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The Geometrical Formulation of Quantum Mechanics

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Abstract

The approaches to Classical and Quantum Mechanics are quite different in many aspects, the most striking one being the linear structure which is present in the Hilbert space $\mathcal{H}$ and which is considered usually as one of the most relevant aspects of the formalism. There are also suggestive similarities, as has been noted often (see [31, 32, 41, 49]) but they have been approached mainly from the algebraic point of view. Our goal in this paper is to describe an alternative description of Quantum Mechanics which is formally analogue to the description of nonrelativistic Classical Mechanics from a geometrical perspective. We will also discuss the main advantages of this new approach, and the most significative differences. We also present two applications to physically relevant examples: the ability to discuss independence of quantum observables (in the context of entanglement witnesses) and a Hamiltonian description of Ehrenfest equations for molecular systems.

1 Introduction

The aim of this paper is to summarize the most relevant aspects of a geometrical formulation of Quantum Mechanics, which is being developed since the last seventies and has been the main line of research of the author in the last five years. For the sake of simplicity, we will consider only the case of finite dimensional systems, although from a formal point of view, most of the results presented here can be extended to the infinite dimensional case. The original references to the results presented in this work can be found in [2, 3, 4, 7, 8, 24, 28, 29, 30] and are due to several people, who were kind enough

to share part of their knowledge and time with the author along these years. He would like that this work serve also as a small tribute for all of them.

The origins of the construction, though, go back to the end of the seventies, and has been developed by many different researchers. Just to mention the most relevant references ordered chronologically, let us refer to former interesting approaches as [48], the seminal work by Kibble [39], the works by Cantoni ([19, 20, 21, 22, 23]), by Cirelly and co-workers ([25, 26, 27]), the more physically oriented approach by Heslot [37], Bloch's paper ([11]), the work by Anandan[5, 6], and then Ashtekar and Schilling [9]. There are several interesting works by Brody and coworkers ([14] is the one closer to the work presented here, although other results, more oriented to Statistical Mechanics such as [13, 15, 16, 17, 18] are also relevant) and also from Spera and coworkers ([10, 47]) .

Abstracting from all these works, let us begin our study in a very general framework. If we want to describe a physical system, what would the minimal mathematical apparatus we need? From a fairly general point of view, the minimal mathematical structure we can think of contains:

- a space of states, which we denote as $\mathcal{S}$ and which encodes the information that we consider relevant to describe the physical system in an unambiguous way,
- a space of observables, that we denote as $\mathcal{O}$, and which encodes the set of possible representations of physical magnitudes,
- and finally, a way of representing the measurement process, i.e., a pairing $\mathcal{O}\times\mathcal{S} \to \mathbb{R}$ which assigns a real number to any magnitude and a given state.
- If we want to describe some sort of evolution, we must define also a differential (or difference, if the system is discrete) equation whose solutions define the trajectories of the physical system.

For instance, in the case of the the Hamiltonian (or Lagrangian) nonrelativistic Classical Mechanics, the situation is very well known:

- The states of the physical system are described by a phase space which contains the set of positions and momenta of the system (or the set of positions and the set of velocities if we are considering a Lagrangian description). Depending on the situation, $\mathcal{S}$ takes some extra structure, which is used to provide a tensorial description of the dynamics and the rest of the tools we use. Thus, we can find the form of a vector space, a cotangent bundle, a symplectic, a Poisson (or even, in a more general framework, a Dirac) manifold. Also, Riemannian metrics may be introduced in order to describe special systems.

- The set of observables corresponds to the set of functions defined on the phase space, the corresponding pairing being the evaluation of the functions on the corresponding point.

