for Banach symplectic manifolds [5, 45, 57].

The extension of the standard Darboux theorem to Banach symplectic manifolds is accomplished through *constant differential forms*. Let us describe this notion. Every skew-symmetric continuous bilinear form on a normed space E, let us say $B : E \times E \to \mathbb{R}$, gives rise to a unique differential two-form ω_0 on E by considering the natural isomorphism $\lambda_u : E \simeq \mathrm{T}_uE$ and defining ω_0 to be the only differential form satisfying that $\lambda_u^*(\omega_0)_u = B$ for every $u \in E$. Such a type of differential two-form on a normed space E defined from of a skew-symmetric bilinear form on E is called a *constant* differential two-form.

Theorem 4.2. (The strong Darboux theorem [1]) *If (P, ω) is a strong Banach symplectic manifold, then there exists an open neighbourhood around every $u \in P$ where ω is the pull-back of a constant differential two-form.*

Every cotangent bundle on a finite-dimensional manifold admits a so-called *tautological differential one-form* whose differential gives rise to a strong symplectic form [2]. Similarly, the cotangent bundle of a Banach manifold P is endowed with a canonical differential one-form and a related symplectic form, which is not strong in general [44].

Definition 4.3. Let P be a manifold modelled on a Banach space $\mathcal{X}$ and let $\pi : \mathrm{T}^*P \to P$ be the cotangent bundle projection. The *tautological differential one-form* on T^*P is the differential one-form θ on T^*P of the form

$$\theta_{\alpha_u}(w_{\alpha_u}) := \alpha_u(\mathrm{T}\pi(w_{\alpha_m}))\,, \qquad \forall \alpha_u \in \mathrm{T}_u^*P\,, \quad \forall w_{\alpha_u} \in \mathrm{T}_{\alpha_u}(\mathrm{T}^*P)\,, \quad \forall u \in P\,,$$

and the *canonical two-form* ω on P is defined as $\omega = -\mathrm{d}\theta$.

Let us give a coordinate expression for θ and ω on a separable Banach manifold P modelled on a Banach space $\mathcal{X}$ with an unconditional Schauder basis. It is worth recalling that the separability does not imply the existence of an unconditional Schauder basis (see [24]). On a sufficiently small open set $U \subset P$, one can consider a coordinate system $\{x^j\}_{j\in\mathbb{N}}$. The coordinate system $\{x^j, p_j\}_{j\in\mathbb{N}}$ adapted to T^*P allows us to establish a local diffeomorphism $\mathrm{T}^*U \simeq U \times \mathcal{X}^*$. In turn, the $\{x^j, p_j\}_{j\in\mathbb{N}}$ induce another adapted coordinate system to TT^*U, namely $\{x^j, p_j, \dot{x}^j, \dot{p}_j\}_{j\in\mathbb{N}}$, allowing us to define a diffeomorphism $\mathrm{TT}^*U \simeq (U \times \mathcal{X}^*) \times (\mathcal{X} \times \mathcal{X}^*)$. In these coordinates,

$$\sum_{j\in\mathbb{N}} \theta_{(x,p)}(\dot{x}^j(x,p)\partial_{x^j} + \dot{p}_j(x,p)\partial_{p_j}) = \sum_{j\in\mathbb{N}} p_j \dot{x}^j \quad \Longrightarrow \quad \theta = \sum_{j\in\mathbb{N}} p_j \mathrm{d}x^j .$$

Then, $\omega = -\mathrm{d}\theta = \sum_{j\in\mathbb{N}} \mathrm{d}x_j \wedge \mathrm{d}p^j$.

More generally, one has the following result for Banach spaces (see [44] for details).

Theorem 4.4. *The canonical two-form ω on T^*P is a symplectic form. Additionally, ω is a strong symplectic form if and only if P is modelled on a reflexive Banach space.*

Definition 4.5. Let P be a Banach manifold and let $\{\cdot,\cdot\}$ denote a bilinear operation on $\mathscr{C}^\infty(P)$. If $(\mathscr{C}^\infty(P), \{\cdot,\cdot\})$ is a Lie algebra and $\{\cdot,\cdot\}$ satisfies the *Leibniz rule*, namely $\{fg, h\} = \{f, h\}g + f\{g, h\}$ for all $f, g, h \in \mathscr{C}^\infty(P)$, then $\{\cdot,\cdot\}$ is called a *Poisson bracket* or a *Poisson structure* on P and in this case $(P, \{\cdot,\cdot\})$ is said to be a *Poisson manifold*.

Definition 4.6. Let (P, ω) be a symplectic manifold. A vector field $X : P \to \mathrm{T}P$ is called *Hamiltonian* if there exists a function $h \in \mathscr{C}^\infty(P)$ such that $\iota_X\omega = \mathrm{d}h$. The function h is called a *Hamiltonian function* of X. Whenever $\iota_X\omega$ is closed, and thus locally exact (see [43, 44]), we say that X is a *locally Hamiltonian vector field.*

The set of (locally) Hamiltonian vector fields on (P, ω) will be denoted by (resp. $\mathrm{Ham}_{\mathrm{loc}}(P, \omega)$) $\mathrm{Ham}(P, \omega)$ or (resp. $\mathrm{Ham}_{\mathrm{loc}}(P)$) $\mathrm{Ham}(P)$ when ω is understood from context.

If ω is a strong symplectic form, then every $h \in \mathscr{C}^\infty(P)$ is the Hamiltonian function of a Hamiltonian vector field as in the case of symplectic forms on finite-dimensional manifolds. For general Banach symplectic manifolds, each $\omega_u^\flat$, with $u \in P$, is only in general injective and a certain $h \in \mathscr{C}^\infty(P)$ may not give rise to any Hamiltonian vector field. If it does, the Hamiltonian vector field is unique. This motivates the following definition.

Definition 4.7. Let (P, ω) be a Banach symplectic manifold. An *admissible function* for (P, ω) is a function $h \in \mathscr{C}^\infty(P)$ that is a Hamiltonian function for some Hamiltonian vector field.

We will write X_h for the unique Hamiltonian vector field associated with an admissible function h. The following result is immediate.

Proposition 4.8. *Let (P, ω) be a symplectic manifold. The set $\mathrm{Ham}_{\mathrm{loc}}(P)$ is a Lie algebra, while $\mathrm{Ham}(P)$ is an ideal of $\mathrm{Ham}_{\mathrm{loc}}(P)$ and $[\mathrm{Ham}_{\mathrm{loc}}(P), \mathrm{Ham}_{\mathrm{loc}}(P)] \subset \mathrm{Ham}(P)$. In particular, if $X_1, X_2 \in \mathrm{Ham}_{\mathrm{loc}}(P)$, then $[X_1, X_2] = -X_{\omega(X_1,X_2)}$.*

Every symplectic form on a finite-dimensional manifold gives rise to a Poisson structure. This is no longer true for a general symplectic form, as not every function is associated with a Hamiltonian vector field. A way to ensure this is given by the following proposition.

Proposition 4.9. *A strong symplectic manifold (P, ω) induces a Poisson structure on P given by*

$$\{f, g\}_\omega := \omega(X_f, X_g) , \qquad \forall f, g \in \mathscr{C}^\infty(P) .$$

Definition 4.10. Let (P_1, ω_1) and (P_2, ω_2) be symplectic manifolds. A diffeomorphism $\phi : P_1 \to P_2$ is called a *symplectic map* if $\phi^*\omega_2 = \omega_1$.

We hereafter focus on physical systems determined by the so-called Hamiltonian systems.

Definition 4.11. A *Hamiltonian system* is a triple (P, ω, h), where (P, ω) is a symplectic manifold and h is a time-dependent on P such that $h_t \in \mathscr{C}^\infty(P)$ for every $t \in \mathbb{R}$ is an admissible function for (P, ω), called the *Hamiltonian function* of the system.

Every Hamiltonian system (P, ω, h) gives rise to a unique time-dependent vector field X_t, called the *Hamiltonian vector field*, satisfying that $\iota_{X_t}\omega = \mathrm{d}h_t$, where we recall that h_t is the function $h_t : u \in P \mapsto h_t(u) \in \mathbb{R}$ for every $t \in \mathbb{R}$. The system of differential equations describing the integral curves $c : t \in \mathbb{R} \to c(t) \in P$ of X_t takes the form

$$\frac{\mathrm{d}c(t)}{\mathrm{d}t} = X_t(c(t))\,.$$

This system of differential equations is called the *Hamilton's equations* for (P, ω, h). In order to emphasize the Hamiltonian function h, we will sometimes write $X_h = X_t$. In the Marsden–Weinstein reduction, one is interested in a special family of Hamiltonian systems admitting a particular type of symmetries described next.