- The dynamics can be introduced in several equivalent ways, which encode within the different structures introduced, the content of Newton equations. In the case of Hamiltonian Mechanics, dynamics arises as the integral curves of the Hamiltonian vector field associated to a special function, called the Hamiltonian and denoted as h, which represents the energy of the system. If we denote as $\{\cdot,\cdot\}$ the Poisson bracket defined on the set of functions of $\mathcal{S}$ and associated to the tensor chosen we can write the vector field representing the dynamics in an intrinsic way as

$$X_h = \{h, \cdot\} \tag{1}$$

That is a brief summary of the mathematical description of a classical system. What about a quantum one? The usual approaches to Quantum Mechanics present a situation quite different to the above. The standard presentations, split the description in two "pictures", one where the primary object are the physical states (the Schrödinger picture) and one where the main objects are the physical observables (the Heisenberg picture). Let us review very quickly both of them from the perspective above:

- In the Schrödinger picture of Quantum Mechanics,

  - the states of the physical system are considered to belong to a Hilbert space $\mathcal{H}$, or rather, to the corresponding projective space, i.e. the space of complex rays in $\mathcal{H}$, since all the points differing by a phase are considered physically equivalent, and the norm of the states must be equal to one, since it is probabilistic in nature.

  - On the other hand, the physical magnitudes are modelled as self-adjoint operators defined on $\mathcal{H}$, i.e., modulo the complex unit, the set of observables is identified with the Lie algebra $\mathfrak{u}(\mathcal{H})$ of the unitary group $U(\mathcal{H})$ associated to the Hilbert space $\mathcal{H}$.

  - The pairing is defined as the quadratic function

$$\mathcal{O} \times \mathcal{S} \to \mathbb{R}; \qquad (A, |\psi\rangle) \mapsto \frac{\langle\psi|A\psi\rangle}{\langle\psi|\psi\rangle},$$

    even if the measure process is still a challenging problem (see [50, 51] and references therein).

– Dynamics is introduced on $\mathcal{H}$ via the Schrödinger equation, defining the evolution as the solutions of the differential equation:

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle, \tag{2}$$

where H is the Hermitian operator which represents the energy of the system.

- In the Heisenberg picture of Quantum Mechanics, that we can present following the algebraic approach by Segal [46] or Haag and Kastler [36], we find that:
  - The physical magnitudes are the primary object and are supposed to define the real part of a $\mathbb{C}^*$–algebra $\mathcal{A}$ (see [33] for a classical presentation of the concept),
  - the states of the physical system are defined as positive linear functionals ρ on $\mathcal{A}$, normalized by the condition

$$\mathrm{Tr}\rho = 1$$

  - The pairing is defined via the trace operation (see [34] for the theorem proving the result in general)

$$\mathcal{O}\times\mathcal{S}\to\mathbb{R}; \qquad (A,\rho)\mapsto \mathrm{Tr}(\rho A)$$

  - Dynamics is introduced on $\mathcal{A}$ via the Heisenberg equation, defining the evolution as the solutions of the differential equation:

$$i\hbar\frac{\partial A(t)}{\partial t} = (A(t)H - HA(t)), \tag{3}$$

where again H denotes the Hamiltonian operator.

We can notice then that the approaches to Classical and Quantum Mechanics are quite different in many aspects, the most striking one being the linear structure which is present in the Hilbert space $\mathcal{H}$ and which is considered usually as one of the most relevant aspects of the formalism. There are also suggestive similarities, as has been noted often (see [31, 32, 41, 49]) but they have been approached mainly from the algebraic point of view. Our goal in this paper is to describe an alternative description of Quantum Mechanics which is formally analogue to the description of nonrelativistic Classical Mechanics from a geometrical perspective. We will also discuss the main advantages of this new approach, and the most significative differences. We also present two applications to physically relevant examples: the ability to discuss independence of quantum observables (we will use the concept in the context of entanglement witnesses) and a Hamiltonian description of Ehrenfest equations for molecular systems, which allows, for instance, to define a simple

measure, which is preserved by the dynamics, and which allows us to formulate a rigorous extension to Statistical Mechanics (see [2, 4]).

The structure of the paper is as follows. In Section 2 we introduce the geometrical construction for a quantum mechanical system on a pure state for both the Schrödinger and the Heisenberg pictures, and prove that they are actually related by the momentum mapping of the action of the unitary group on the Hilbert space. Both approaches are then equivalent and we are able to define the equivalence explicitly. Section 3 is devoted to the analysis of the mixed states: we will see how we can use the geometrical structures of the dual of the Lie algebra of the unitary group of the Hilbert space, to endow the set with tensorial objects which are analogue to the ones introduced in the case of pure states. Finally, the last two sections present two simple applications where the geometrical formalism introduced provide us with tools which have no analogue in the usual description of Quantum Mechanics. In particular, in Section 4 we introduce a notion of independence of operators which is not available in the usual framework because of the lack of a consistent non-commutative calculus. We exemplify it by proving the independence of two entanglement witnesses defined on mixed states and used vastly in Quantum Information Theory. Finally, Section 5 presents a recent application of the geometric formalism introduced to define a Hamiltonian formalism for the Ehrenfest description of mixed quantum-classical systems (used often to describe, in an approximate way, molecular systems). We will see how the symplectic description we introduce for quantum dynamics allows us to combine the description of a quantum system with the description of a classical system and couple their dynamics together.

2 Geometric formulation of Quantum Mechanics

As we just mentioned, the aim of this section is simply to provide a tensorial characterization of Quantum Mechanics which is similar to the description of geometric Classical Mechanics. We will proceed step-by-step and study the construction first at the level of a pure-state description and later at a general level. Therefore, the first sections refer mainly to the Schrödinger representation, even if we will discuss some aspects of the Heisenberg approach also.

2.1 Representation of pure states

To introduce the real manifold point of view, we start by replacing the Hilbert space $\mathcal{H}$ with its realification $\mathcal{H}_{\mathbb{R}} := M_Q$. In this realification process the complex structure on $\mathcal{H}$ will be represented by a tensor J on M_Q as we will see.

The natural identification is then provided by choosing a basis $\{|z_k\rangle\}$ in $\mathcal{H}$ and splitting the corresponding coordinates into their real and imaginary parts:

$$|\psi\rangle = \sum_k \psi_k |z_k\rangle \qquad \psi_k \to \psi_k^R + i\psi_k^I$$

Then,

$$\{\psi_1, \cdots, \psi_n\} \in \mathcal{H} \mapsto \{\psi_1^R, \cdots, \psi_n^R, \psi_1^I, \cdots \psi_n^I\} \equiv (\Psi_R, \Psi_I) \in \mathcal{H}_{\mathbb{R}}.$$

Under this transformation, the Hermitian product becomes, for $\psi^1, \psi^2 \in \mathcal{H}$

$$\langle (\Psi_R^1, \Psi_I^1), (\Psi_R^2, \Psi_I^2) \rangle = (\langle \Psi_R^1, \Psi_R^2 \rangle + \langle \Psi_I^1, \Psi_I^2 \rangle) + i(\langle \Psi_R^1, \Psi_I^2 \rangle - \langle \Psi_I^1, \Psi_R^2 \rangle).$$

To consider $\mathcal{H}_{\mathbb{R}}$ just as a real differential manifold, the algebraic structures available on $\mathcal{H}$ must be converted into tensor fields on $\mathcal{H}_{\mathbb{R}}$. Consider first the tangent and cotangent bundles $T\mathcal{H}$ and $T^*\mathcal{H}$ and the following structures:

- The complex structure of $\mathcal{H}$ is translated into a tensor

  $$J : M_Q \to M_Q,$$

  satisfying $J(\Psi_R, \Psi_I) = (-\Psi_I, \Psi_R)$ for any point $(\Psi_R, \Psi_I) \in M_Q$. It is immediate to verify that in this case

  $$J^2 = -\mathbb{I}.$$

- The linear structure available in M_Q is encoded in the vector field Δ

  $$\Delta : M_Q \to TM_Q \quad \psi \mapsto (\psi, \psi).$$

- With every vector we can associate a vector field

  $$X_\psi : M_Q \to TM_Q \quad \phi \to (\phi, \psi)$$

  These vector fields are the infinitesimal generators of the vector group M_Q acting on itself.