Definition 4.12. A *G-invariant Hamiltonian system* relative to the Lie group action $\Phi : G \times P \to P$ is a Hamiltonian system (P, ω, h) satisfying that

$$(\Phi_g^* h_t) = h_t\,, \qquad \Phi_g^*\omega = \omega\,, \qquad \forall g \in G\,, \quad \forall t \in \mathbb{R}\,.$$

If $\Phi : G \times P \to P$ is known from context, then we will simply talk about G-invariant Hamiltonian systems.

Definition 4.13. A Lie group action $\Phi : G \times P \to P$ on a symplectic manifold (P, ω) is called *symplectic* if, for every $g \in G$, the mapping $\Phi_g : P \to P$ is a symplectic map. Meanwhile, Φ is called *Hamiltonian* if the fundamental vector fields of Φ are Hamiltonian relative to ω.

Example 4.14. Let $\mathcal{H}$ be a complex Hilbert space and consider the constant symplectic form ω_B on $\mathcal{H}$ induced by the continuous skew-symmetric bilinear form $B : (\psi_1, \psi_2) \in \mathcal{H} \times \mathcal{H} \mapsto \mathfrak{Im}\langle\psi_1|\psi_2\rangle \in \mathbb{R}$. Given the skew-adjoint operator $\mathrm{iId}_\mathcal{H}$, the Stone–von Neumann Theorem [33, 53] states that each $\exp(it\mathrm{Id}_\mathcal{H})$ is a continuous mapping on $\mathcal{H}$ and, since it is linear, it is also smooth (cf. [46]). Since $t\mathrm{iId}_\mathcal{H}$ is continuous, $\exp(t\mathrm{iId}_\mathcal{H}) = \mathrm{e}^{\mathrm{i}t}\mathrm{Id}_\mathcal{H}$ and the operators $\exp(it\mathrm{Id}_\mathcal{H})$, for $t \in \mathbb{R}$, span a group isomorphic to $U(1)$, namely the unitary group of transformations on a one-dimensional Hilbert space. Define the Lie group action

$$\Phi : (\exp(t\mathrm{iId}_\mathcal{H}), \psi) \in U(1) \times \mathcal{H} \longmapsto \mathrm{e}^{\mathrm{i}t}\psi \in \mathcal{H}\,.$$

Then, $B(\Phi_g\psi_1, \Phi_g\psi_2) = B(\psi_1, \psi_2)$ for every $\psi_1, \psi_2 \in \mathcal{H}$ and $g \in U(1)$. Consequently, $\Phi_g^*\omega_B = \omega_B$ for every $g \in G$ and Φ is a symplectic action. △

Definition 4.15. Let (P, ω) be a symplectic manifold. A *momentum map* for a Lie group action $\Phi : G \times P \to P$ is a mapping $J : P \to \mathfrak{g}^*$ such that

$$(\iota_{\xi_P}\omega)_u = \mathrm{d}\langle J(u), \xi\rangle\,, \qquad \forall \xi \in \mathfrak{g}\,, \quad \forall u \in P\,,$$

where ξ_P is the fundamental vector field of Φ related to $\xi \in \mathfrak{g}$, i.e.

$$\xi_P(u) := \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \Phi(\exp(t\xi), u)\,, \qquad \forall u \in P\,.$$

Thus, $J_\xi : u \in P \mapsto \langle J(u), \xi\rangle \in \mathbb{R}$ is a Hamiltonian function of ξ_P for each $\xi \in \mathfrak{g}$.

Theorem 4.16. (Hamiltonian Noether's theorem [43]) *Consider a Hamiltonian system (P, ω, h). Let $\Phi : G \times P \to P$ be a Lie group action on a symplectic manifold (P, ω) with a momentum map $J : P \to \mathfrak{g}^*$. If the time-dependent function h_t on P is G-invariant, namely $h_t \circ \Phi_g = h_t$ for all $g \in G$ and $t \in \mathbb{R}$, then J is conserved on the trajectories of X_h, that is $J \circ F_t = J$, for all $t \in \mathbb{R}$,where F is the flow of X_h.*

To introduce the Marsden–Weinstein symplectic reduction, one has to consider a quite general property of momentum maps given by the following definition (cf. [1]), which makes use of the adjoint action $\mathrm{Ad} : G \times \mathfrak{g} \to \mathfrak{g}$ on the Lie algebra $\mathfrak{g}$ of G.

$$\begin{tikzcd} P \arrow[r, "J"] \arrow[d, "\Phi_g"'] & \mathfrak{g}^* \arrow[d, "(\mathrm{Ad}^*)_g"] \\ P \arrow[r, "J"'] & \mathfrak{g}^* \end{tikzcd}$$

Definition 4.17. A momentum map $J : P \to \mathfrak{g}^*$ of a Hamiltonian Lie group action $\Phi : G \times P \to P$ is said to be Ad^*-*equivariant* when $J \circ \Phi_g = (\mathrm{Ad}^*)_g \circ J$ for all $g \in G$, where Ad^* is the coadjoint action of G, namely $\mathrm{Ad}^* : (g, \theta) \in G \times \mathfrak{g}^* \mapsto (\mathrm{Ad}^*)_g := \theta \circ \mathrm{Ad}^*_{g^{-1}} \in \mathfrak{g}^*$ and Ad^*_g is the transpose of the morphism $\mathrm{Ad}_g : \mathfrak{g} \to \mathfrak{g}$. In other words, J is *equivariant* if the diagram aside is commutative for every $g \in G$.

When (P, ω, h) is a G-invariant Hamiltonian system, one expects that the G-invariance of the system will allow for the simplification of the system, e.g. giving rise to a new symplectic manifold of a 'smaller' dimension. This is next accomplished through the Marsden–Weinstein theorem allowing us to pass from a symplectic manifold having a Hamiltonian Lie group action of symmetries of h to another 'reduced' symplectic manifold. Then, the initial h will also give rise to a new time-dependent function on the 'reduced' manifold, which finishes the reduction process (see [43] for details). To do so, we first need the give the following definition.

Definition 4.18. Given a map $f : P \to N$ between manifolds, we say that $n \in N$ is a *weakly regular value* of f if $f^{-1}(n)$ is a submanifold of P and $\mathrm{T}_u f^{-1}(n) = \ker \mathrm{T}_u f$ for every $u \in f^{-1}(n)$.

Theorem 4.19. (The Marsden–Weinstein reduction theorem) *Let G be a Lie group acting on P and let $J : P \to \mathfrak{g}^*$ be an associated Ad^*-equivariant momentum map. Let μ be a weakly regular value of J and suppose that G_μ acts freely and properly on the submanifold $J^{-1}(\mu)$. If $\jmath_\mu : J^{-1}(\mu) \hookrightarrow P$ is the natural embedding of $J^{-1}(\mu)$ within P and $\pi_\mu : J^{-1}(\mu) \to P_\mu$ is the canonical projection, then there exists a unique symplectic form ω_μ on $P_\mu := J^{-1}(\mu)/G_\mu$ such that*

$$\pi_\mu^* \omega_\mu = \jmath_\mu^* \omega\,.$$

It is important to point out that Theorem 4.19 does not require the Banach symplectic manifold P to be strongly symplectic [43]. The following theorem uses the Marsden–Weinstein reduction theorem to reduce the dynamics.

Theorem 4.20. *Let the conditions of Theorem 4.19 hold. Let $(P, \omega, h(t))$ be a G-invariant Hamiltonian relative to the Lie group action $\Phi : G \times P \to P$. Then,*

- *The flow, F, of X_h leaves $J^{-1}(\mu)$ invariant,*
- *The diffeomorphisms F_t commute with every Φ_g, for $g \in G_\mu$, giving rise to a flow K on P_μ such that $\pi_\mu \circ F_t = K_t \circ \pi_\mu$,*
- *The flow K corresponds to a vector field with a Hamiltonian function $h_\mu \in \mathscr{C}^\infty(P_\mu)$ determined by $h_\mu \circ \pi_\mu = h \circ \jmath_\mu$.*

It is remarkable that the proper description of the theorem in the infinite-dimensional case requires Theorem 3.8 so as to ensure that $J^{-1}(\mu)/G_\mu$ is a submanifold.