- The Hermitian tensor $\langle \cdot, \cdot \rangle$ defined on the complex vector space $\mathcal{H}$, can be written in geometrical terms as

  $$\langle X_{\psi_1}, X_{\psi_2} \rangle(\phi) = \langle \psi_1, \psi_2 \rangle.$$

  On the "real manifold" the Hermitian scalar product may be written as

  $$\langle \psi_1, \psi_2 \rangle = g(X_{\psi_1}, X_{\psi_2}) + i\,\omega(X_{\psi_1}, X_{\psi_2}),$$

  where g is now a symmetric tensor and ω a skew-symmetric one.

The properties of the Hermitian product ensure that:

- the symmetric tensor is positive definite and non-degenerate, and hence defines a Riemannian structure on the real vector manifold.
- the skew-symmetric tensor is also non degenerate, and is closed with respect to the natural differential structure of the vector space. Hence, the tensor is a symplectic form (see also [42])

As the inner product is sesquilinear, it satisfies

$$\langle \psi_1, i\psi_2 \rangle = i\langle \psi_1, \psi_2 \rangle, \qquad \langle i\psi_1, \psi_2 \rangle = -i\langle \psi_1, \psi_2 \rangle.$$

This implies

$$g(X_{\psi_1}, X_{\psi_2}) = \omega(JX_{\psi_1}, X_{\psi_2}).$$

We also have that $J^2 = -\mathbb{I}$, and hence that the triple (J, g, ω) defines a Kähler structure (see [25, 27]). This implies, among other things, that the tensor J generates both finite and infinitesimal transformations which are orthogonal and symplectic.

The choice of the basis also allows us to introduce adapted coordinates for the realified structure:

$$\langle z_k, \psi \rangle = (q_k + ip_k)(\psi),$$

and write the geometrical structures introduced above as:

$$J = \partial_{p_k} \otimes dq_k - \partial_{q_k} \otimes dp_k \quad g = dq_k \otimes dq_k + dp_k \otimes dp_k \quad \omega = dq_k \wedge dp_k$$

Note 1. *If we represent the points of $\mathcal{H}$ by using complex coordinates we can write the Hermitian structure by means of $z_n = q^n + ip_n$:*

$$h = \sum_k d\bar{z}_k \otimes dz_k,$$

where of course

$$\langle X_{\psi_1} | X_{\psi_2} \rangle = h(X_{\psi_1}, X_{\psi_2}),$$

the vector fields now being the corresponding ones on the complex manifold.

In an analogous way we can consider a contravariant version of these tensors. The coordinate expressions with respect to the natural basis are:

- the Riemannian structure $G = \sum_{k=1}^{n} \left(\frac{\partial}{\partial qk} \otimes \frac{\partial}{\partial q^k} + \frac{\partial}{\partial p_k} \otimes \frac{\partial}{\partial p_k} \right)$,
- the Poisson tensor $\Omega = \sum_{k=1}^{n} \left(\frac{\partial}{\partial q^k} \wedge \frac{\partial}{\partial p_k} \right)$
- while the complex structure has the form

$$J = \sum_{k=1}^{n} \left(\frac{\partial}{\partial p_k} \otimes dq^k - \frac{\partial}{\partial q^k} \otimes dp_k \right)$$

2.1.1 Example I: the Hilbert space of a two level quantum system

For a two levels system we will consider an orthonormal basis on $\mathbb{C}^2$, say $\{|e_1\rangle, |e_2\rangle\}$. We introduce thus a set of coordinates

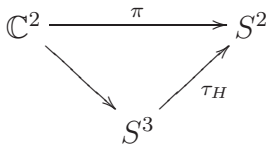
$$\langle e_j|\psi\rangle = z^j(\psi) = q^j(\psi) + ip_j(\psi) \qquad j = 1, 2.$$

In the following we will use z^j or q^j, p_j omitting the dependence in the state ψ as it is usually done in differential geometry.