5 Symplectic forms on separable Hilbert spaces

Standard quantum mechanical theories assume Hilbert spaces to be separable, i.e. to admit a countable dense subset of vectors [59]. So we will skip some non-standard approaches [56, 59]. Let us now endow a separable Hilbert space with a strong symplectic form. This will provide a rigorous mathematical extension to the infinite-dimensional setting of the standard approach to finite-dimensional Hilbert spaces [10, 12, 14, 18]. We will indeed provide certain details that are frequently absent in the literature [4].

A complex Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle)$ is separable if and only if it admits a countable orthonormal basis $\{\psi^j\}_{j\in\mathbb{N}}$ (see [49]). This is quite a ubiquitous condition in quantum problems, but it may fail to hold, for instance, in scattering processes [50]. When $\mathcal{H}$ is separable, it admits an orthonormal basis [49] that enables us to endow $\mathcal{H}$ with a real differentiable structure modelled on a Hilbert space.

Choose real-valued coordinates $\{q^j, p_j\}_{j\in\mathbb{N}}$ on $\mathcal{H}$ given by

$$q^j(\psi) := \mathfrak{Re}\langle\psi^j|\psi\rangle, \qquad p_j(\psi) := \mathfrak{Im}\langle\psi^j|\psi\rangle, \qquad \forall j \in \mathbb{N}, \quad \forall \psi \in \mathcal{H}.$$

Let ℓ_2 be the Hilbert space of complex square-summable series considered in the natural way as a real vector space. One can then construct a global chart $\varphi : \psi \in \mathcal{H} \mapsto (q^j, p_j)_{j\in\mathbb{N}} \in \ell_2$. In fact, every $\psi \in \mathcal{H}$ admits a unique family of complex constants $c_j \in \mathbb{C}$ such that $\psi = \sum_{j\in\mathbb{N}} c_j\psi^j$. It is worth recalling that since $\mathcal{H}$ is a Hilbert space $\lim_{j\to\infty}\sum_{j=1}^n c_j\psi^j = \psi$ and this holds independently of the order of the elements of the basis. This is not true for a Schauder basis of a Banach space. Consequently, $\|\psi\|_{\mathcal{H}} := \sqrt{\langle\psi|\psi\rangle} = \sum_{j\in\mathbb{N}} |c_j|^2 < \infty$ and

$$\sum_{j\in\mathbb{N}} |c_j|^2 = \sum_{j\in\mathbb{N}}([\mathfrak{Re}(c_j)]^2 + [\mathfrak{Im}(c_j)]^2) = \sum_{j\in\mathbb{N}}([q^j(\psi)]^2 + [p_j(\psi)]^2) < \infty. \tag{2}$$

Thus, $\varphi(\psi) = (q^j(\psi), p_j(\psi))_{j\in\mathbb{N}} \in \ell_2$. Conversely, every sequence $(x_0^j, p_{0j})_{j\in\mathbb{N}} \in \ell_2$ is the image of a unique element $\sum_{j\in\mathbb{N}}(x_0^j + \mathrm{i}p_{0j})\psi^j \in \mathcal{H}$. In view of (2), one has that $\|\varphi(\psi)\|_{\ell_2} = \|\psi\|_{\mathcal{H}}$ and φ is an isometry. Since φ is an isometry and it has an inverse, its inverse is also an isometry and it is therefore continuous. Consequently, $\mathcal{H}$ and ℓ^2 are homeomorphic. This gives rise to a real differentiable structure on $\mathcal{H}$.

Recall that the tangent space to $\mathcal{H}$ at ψ is the space of equivalence classes of curves $\gamma_\psi : \mathbb{R} \to \mathcal{H}$ such that $\gamma_\psi(0) = \phi$ and $\mathrm{d}\gamma_\psi/\mathrm{d}t(0) = \psi$. Moreover, $\mathrm{T}_\psi\mathcal{H} = \{\dot\phi_\psi : \phi \in \mathcal{H}\}$ and there exists an isomorphism $\lambda_\phi : \psi \in \mathcal{H} \mapsto \dot\psi_\phi \in \mathrm{T}_\phi\mathcal{H}$. Moreover, we represent $\lambda_\phi(\psi^j)$ and $\lambda_\phi(\mathrm{i}\psi^j)$ by $(\partial_{q^j})_\phi$ and $(\partial_{p_j})_\phi$, respectively. Hence, $\{(\partial_{q^j})_\phi, (\partial_{p_j})_\phi\}_{j\in\mathbb{N}}$ becomes a basis of $\mathrm{T}_\phi\mathcal{H}$ and $\lambda_\phi(\psi) = \sum_{j\in\mathbb{N}}[q^j(\psi)(\partial_{q^j})_\phi + p_j(\psi)(\partial_{p_j})_\phi]$.

The cotangent space of $\mathcal{H}$ at ϕ, i.e. $\mathrm{T}^*_\phi\mathcal{H} := (\mathrm{T}_\phi\mathcal{H})^*$, admits a basis $\{(\mathrm{d}q^j)_\phi, (\mathrm{d}p_j)_\phi\}_{j\in\mathbb{N}}$ dual to $\{(\partial_{q^j})_\phi, (\partial_{p_j})_\phi\}_{j\in\mathbb{N}}$. Then,

$$(\mathrm{d}q^j)_\phi(\lambda_\phi(\psi)) = q^j(\psi) = \mathfrak{Re}\langle\psi^j|\psi\rangle\,, \qquad (\mathrm{d}p_j)_\psi(\lambda_\phi(\psi)) = p_j(\psi) = \mathfrak{Im}\langle\psi^j|\psi\rangle\,.$$

Observe that $B : (\phi, \psi) \in \mathcal{H}\times\mathcal{H} \mapsto \mathfrak{Im}\langle\phi|\psi\rangle \in \mathbb{R}$ is a non-degenerate bilinear (over $\mathbb{R}$) form. Since

$$B(\psi_1, \psi_2) = \mathfrak{Im}\langle\psi_1|\psi_2\rangle = \mathfrak{Im}\overline{\langle\psi_2|\psi_1\rangle} = -\mathfrak{Im}\langle\psi_2|\psi_1\rangle = -B(\psi_2, \psi_1)\,, \qquad \forall\psi_1, \psi_2 \in \mathcal{H}\,,$$

we obtain that B is skew-symmetric. Then, B allows us to endow $\mathcal{H}$ with a unique constant differential two-form ω such that $B = \lambda_\phi^*\omega_\phi$ on every $\phi \in \mathcal{H}$. By using the isomorphism λ_ϕ, one has that $\omega_\phi : \mathrm{T}_\phi\mathcal{H}\times\mathrm{T}_\phi\mathcal{H} \to \mathbb{R}$ takes the local form

$$\omega_\phi(\dot\psi_1, \dot\psi_2) := \mathfrak{Im}\langle\psi_1|\psi_2\rangle = \sum_{j\in\mathbb{N}}(q^j(\psi_1)p_j(\psi_2) - q^j(\psi_2)p_j(\psi_1)) = \sum_{j\in\mathbb{N}}\left(\mathrm{d}q^j \wedge \mathrm{d}p_j\right)(\dot\psi_1, \dot\psi_2)\,. \tag{3}$$

Then, $\mathrm{d}\omega = 0$ and ω is a non-degenerate form.

To see that ω is a strong symplectic form, note that $\mathcal{H}$ admits a submanifold $\mathcal{Q}$ given by the zeroes of the functions $\{p^j\}_{j\in\mathbb{N}}$. In fact, the $\{q^j\}_{j\in\mathbb{N}}$ form a coordinate system on $\mathcal{Q}$ taking values in the real vector space of square-summable sequences $(q_j)_{j\in\mathbb{N}}$, making $\mathcal{Q}$ into a manifold modelled on a Hilbert space. Then, the variables $\{q^j, p_j\}_{j\in\mathbb{N}}$ can be understood as the adapted variables to $\mathrm{T}^*\mathcal{Q} = \mathcal{H}$. In view of (3), we get that ω is the canonical two-form of $\mathrm{T}^*\mathcal{Q}$. Since $\mathrm{T}^*\mathcal{Q}$ is modelled on a Hilbert space, which is always reflexive [49], Theorem 4.4 shows that ω is a strong symplectic form.

6 Vector fields related to self-adjoint operators

In geometric finite-dimensional quantum mechanics, operators can easily be described via the so-called *linear vector fields*, which are smooth [12, 44]. Let us extend this idea to bounded, first, and next to general (possibly unbounded) operators on infinite-dimensional Hilbert spaces. This will involve addressing several issues concerning the lack of differentiability of the linear vector fields related to unbounded operators.

We showed in Section 5 that $\mathcal{H}$ is a smooth manifold modelled on a real Hilbert space through a global chart given by the coordinates $\{q^j, p_j\}_{j\in\mathbb{N}}$. This gives rise to a global coordinate system $\{q^j, p_j, \dot{q}^j, \dot{p}_j\}_{j\in\mathbb{N}}$ adapted to $\mathrm{T}\mathcal{H}$. This coordinate system gives rise to a diffeomorphism between $\mathrm{T}\mathcal{H}$ and $\mathcal{H}\oplus\mathcal{H}$. Then, every bounded operator $B:\mathcal{H}\to\mathcal{H}$ gives rise to a vector field

$$X_B:\phi\in\mathcal{H}\mapsto(\phi, B\phi)\in\mathrm{T}_\phi\mathcal{H}\subset\mathrm{T}\mathcal{H}\,.$$

Since B is bounded, it is continuous and $B:\mathcal{H}\to\mathcal{H}$ is also a smooth mapping. It follows immediately that X_B, which amounts to a bounded operator $\mathrm{Id}_{\mathcal{H}}\times B:\phi\in\mathcal{H}\mapsto(\phi,B\phi)\in\mathcal{H}\times\mathcal{H}$, where $\mathcal{H}\times\mathcal{H}$ is endowed with its natural Hilbert structure induced by the one on $\mathcal{H}$, is a smooth vector field.

In infinite-dimensional quantum mechanics, operators are standardly unbounded, they have a domain, and it is non-trivial to provide a process to ensure that they can be described somehow through linear vector fields on a domain that will be smooth enough for their differential geometric treatment. Let us detail this process by means of the theory of analytic vectors (see [27, 33, 47, 51] for details).

Definition 6.1. An *analytic vector* for an operator $B: D(B)\subset\mathcal{H}\to\mathcal{H}$ is an element $\phi\in\mathcal{H}$ such that $\phi\in D^\infty(B):=\bigcap_{n\in\bar{\mathbb{N}}}D(B^n)$ and $\sum_{n\in\bar{\mathbb{N}}}t^n\|B^n\phi\|/n!<+\infty$ for a certain $t>0$. The elements of $\phi\in D^\infty(B)$ are called *smooth* vectors [52].

We hereafter assume B to be skew-self adjoint. We write $D^a(B)$ for the space of analytic vectors of B. The terms (resp. 'analytic') 'smooth' come from the fact that the mapping $\gamma: t\in\mathbb{R}\mapsto\exp(tB)\psi\in\mathcal{H}$ is (resp. analytic) smooth if and only if (resp. $\psi\in D^a(B)$) $\psi\in D^\infty(B)$ (see [51, p. 145]). Obviously, $D^a(B)\subset D^\infty(B)$.

The existence of analytic vectors for operators can be illustrated by the *Nelson's analytic vectors theorem*, which states that a symmetric operator A on a Hilbert space $\mathcal{H}$ is essentially self-adjoint if and only if A admits contains a dense domain $D^a(A)$ of analytic vectors [36]. Analytic vectors allow for many other interesting simplifications in the theory of skew-adjoint operators. They will also allow for the differential geometric study of quantum mechanical problems. Let us consider the following example.

Proposition 6.2. ([51, Theorem 7.8]) *Let A be a skew-self-adjoint operator and consider an element $\psi\in D^a(A)$. Let $C_\psi\in\mathbb{C}$ be such that $\|A^n\psi\|\leq|C_\psi|^n n!$ for every $n\in\mathbb{N}$. If $z\in\mathbb{C}$ and $|z|<C_\psi^{-1}$, then $\psi\in D(e^{zA})$ and $e^{zA}\psi=\lim_{n\to+\infty}\sum_{k=0}^n\frac{z^k}{k!}A^k\psi$.*

Since e^{tA} is a continuous operator defined on $\mathcal{H}$, it stems from the definitions of smooth and analytic vectors for A that $\exp(tA)D^\infty(A)\subset D^\infty(A)$ and $\exp(tA)D^a(A)\subset D^a(A)$ for every $t\in\mathbb{R}$ (cf. [51, p. 149]).

Assume that V is a finite-dimensional Lie algebra of self-adjoint operators on $\mathcal{H}$. One may wonder when the exponential of the elements of V, which are continuous automorphisms on $\mathcal{H}$ by the Stone–von Neumann Theorem [33, 53], can be understood as automorphisms on $\mathcal{H}$ related to a continuous Lie group representation on $\mathcal{H}$. The following definition, based on the one given in [25] establishes the family of Lie algebras V admitting such a property and defines rigorously what we meant.

Definition 6.3. A finite-dimensional Lie algebra V of operators with a common domain $\mathcal{D}$ within a Hilbert space $\mathcal{H}$ is *integrable* if there exists an injective Lie algebra representation $\rho:\mathfrak{g}\to V$ and a continuous Lie group action $\Phi : G \times \mathcal{H} \to \mathcal{H}$ (relative to the natural topologies on $G \times \mathcal{H}$ and $\mathcal{H}$), where G is the connected and simply connected Lie group of $\mathfrak{g}$, such that

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \Phi(\exp(tv), \psi) = \rho(v)\psi, \qquad \forall \psi \in \mathcal{D}, \qquad \forall v \in \mathfrak{g}.$$

We call ρ the *infinitesimal Lie group action* associated with Φ.

Geometrically, the above definition tells us that the fundamental vector fields of the Lie group action G on $\mathcal{D}$ coincide with the restriction of the elements of V in D. Moreover, the fundamental vector fields of this action satisfy that

$$[X_{\rho(v_1)}, X_{\rho(v_2)}]\psi = \frac{1}{2}\frac{\partial^2}{\partial t^2} \exp(-t\rho(v_2)) \exp(-t\rho(v_1)) \exp(t\rho(v_2)) \exp(t\rho(v_1))\psi, \qquad \forall \psi \in \mathcal{D}.$$

In other words, despite the lack of differentiability of the vector fields related to operators, the geometric expression of the Lie derivative of vector fields still holds.

It is a consequence of an argument given by Nelson [47] and Goodman [29] that if a finite-dimensional real Lie algebra of skew-symmetric operators is integrable, then the next criterium holds (cf. [27]).

Theorem 6.4. **(FS^3 criterium [27])** *Every finite-dimensional Lie algebra of skew-symmetric operators on a Hilbert space $\mathcal{H}$ is integrable if it admits a basis with a common dense invariant subspace of analytic vectors.*

There are other criteria of integrability of finite-dimensional Lie algebras of skew-symmetric operators on Hilbert spaces [47, 52], but they are more complicated to use. On the other hand, the FS^3 criterium can be relatively easily proved to hold in many physically relevant problems appearing in physics (cf. [12, 13, 15, 16]).

Assume then that the skew-symmetric operators of the Lie algebra V have a common invariant domain D_V of analytic vectors on $\mathcal{H}$. The related continuous unitary action $\Phi : G \times \mathcal{H} \to \mathcal{H}$ satisfies that $\Phi_\psi : g \in G \mapsto \Phi(g, \psi) \in \mathcal{H}$ is an analytical function on the space of analytic elements D_V. If D_V^∞ is a common invariant domain of smooth vectors for the elements of V, then Φ_ψ is smooth on D_V^∞ (cf. [35])

Let us now prove the following useful result.

Theorem 6.5. *Every skew-adjoint operator B on a Hilbert space $\mathcal{H}$ gives rise to an integrable vector field on a domain $X_B : \psi \in D^\infty(B) \subset \mathcal{H} \mapsto (\psi, B\psi) \in \mathcal{H} \oplus \mathcal{H} \simeq \mathrm{T}\mathcal{H}$ and $X_B(\psi) \in \mathrm{T}_\psi D^\infty(B)$.*

Proof. We know that $\mathrm{T}\mathcal{H}$ is diffeomorphic to $\mathcal{H} \oplus \mathcal{H}$. Hence, B can be associated with the vector field on a domain given by X_B. Moreover, $BD^a(B) \subset D^a(B)$ and the Nelson's analytic vectors theorem shows that $D^a(B)$ is dense in $\mathcal{H}$. The norm of $\mathcal{H}$ can be restricted to $D^\infty(B)$, which becomes a normed space. The maps of the global atlas on $\mathcal{H}$ can be restricted to $D^\infty(B)$, which makes $D^\infty(B)$ into a manifold modelled on a normed space. The inclusion $\jmath : D^\infty(B) \hookrightarrow \mathcal{H}$ is smooth relative to the previous differential structures because every smooth function on $\mathcal{H}$ remains smooth when restricted to $D^\infty(B)$.