The set of physical states is not equal to $\mathbb{C}^2$, since we have to consider the equivalence relation given by the multiplication by a complex number i.e.

$$\psi_1 \sim \psi_2 \Leftrightarrow \psi_2 = \lambda\psi_1 \qquad \lambda \in \mathbb{C}_0 = \mathbb{C} - \{0\}.$$

And besides, the norm of the state must be equal to one. These two properties can be encoded in the following diagram:



where S^2 and S^3 stand for the two and three dimensional spheres, and the projection τ_H is the Hopf fibration. The projection π is associating each vector with the one-dimensional complex vector space to which it belongs. Thus we see how this projection factorizes through a projection onto S^3 and a further projection given by the Hopf fibration, which is a $U(1)$–fibration.

The Hermitian inner product on $\mathbb{C}^2$ can be written in the coordinates z_1, z_2 as

$$\langle\psi|\psi\rangle = \bar{z}_j z^k \langle e_k|e_j\rangle = \bar{z}_j z^j.$$

Equivalently we can write it in real coordinates q, p and obtain:

$$\langle\psi|\psi\rangle = p_1^2 + p_2^2 + (q^1)^2 + (q^2)^2$$

We can also obtain these tensors in contravariant form if we take as starting point the Hilbert space $\mathcal{H} = \mathbb{C}^2$. If we repeat the steps above, we obtain the two contravariant tensors:

$$G = \frac{\partial}{\partial q^k} \otimes \frac{\partial}{\partial q^k} + \frac{\partial}{\partial p_k} \otimes \frac{\partial}{\partial p_k} \qquad \Lambda = \frac{\partial}{\partial q^k} \wedge \frac{\partial}{\partial p_k}.$$

Other tensors encode the complex vector space structure of $\mathcal{H} = \mathbb{C}^2$:

- the dilation vector field $\Delta = q^1 \frac{\partial}{\partial q^1} + p_1 \frac{\partial}{\partial p_1} + q^2 \frac{\partial}{\partial q^2} + p_2 \frac{\partial}{\partial p_2}$,
- and the complex structure tensor $J = dp_1 \otimes \frac{\partial}{\partial q^1} - dq^1 \otimes \frac{\partial}{\partial p_1} + dp_2 \otimes \frac{\partial}{\partial q^2} - dq^2 \otimes \frac{\partial}{\partial p_2}$.

2.2 The complex projective space

Another important aspect of the Hilbert space description of Quantum Mechanics is the study of the global phase of the state. It is a well known fact that physical states are independent of the global phase of the element of the Hilbert space that we choose to represent them. In the formulation as a real vector space, we can represent the multiplication by a phase on the manifold M_Q as a transformation whose infinitesimal generator is written as:

$$\Gamma = \sum_k \left(p_k \frac{\partial}{\partial q^k} - q^k \frac{\partial}{\partial p_k} \right). \tag{4}$$

The meaning of this vector field is simple to understand if we realize that a phase change changes the angle of the complex number representing the state, when considered in polar form (i.e. in polar coordinates $\{r^i, \theta^i\}_{i=1,\cdots,n}$, Eq. (4) becomes just

$$\Gamma = \sum_k \frac{\partial}{\partial \theta^k}.$$

Then, from a geometrical point of view we can use Eq. (4) in two ways:

- Computing its integral curves, which are the different states which are obtained from an initial one by a global phase multiplication.
- Acting with the vector field on functions of M_Q (which will represent our observables) providing us with the effect of the global phase transformation on the observables.

We can also consider another important vector field, which encodes the linear space structure of the tangent bundle TM_Q. In order to avoid singularities let us eliminate the zero section of the bundle TM_Q and denote the resulting space by T_0M_Q. We remind the reader that M_Q is just the realification of a complex vector space and, as such, we can encode its linear structure in the dilation vector field, which reads:

$$\Delta : M_Q \to T_0 M_Q; \qquad \psi \mapsto (\psi, \psi) \tag{5}$$

In the coordinate system (q^k, p_j), it takes the form

$$\Delta = q^k \frac{\partial}{\partial q^k} + p_k \frac{\partial}{\partial p_k} \tag{6}$$

We are particularly interested in the relation of the vector fields Δ and Γ. In particular:

Lemma 1. *Δ and Γ define a foliation on the manifold M_Q.*

Proof. It is simple to relate Δ with Γ via the complex structure, in the form:

$$\Gamma = J(\Delta). \tag{7}$$

Then it is straightforward to prove that both vector fields commute. □

We thus have an integrable distribution defined on the manifold M_Q. We can thus define the corresponding quotient manifold identifying the points which belong to the same orbit of the generators Γ and Δ. Notice that, from the physical point of view, this corresponds to the identification of points in the same ray of the Hilbert space.

Definition 1. *The resulting quotient manifold, denoted as $\mathcal{P}$, defined as*

$$\pi : M_Q \to \mathcal{P} \tag{8}$$

is called the ***complex projective space*** *and its points represent the physical pure states of a quantum system. We will denote by $[\psi]$ the point in $\mathcal{P}$ which is the image by π of a point $\psi \in M_Q$:*

$$\mathcal{P} \ni [\psi] := \pi(\psi) \qquad \psi \in M_Q \tag{9}$$

2.3 The observables

Our aim now is to provide a representation of the physical magnitudes, such as the energy or the angular momentum, in terms of the geometric objects introduced in the previous section. There are several possibilities, but we will consider only the simplest one from the mathematical point of view, and, at the same time, the most meaningful one from a physical point of view.

We know that in the usual formulation of Quantum Mechanics, physical observables are represented by linear operators on the Hilbert space $\mathcal{H}$, which are self-adjoint with respect to the inner product. The information which is physically relevant, though, corresponds to the expectation value associated to each observable (the pairing we introduced in the introduction), at each normalized state $|\psi\rangle \in \mathcal{H}$:

$$A \mapsto f_A(\psi) = \frac{1}{2}\langle\psi|A\psi\rangle \qquad |\psi\rangle \in \mathcal{H} \quad \langle\psi|\psi\rangle = 1 \tag{10}$$

If we think in the point $|\psi\rangle$ as an element of the differentiable manifold M_Q instead, the function f_A turns out to be a quadratic function defined on M_Q. For arbitrary operators, the function f_A is complex-valued. Hermitian operators give rise thus to quadratic real valued functions. We will denote:

Definition 2. *We will represent as $\mathcal{F}(M_Q)$ the set of all possible quadratic functions on M_Q and as $\mathcal{F}_{\mathbb{R}}(M_Q)$ the subset of real functions associated to the set of Hermitian operators.*

An interesting issue is how to characterize, by using the quadratic functions $\mathcal{F}(M_Q)$, the algebraic structures the set of operators in endowed with and which are physically relevant, for instance, in Heisenberg approach

2.3.1 The algebraic structures

We know that on the set $\mathrm{End}(\mathcal{H})$ there are three relevant ones:

- an associative product

$$\cdot : \mathrm{End}(\mathcal{H}) \times \mathrm{End}(\mathcal{H}) \to \mathrm{End}(\mathcal{H}) \qquad (A, B) \mapsto AB \tag{11}$$

- its symmetric part

$$\circ : \mathrm{End}(\mathcal{H}) \times \mathrm{End}(\mathcal{H}) \to \mathrm{End}(\mathcal{H}) \qquad (A, B) \mapsto A \circ B = AB + BA \tag{12}$$

  which defines a structure called **Jordan algebra** (see [38, 40]). The definition is as follows:

  Definition 3. *A commutative algebra $(\mathcal{A}, \circ)$ over a field $\mathbb{K}$ is called a **Jordan algebra** if*

$$(x \circ y) \circ (x \circ x) = x \circ (y \circ (x \circ x)) \qquad \forall x, y \in \mathcal{A}$$

  It can be easily proved that $(\mathrm{End}(\mathcal{H}, \circ)$ defines a Jordan algebra.