To show that X_B is an integrable vector field, we still have to prove that $X_B : D^\infty(B) \to \mathrm{T}\mathcal{H}$ has a flow. The Stone–von Neumann Theorem [33, 53] states that B admits a continuous flow $F : (t, \psi) \in \mathbb{R} \times \mathcal{H} \mapsto \exp(tB)\psi \in \mathcal{H}$. On an element $\psi \in D^\infty(B)$, one has that F_ψ is smooth. In view of this, one can see that X_B is a vector field on the domain $D^\infty(B)$ and $BD^\infty(B) \subset D^\infty(B)$ (see [35] for further details). Hence, X_B is an integrable vector field on the domain $D^\infty(B)$. Since $BD^\infty(B) \subset D^\infty(B)$, one has that X_B can be considered also as a vector field on a domain $D^\infty(B)$ taking values in $\mathrm{T}D^\infty(B)$. $\square$

7 Hamiltonian functions induced by self-adjoint operators

Previous section showed that vector fields generated by skew-adjoint operators may be well-defined on an appropriate domain. We will show that these vector fields can be considered as Hamiltonian vector fields in a domain by using functions on domains. For instance, we will have to deal with functions on Hilbert spaces of the type

$$f_H : \psi \in D(H) \subset \mathcal{H} \mapsto \langle \psi | H\psi \rangle \in \mathbb{R}\,,$$

where H is a skew-symmetric operator. The function f_H is called the *average value* of the operator H [33] and it is only defined on the domain of H, which is dense in $\mathcal{H}$.

In general, the whole symplectic formalism can be modified to deal with quantum mechanical systems by considering that structures are defined on a dense subset of $\mathcal{H}$ having the structure of a normed space and using the fact that the operators of the theory are self- or skew-self-adjoint.

Let us start defining how to write in terms of quantum operators the differentials of the real and imaginary parts of certain average functions. This is done in the following lemma.

Lemma 7.1. *If f_A is the average function of a symmetric operator $A : D(A) \subset \mathcal{H} \to \mathcal{H}$, then*

$$\iota_{\dot\phi}(\mathrm{d}f_A)_\psi = 2\mathfrak{Re}\langle \phi | A\psi \rangle\,, \qquad \forall \dot\phi \in \mathrm{T}_\psi D(A)\,.$$

Therefore, $(\mathrm{d}f_A)_\psi$ can be extended to a unique element of $\mathrm{T}^*_\psi\mathcal{H}$.

Proof. By definition of the contraction of the differential of a function with a vector field

$$(\mathrm{d}f_A)_\psi(\dot\phi) = \lim_{t\to 0} \frac{f_A(\psi + t\phi) - f_A(\psi)}{t} = \langle \psi | A\phi \rangle + \langle \phi | A\psi \rangle = 2\mathfrak{Re}\langle \phi | A\psi \rangle\,,$$

for all $\phi, \psi \in D(A)$. Now, observe that $(\mathrm{d}f_A)_\psi(\dot\phi) = 2\mathfrak{Re}\langle A\psi | \phi \rangle \leq 2\|A\psi\|\|\phi\|$, so that $(\mathrm{d}f_H)_\psi$ is bounded on $D(A)$. Since the topology of $D(A)$ is the restriction of the one in $\mathcal{H}$ to $D(A)$ and in view of the Hahn–Banach Theorem, $(\mathrm{d}f_A)_\psi$ may be continuously extended to a linear continuous form on $\mathrm{T}_\psi\mathcal{H}$. Since $D(A)$ is dense in $\mathcal{H}$, the extension is unique. □

The above lemma shows that f_A is Fréchet differentiable at every point of $D(A)$ and it allows us to introduce the following definition.

Definition 7.2. Let f_H be the average value of a symmetric operator $H : D(H) \subset \mathcal{H} \to \mathcal{H}$. Its *differential* is the mapping $\mathrm{d}f_H : \psi \in D(H) \subset \mathcal{H} \mapsto (\mathrm{d}f_H)_\psi \in \mathrm{T}^*_\psi\mathcal{H} \subset \mathrm{T}^*\mathcal{H}$, where $(\mathrm{d}f_H)_\psi(\dot\phi) = 2\mathfrak{Re}\langle \phi | H\psi \rangle$.

Definitions of symplectic geometry can be adapted to the context of quantum mechanics by assuming that they must be restricted appropriately to domains.

Definition 7.3. We say that a vector field on a domain $X : D(H) \subset \mathcal{H} \to \mathrm{T}\mathcal{H}$ is *Hamiltonian* relative to a symplectic manifold $(\mathcal{H}, \omega)$ if $\iota_X\omega = \mathrm{d}h$, where the right-hand side is understood as the Gâteaux differential of a function $h : D(H) \subset \mathcal{H} \to \mathbb{R}$.

Proposition 7.4. *The vector field with a domain $X_{-\mathrm{i}H}$ on $\mathcal{H}$ induced by a symmetric operator $H : D(H) \subset \mathcal{H} \to \mathcal{H}$, where $D(H)$ is a domain of analytic vectors of H, is Hamiltonian relative to the Hamiltonian function $f_H : \psi \in D(H) \mapsto \frac{1}{2}\langle \psi | H\psi \rangle$.*

Proof. Using the expression for the canonical symplectic form on $\mathcal{H}$, we obtain in view of Lemma 7.1 that

$$(\iota_{X_{-\mathrm{i}H}}\omega)_\psi(\dot\phi) = \mathfrak{Im}\langle -\mathrm{i}H\psi | \phi \rangle = \mathfrak{Re}\langle H\psi | \phi \rangle = \frac{1}{2}\iota_{\dot\phi}\mathrm{d}\langle \psi | H\psi \rangle\,, \qquad \forall \dot\phi \in \mathrm{T}_\psi\mathcal{D}(H)\,, \quad \forall \psi \in \mathcal{H}\,.$$

□

8 On t-dependent Hamiltonian operators

To make a differential geometric approach possible, this section presents the type of non-autonomous Schrödinger equations to be studied. In particular, we are concerned with the ones of the form

$$\frac{\partial\psi}{\partial t} = -\mathrm{i}H(t)\psi\,, \qquad \psi\in\mathcal{H}\,, \tag{4}$$

where the time-dependent $H(t)$ are determined by the following proposition. Let us define precisely the type of operators $H(t)$ that we study.

Definition 8.1. A *time-dependent Hamiltonian operator* is a time-parametrised family of self-adjoint operators $H(t)$ on a Hilbert space $\mathcal{H}$ such that all the $H(t)$ admit a common invariant domain $\mathcal{D}$ of analytic vectors in $\mathcal{H}$.

Note that we do not impose each $H(t)$ to be self-adjoint on $\mathcal{D}$. Since $\mathcal{D}$ will be a subset of the domains $D(H(t))$, with $t\in\mathbb{R}$, where each $H(t)$, for a fixed t, is self-adjoint, the operators $H(t)$ are only symmetric on $\mathcal{D}$. Definition 8.1 is satisfied by relevant physical systems. The following example shows one of them.

Example 8.2. The quantum operators

$$H_1 := \mathrm{i}\hat{p}^2, \qquad H_2 := \mathrm{i}\hat{x}^2, \qquad H_3 := \mathrm{i}(\hat{x}\hat{p}+\hat{p}\hat{x}), \qquad H_4 := \mathrm{i}\hat{p}, \qquad H_5 := \mathrm{i}\hat{x}, \qquad H_6 := \mathrm{i}\mathrm{Id}$$

are self-adjoint operators on $L^2(\mathbb{R})$ with respect to appropriate domains (cf. [30, 33, 51]). The operators $H_1,\ldots,H_6$ span a Lie algebra of skew-symmetric operators on a common domain $\mathcal{D}$ of functions of the form $e^{-x^2/2}P(x)$, where $P(x)$ is any polynomial (cf. [51]). The space $\mathcal{D}$ admits an algebraic basis $e^{-x^2/2}H_n(x)$, where the $H_n(x)$ are the so-called *Hermite polynomials,* which constitute a basis of $L^2(\mathbb{R}^2)$ and, in consequence, $\mathcal{D}$ is dense in $L^2(\mathbb{R}^2)$ (see [54]). The operators $H_1,\ldots,H_6$ are only symmetric on $\mathcal{D}$, which is contained in all their domains as self-adjoint operators. Moreover, $\mathcal{D}$ is also invariant relative to the action of the $H_1,\ldots,H_6$. Hence, every time-dependent Hamiltonian operator on $L^2(\mathbb{R})$ of the form

$$H(t) := \sum_{\alpha=1}^{6} b_\alpha(t)H_\alpha, \tag{5}$$

where the functions $b_\alpha(t)$ are any real time-dependent functions, is a time-dependent Hamiltonian operator with a domain $\mathcal{D}$.

The time-dependent Hamiltonian (5) embraces time-dependent harmonic oscillators and other related systems [12]. Note that $V=\langle H_1,\ldots,H_6\rangle$ is a Lie algebra of symmetric operators on $\mathcal{D}$. Therefore, they can be integrated giving rise to the so-called *metaplectic representation* of the *metaplectic group* (see [30, 55] for details).

Note that $\mathcal{D}$ is not invariant relative to the operators $\exp(-\mathrm{i}H_i)$, with $i=1,\ldots 6$. Nevertheless, the exponentials of the operators of V acting on elements of $\mathcal{D}$ do not change their smooth or analytic character, so one can extend $\mathcal{D}$ to obtain a new domain that will be invariant under the exponentials of the elements of V. △

Non-autonomous Schrödinger equations on $\mathcal{H}$ describe the dynamics of quantum systems and the elements of $\mathcal{H}$ represent its quantum states. Under the conditions given in Definition 8.1 on the associated $H(t)$, we can prove that the non-autonomous Schrödinger equation can be considered as a Hamiltonian system.

Using the diffeomorphism $\mathrm{T}\mathcal{H}=\mathcal{H}\oplus\mathcal{H}$, we can understand the solutions to (4) as curves in $\mathcal{H}$ whose tangent vectors at $\psi(t)$ are given by $X(t,\psi(t))=(\psi(t),-\mathrm{i}H(t)\psi(t))$. This gives rise to a time-dependent vector field with a domain $X:(t,\psi)\in\mathbb{R}\times D\mapsto X(t,\psi)\in\mathrm{T}\mathcal{H}$. It is easy to prove that the time-dependent vector field on a domain, X, is well-defined as it is a linear combination with time-dependent functions of the vector fields related to the skew-symmetric operators related to $-\mathrm{i}H_\alpha$, with $\alpha = 1, \ldots, r$.

Finally, the Proposition 7.4 ensures that the time-dependent vector field X is, for every $t \in \mathbb{R}$, a Hamiltonian vector field with a Hamiltonian function $\langle\psi|H(t)\psi\rangle/2$. In consequence, we obtain the following theorem.

Theorem 8.3. *A non-autonomous Schrödinger equation related to a time-dependent Hamiltonian $H(t)$ is the differential equation for the integral curves of the time-dependent vector field on a domain associated with the time-dependent Hamiltonian system $(\mathcal{H}, \omega, \langle\psi|H(t)\psi\rangle/2)$.*

As considered in Example 8.2, the domain of the Hamiltonian system $(\mathcal{H}, \omega, \langle\psi|H(t)\psi\rangle/2)$ can be considered to be invariant under the exponentials of the elements of $H(t)$.

The previous theorem justifies to provide the following definition.

Definition 8.4. A *quantum time-dependent Hamiltonian system* is a Hamiltonian system of the form $(\mathcal{H}, \omega, \langle\psi|H(t)\psi\rangle/2)$, where $H(t)$ is a time-dependent Hamiltonian operator on $\mathcal{H}$.

Hence, the above states that the non-autonomous Schrödinger equations defined by a time-dependent Hamiltonian are the Hamilton equations of the time-dependent Hamiltonian.

9 Reduction process for non-autonomous Schrödinger equations

This section describes the projection of an autonomous Schrödinger equation determined by a time-dependent Hamiltonian operator onto its projective space via a Marsden–Weinstein reduction.

Recall that the projective space, $\mathcal{PH}$, of a Hilbert space $\mathcal{H}$ is the space of equivalence classes of proportional non-zero elements of $\mathcal{H}$. Every equivalence class in $\mathcal{PH}$ is called a *ray* of $\mathcal{H}/\{0\}$. Physically, the projective space $\mathcal{PH}$ is what is really relevant, as different elements of $\mathcal{H}$ belonging to the same ray have the same physical meaning [50].

Let us apply the Marsden–Weinstein reduction to a non-autonomous Schrödinger equation determined by a time-dependent Hamiltonian $H(t)$ on a Hilbert space $\mathcal{H}$ to describe its projection onto the projective space $P\mathcal{H}$ as a Hamiltonian system relative to a reduced symplectic form.

To accomplish the quantum analogue of the process, we will first define what an invariant function is. As in previous section, one just considers an appropriate restriction of the infinite-dimensional case to an appropriate domain.

Assume that Hamiltonian functions in quantum mechanics are only defined on dense subspaces of Hilbert space. Due to this, it is convenient to recall what it has to be meant the symmetry of the function relative to a group action.

Definition 9.1. Let $\Phi : G \times \mathcal{H} \to \mathcal{H}$ be a Lie group action and let D be a dense complex subspace of $\mathcal{H}$. A time-dependent function $f : (t, \psi) \in \mathbb{R} \times D \mapsto f_t(\psi) := f(t, \psi) \in \mathbb{R}$ is said to be invariant under Φ (or *G-invariant* when G is known from context) if $f_t \circ \Phi_g = f_t$ for all $g \in G$ and every $t \in \mathbb{R}$.

Implicitly, the above implies that $\Phi_g(D) \subset D$. Otherwise $\Phi_g(\psi) \notin D$ for certain $g \in G$ and $\psi \in D$, and the $f(\Phi_g(\psi)) \neq f(\psi)$ since the first would not be defined.

Naturally, one says that a time-independent function $f : D \to \mathbb{R}$ is G-invariant relative to the Lie group action $G \times \mathcal{H} \to \mathcal{H}$ if $\jmath^* f$, where $\jmath : \psi \in D \mapsto (\psi, t) \in \mathbb{R} \times D$, is G-invariant in the sense given in Definition 9.1.

Example 9.2. Consider the multiplicative group $U(1) = \{e^{\mathrm{i}\theta} \,|\, \theta \in [0, 2\pi[\}$ and the Lie group action $\Phi : U(1) \times \mathcal{H} \to \mathcal{H};\ (e^{\mathrm{i}\theta}, \psi) \mapsto e^{\mathrm{i}\theta}\psi$. Let us prove that if H is a symmetric operator with domain

$D(H)$, then the average function f_H is $U(1)$-invariant. In fact, the domain $D(H)$ is a $\mathbb{C}$-linear subspace of $\mathcal{H}$. Moreover,

$$f_H \circ \Phi_g(\psi) = \langle e^{\mathrm{i}\theta}\psi | H e^{\mathrm{i}\theta}\psi\rangle = e^{-\mathrm{i}\theta} e^{\mathrm{i}\theta}\langle\psi|H\psi\rangle = f_H(\psi)\,, \qquad \forall \psi \in D(H)\,.$$

Therefore, f_H is invariant relative to the Φ_g with $g \in U(1)$. Consequently, f_H is a $U(1)$-invariant function. It is worth noting, that if $\psi \in D(H)$, then $e^{\mathrm{i}\theta}\psi \in D(H)$ for every $\theta \in \mathbb{R}$ and $\Phi_g(\psi) \in D(H)$ for every $g = e^{\mathrm{i}\theta} \in U(1)$. Hence, $D(H)$ is invariant under Φ. △

Let us now accomplish the reduction of a non-autonomous Schrödinger equation (4) associated with a time-dependent Hamiltonian operator $H(t)$ on a separable Hilbert space $\mathcal{H}$ onto its projective Hilbert space, $\mathcal{PH}$, via a Marsden–Weinstein symplectic reduction.

Consider global real-valued coordinates $\{q_j, p^j\}_{j\in\mathbb{N}}$ on $\mathcal{H}$ as mentioned in Section 5. The initial data for the reduction is given by

$$\omega := \sum_{j\in\mathbb{N}} \mathrm{d}q^j \wedge \mathrm{d}p_j\,, \qquad H(t) := \sum_{\alpha=1}^{r} b_\alpha(t) H_\alpha\,,$$

where the $b_1(t), \ldots, b_r(t)$ are arbitrary time-dependent real-valued functions and the H_α, with $\alpha \in \overline{1,r}$, are self-adjoint operators such that all elements of $\langle H_1, \ldots H_r\rangle$ share a common domain D of $\mathcal{H}$. We stress that we do not demand $H_1, \ldots, H_r$ to be self-adjoint on D.

The non-autonomous Schrödinger equation (4) induced by $H(t)$ defines a time-dependent Hamiltonian vector field on $\mathcal{H}$ with a domain $D \subset \mathcal{H}$ of the form

$$X(t,\psi) := \sum_{\alpha=1}^{r} b_\alpha(t) X_\alpha(\psi)\,, \qquad \forall \psi \in D\,,$$

such that $X_\alpha(\psi) := -\mathrm{i}H_\alpha\psi$ for all $\alpha \in \overline{1,r}$ and $\psi \in D$. We will hereafter consider the reduction of ω to the projective space, and then the reduction of the Schrödinger equation associated with $H(t)$.

9.1 The Marsden–Weinstein reduction of the symplectic form on $\mathcal{H}$

Consider the Lie group action $\Phi : U(1) \times \mathcal{H} \ni (e^{\theta \mathrm{i}\mathrm{Id}_{\mathcal{H}}}, \psi) \mapsto e^{\mathrm{i}\theta}\psi \in \mathcal{H}$. This Lie group action is symplectic as relative to the symplectic form (3) as proved in Example 4.14.

To obtain the momentum map associated with Φ, we must relate every fundamental vector field of Φ to a Hamiltonian function. The Lie algebra of $U(1)$, say $\mathfrak{u}(1)$, consists of imaginary numbers. Thus, $\mathfrak{u}(1) = \{a\mathrm{i} \mid a \in \mathbb{R}\}$. The fundamental vector field of Φ generated by $\mathrm{i} \in \mathfrak{u}(1)$, takes the form

$$X_{\mathrm{i}}(\psi) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \Phi(e^{\mathrm{i}t}, \psi) = \mathrm{i}\psi\,, \qquad \forall \psi \in \mathcal{H}\,.$$

This is the vector field associated with the skew-self-adjoint operator $A = \mathrm{i}\mathrm{Id}$. In view of these results and Proposition 7.4, an appropriate momentum map J corresponding to the action Φ is given by

$$J : \mathcal{H} \ni \psi \longmapsto -\frac{1}{2}\langle\psi|\psi\rangle \in \mathfrak{u}^*(1) \simeq \mathbb{R}^*\,,$$

so that the values of J at every $\psi \in \mathcal{H}$ are proportional to the square of the norm of ψ. Let us prove that J is smooth. The directional derivative of J along $\dot{\psi}$ at ψ_0, i.e. $\dot{\psi}_{\psi_0} J$, becomes

$$\dot{\psi}_{\psi_0} J = \lim_{t\to 0} \frac{J(\psi_0 + t\psi) - J(\psi_0)}{t} = -\mathfrak{Re}\langle\psi_0|\psi\rangle\,, \qquad \forall \psi_0 \in \mathcal{H}\,, \quad \forall \dot{\psi} \in \mathrm{T}_{\psi_0}\mathcal{H}\,.$$

This gives rise to a linear and bounded function on $\mathcal{H}$ for each $\psi \in \mathcal{H}$. Hence, they are continuous and J is $\mathscr{C}^1$. Let us write $\nabla_{\dot\psi} J$ for the partial derivative function of J in the direction $\dot\psi$. The directional derivative of the second order of J along ϕ and ψ is constant.

$$
\begin{aligned}
[\nabla_{\dot\phi}\nabla_{\dot\psi} J]_{\psi_0} &= \lim_{t\to 0}\frac{1}{t}((\nabla_{\dot\psi}J)(\psi_0+t\phi)-(\nabla_{\dot\psi}J)(\psi_0))\\
&= -\lim_{t\to 0}\frac{1}{t}(\mathfrak{Re}\langle\psi_0+t\phi|\psi\rangle-\mathfrak{Re}\langle\psi_0|\psi\rangle) = -\mathfrak{Re}\langle\phi|\psi\rangle\,,\qquad \forall\psi_0\in\mathcal{H}\,,\quad \forall\psi,\phi\in \mathrm{T}_{\psi_0}\mathcal{H}\,.
\end{aligned}
$$

Hence, all derivatives of second-order are constant and therefore continuous. Derivatives of higher-order are zero. Hence, J is smooth.

Let us show that Φ is Ad^*-adjoint. Since $U(1)$ is an Abelian Lie group, its adjoint action Ad is trivial, i.e. $\mathrm{Ad}_g = \mathrm{Id}_{\mathfrak{u}(1)}$ for every $g\in U(1)$, and the coadjoint action is also trivial. Moreover, J is invariant with respect to the action of $U(1)$ on $\mathcal{H}$, since unitary transformations do not change the norm of elements of the Hilbert space $\mathcal{H}$. Therefore,

$$
J(\psi) = J\circ\Phi_g(\psi) = \mathrm{Id}_{\mathfrak{u}^*(1)}\circ J(\psi) = (\mathrm{Ad}^*)_g\circ J(\psi)\,,\quad \forall\psi\in\mathcal{H}\,,\quad \forall g\in U(1)\,.
$$

Thus, J is an Ad^*-equivariant momentum map.

Let us prove that all $\mu\in\mathbb{R}_- := \{\lambda\in\mathbb{R}\mid \lambda<0\}$ are regular values of J. Since J is smooth, it is enough to prove that $\mathrm{T}_\psi J:\mathrm{T}_\psi\mathcal{H}\to\mathbb{R}^*$ is a surjection with a split kernel for all non-zero elements $\psi\in\mathcal{H}$ [2]. The tangent map is of the form $\mathrm{T}_\psi J(\dot\phi) = \dot\phi_\psi J = -\mathfrak{Re}\langle\psi|\phi\rangle$. Note that $\mathrm{T}_\psi J\neq 0$ if and only if $\psi\neq 0$. Therefore, $\dim(\mathrm{Im}\,\mathrm{T}_\psi J)=1$ and $\mathrm{T}_\psi J$ is therefore surjective if and only if $\psi\in\mathcal{H}\backslash\{0\}$. Since J is smooth, $\mathrm{T}_\psi J$ is a continuous map, $\ker(\mathrm{T}_\psi J)$ is a closed subspace of $\mathrm{T}_\psi\mathcal{H}$, which becomes a Hilbert space relative to $\mathfrak{Re}\langle\cdot|\cdot\rangle$. Hence, $\mathrm{T}_\psi J$ has a split kernel, as $\ker(\mathrm{T}_\psi J)\oplus\ker(\mathrm{T}_\psi J)^\perp = \mathrm{T}_\psi\mathcal{H}$, where $\ker(\mathrm{T}_\psi J)^\perp$ is a closed subspace. Hence, all $\mu\in\mathbb{R}_-$ are regular values of J, and, for these values, we obtain the submanifolds

$$
J^{-1}(\mu) = \left\{\psi\in\mathcal{H}\ \Big|\ -\frac{1}{2}\langle\psi|\psi\rangle = -\frac{1}{2}\sum_{j\in\mathbb{N}}\left[q_j(\psi)^2+p^j(\psi)^2\right]=\mu\right\},\qquad \forall\mu<0\,.
$$

As mentioned before, $(\mathrm{Ad}^*)_g = \mathrm{Id}_{\mathfrak{u}^*(1)}$ for every $g\in U(1)$. Therefore, the isotropy group at μ takes the form $U(1)_\mu := \{g\in U(1)\mid (\mathrm{Ad}^*)_g(\mu)=\mu\} = U(1)$. Now we will prove that $U(1)$ acts freely and properly on $J^{-1}(\mu)$. The condition $\Phi_{e^{i\theta}}(\psi)=\psi$, where $\theta\in[0,2\pi[$ implies that $\theta=0$, so that $e^{\mathrm{i}\theta}=1$ is the identity element of $U(1)$ and, as a result, Φ is a free action. Moreover, $U(1)$ is homeomorphic to the group $S^1=\{z\in\mathbb{C}\mid |z|=1\}\subset\mathbb{C}\simeq\mathbb{R}^2$. Therefore, $U(1)$ is a compact Lie group. In view of the Proposition 3.9, the Lie group action Φ is also proper. Consequently, Theorem 3.8 ensures that

$$
P_\mu := J^{-1}(\mu)/U(1)
$$

is a smooth manifold for all $\mu<0$. Note that if $\pi_\mu : J^{-1}(\mu)\to P_\mu$ is such that the images of two elements of $J^{-1}(\mu)$ are the same, then both elements are the same up to a proportional complex constant with module one. This amounts to saying that the images of two elements of $J^{-1}(\mu)$ are the same if the images under $\pi:\mathcal{H}_0=\mathcal{H}\setminus\{0\}\to\mathcal{PH}$ are the same. Consequently, $\pi_\mu = \pi|_{J^{-1}(\mu)}$. Since the differentiable structure on P_μ is the only one making $\pi_\mu : J^{-1}(\mu)\to P_\mu$ into a differentiable submersion and $\pi_\mu=\pi|_{J^{-1}(\mu)}$, then the differentiable structure on P_μ is the one of $\pi(J^{-1}(\mu))=\mathcal{PH}$. Hence $P_\mu=\mathcal{PH}$.

We see that all assumptions of the Marsden–Weinstein theorem are satisfied for $\mu<0$. We may now proceed to the reduction process for the symplectic form. Let us rewrite π_μ as $\pi_\mu : J^{-1}(\mu)\to P\mathcal{H};\psi\mapsto[\psi]$, and consider the natural embedding $\jmath_\mu : J^{-1}(\mu)\hookrightarrow\mathcal{H}$.

The symplectic form on the projective space $P\mathcal{H}$ is the only symplectic form on this latter manifold such that $\pi_\mu^*\omega_\mu = \jmath_\mu^*\omega$. In other words,

$$
\omega_{\mu_{[\psi_0]}}([\dot\psi],[\dot\phi]) = \mathfrak{Im}\langle\psi|\phi\rangle\,,\qquad \forall\psi_0\in J^{-1}(\mu)\,,\quad \forall\dot\psi,\dot\phi\in\mathrm{T}_{\psi_0}J^{-1}(\mu)\,.
$$

9.2 Marsden–Weinstein reduction of Schrödinger equations

Observe that the vector fields $X_\alpha = X_{-\mathrm{i}H_\alpha}$, with $\alpha = 1, \ldots, r$, are tangent to $J^{-1}(\mu)$ on those points in which they are defined. In fact, the self-adjointness of H_α implies that, on points of D, we have

$$X_\alpha J(\psi) = \frac{1}{2} X_\alpha \langle\psi|\psi\rangle = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \langle \exp\left(-t\mathrm{i}H_\alpha\right)\psi|\exp\left(-t\mathrm{i}H_\alpha\right)\psi\rangle = 0\,.$$

Then, the restriction of X_α to $J^{-1}(\mu)$ is a well-defined vector field: it is not only tangent where defined, but it is defined on a subset dense in $J^{-1}(\mu)$. Let us prove this.

Since D is dense in $\mathcal{H}$, for every $\psi \in J^{-1}(\mu)$ with $\mu \neq 0$, there exists a sequence $(\psi_n^D)_{n\in\mathbb{N}}$ of non-zero elements of $\mathcal{H}\backslash\{0\}$ that belong to D, such that $\psi_n^D \to \psi$. Now, take some element $\psi \in J^{-1}(\mu) \subset \mathcal{H}\backslash\{0\}$, that is, $\langle\psi|\psi\rangle = -2\mu =: k$. If $\psi_n^D \to \psi$, then $(\sqrt{k}\psi_n^D/\|\psi_n^D\|)_{n\in\mathbb{N}}$ is a sequence in $J^{-1}(\mu)\cap D$, such that $\sqrt{k}\psi_n^D/\|\psi_n^D\| \to \sqrt{k}\psi/\|\psi\|$. Consequently, $D_\mu := J^{-1}(\mu)\cap D$ is dense in $J^{-1}(\mu)$ and $\overline{D_\mu} = J^{-1}(\mu)$.

The flow of X_α, namely $F : (t,\psi) \in \mathbb{R}\times\mathcal{H} \mapsto \exp(-\mathrm{i}H_\alpha)\psi \in \mathcal{H}$, leaves invariant $J^{-1}(\mu)$. Additionally, it commutes with all the Φ_g, since each Φ_g is a multiplication by a phase and the $\exp(-t\mathrm{i}H_\alpha)$ are linear mappings. Therefore, this gives rise to an induced flow on P_μ of the form $K : (t,[\psi]) \in \mathbb{R}\times P_\mu \mapsto [F_t\psi] \in P_\mu$. Then, this flow is related to the projection of X_α^μ to P_μ. Since the projection π_μ amounts to the restriction of π to $J^{-1}(\mu)$ and X_α^μ is the restriction of X_α to $J^{-1}(\mu)$, one obtains that the projection of X_α^μ onto $J^{-1}(\mu)/U(1)_\mu$ is the projection onto $\mathcal{PH}$ of X_α.

To prove that the projection of X_α^μ to P_μ is a vector field K_α^μ, one has to prove that such a projection is well defined on a dense subset of P_μ. In fact, theorem 3.8 shows that $\pi_\mu : J^{-1}(\mu) \to J^{-1}(\mu)/U(1)_\mu \simeq P\mathcal{H}$ is a surjective submersion. Therefore,

$$\overline{\pi_\mu(D_\mu)} = \pi_\mu(\overline{D_\mu}) = \pi_\mu(J^{-1}(\mu)) = J^{-1}(\mu)/U(1) \simeq P\mathcal{H}\,,$$

and $\pi_\mu(D_\mu)$ is dense in $P\mathcal{H}$. We conclude that K_α^μ is well-defined with a domain being a dense subset of $P\mathcal{H}$.

Let us prove that K_α^μ is a Hamiltonian vector field on P_μ with a Hamiltonian function given by

$$f_\alpha^\mu([\psi]) = \frac{1}{2}\langle\psi|H_\alpha\psi\rangle\,, \qquad \forall\alpha\in\overline{1,r}\,, \quad \forall\psi\in D(H_\alpha)\backslash\{0\}\,.$$

In fact,

$$\begin{aligned}\omega_\mu(K_\alpha^\mu, K_\beta^\mu)([\psi]) &= (\omega_\mu)(\pi_{\mu*}X_\alpha^\mu, \pi_{\mu*}X_\beta^\mu)([\psi]) = \pi_\mu^*\omega_\mu(X_\alpha^\mu, X_\beta^\mu)(\psi)\\ &= \jmath_\mu^*\omega(X_\alpha^\mu, X_\beta^\mu)(\psi) = (\mathrm{d}\jmath_\mu^* f_\alpha)(X_\beta^\mu)(\psi) = (\mathrm{d}f_\alpha^\mu)(K_\beta^\mu)([\psi])\,.\end{aligned}$$

Then, f_α^μ is the Hamiltonian function of K_α^μ.

Easily, the above shows how the time-dependent vector field X on the domain D gives rise to the time-dependent vector field $X^\mu = \sum_{\alpha=1}^r b_\alpha(t)X_\alpha^\mu$ on $J^{-1}(\mu)\cup D$ projecting onto a time-dependent vector field $K^\mu = \sum_{\alpha=1}^r b_\alpha(t)K_\alpha^\mu$ on $\pi_\mu(D\cap J^{-1}(\mu)) \subset P^\mu$, whose integral curves are determined by the non-autonomous projective Schrödinger equation.

Since K^μ is defined on a manifold D_μ modelled on a normed space, we cannot ensure straightforwardly the existence of its integral curves. Nevertheless, their existence is easily inferred from the existence of the integral curves of the time-dependent vector field X.

10 Conclusions and Outlook

This paper has presented a careful symplectic geometric approach to the Schrödinger equations on separable Hilbert spaces determined through time-dependent unbounded self-adjoint Hamiltonian operators satisfying a quite general condition. Then, the projection of such equations onto the projective space has been described as a Marsden–Weinstein reduction. The paper has described carefully the necessary technical geometric and functional analysis details to accomplish the description of above describe results.

There is much room for additional developments. In the future, we aim to study how to extend to the infinite-dimensional context several geometric techniques to deal with Schrödinger equations (see [10, 37]). Moreover, other types of Marsden–Weinstein reductions will be contemplated.

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