- and its skew-symmetric part,

$$[\cdot, \cdot] : \mathrm{End}(\mathcal{H}) \times \mathrm{End}(\mathcal{H}) \to \mathrm{End}(\mathcal{H}) \qquad (A, B) \mapsto [A, B] := -i(AB - BA) := -i[A, B]_-, \tag{13}$$

  which defines a Lie algebra structure on $\mathrm{End}(\mathcal{H})$, where we recall that

  Definition 4. *A **Lie algebra** is a vector space $\mathfrak{g}$ over a field $\mathbb{K}$ endowed with a bilinear operation $[\cdot, \cdot]$, which is skewsymmetric and satisfies the Jacobi identity, i.e.,*

$$[x, [y, z]] + [z, [x, y]] + [y, [z, x]] = 0 \qquad \forall x, y, z \in \mathfrak{g}.$$

  Notice that we introduce the imaginary unit in order to make it an inner operation in the subspace of Hermitian operators.

The Jordan and the Lie structures can be combined together to define a Lie-Jordan structure (see [40]):

Definition 5. *A **Lie-Jordan algebra** is a real vector space $\mathcal{L}$ endowed with a Jordan structure $\circ$ and a Lie structure $[\cdot, \cdot]$ which satisfy:*

- *the Lie bracket defines derivations of the Jordan product, i.e. $[a, b \circ c] = [a, b] \circ c + b \circ [a, c]$ for all $a, b, c \in \mathcal{L}$*
- *the associator of the Jordan structure can be obtained from the Lie bracket, i.e. for all $a, b, c \in \mathcal{L}$, $(a \circ b) \circ c - a \circ (b \circ c) = \hbar^2 [b, [c, a]]$ where $\hbar \in \mathbb{R}$.*

The set of physical magnitudes is the subset of $\mathrm{End}(\mathcal{H})$ defined by Hermitian operators. Modulo a multiplication by the imaginary unit, that subset corresponds to $\mathfrak{u}(\mathcal{H})$, the Lie algebra of the unitary group $U(\mathcal{H})$. Being a linear subspace, we can restrict easily the three operations above to the set, and define the corresponding operations on the Lie algebra. Moreover, $\mathfrak{u}(\mathcal{H})$ may be identified with its dual $\mathfrak{u}^*(\mathcal{H})$ by the (regular) scalar product defined as

$$\langle\cdot|\cdot\rangle : \mathfrak{u}(\mathcal{H}) \times \mathfrak{u}(\mathcal{H}) \to \mathbb{R}; \qquad \langle A|B\rangle = \frac{1}{2}\mathrm{Tr}AB, \quad \forall A, B \in \mathfrak{u}(\mathcal{H}).$$

The corresponding isomorphism

$$\zeta : \mathfrak{u}(\mathcal{H}) \to \mathfrak{u}^*(\mathcal{H}) \tag{14}$$

allows us to export the geometric and algebraic structures existing in each space, into the other. We can therefore consider the canonical Lie-Poisson structure of the dual $\mathfrak{u}^*(\mathcal{H})$ as a tensor on the space of observables (and therefore we can consider Hamiltonian dynamics), or extend the Jordan structure defined on $\mathfrak{u}(\mathcal{H})$ (since it is contained in $\mathrm{End}(\mathcal{H})$) into its dual.

In particular we can define two tensors

$$[R(\hat{A}, \hat{B})](\xi) = \langle \xi, A \circ B\rangle_{\mathfrak{u}^*} = \mathrm{Tr}(\xi(AB + BA)) \qquad \forall A, B \in \mathfrak{u}(\mathcal{H}) \tag{15}$$

and

$$[\Lambda(\hat{A}, \hat{B})](\xi) = \langle \xi, [A, B]\rangle_{\mathfrak{u}^*} = -i\mathrm{Tr}(\xi(AB - BA)) \qquad \forall A, B \in \mathfrak{u}(\mathcal{H}). \tag{16}$$

where we represent as $\hat{A}$ and $\hat{B}$ the linear functions defined on $\mathfrak{u}^*$ which correspond to the elements $A.B \in \mathfrak{u}(\mathcal{H})$ respectively. Notice that these R is the tensor defined on $\mathfrak{u}(\mathcal{H})$ by the operation defined in Eq. (12) when restricted to $\mathfrak{u}(\mathcal{H}) \subset \mathrm{End}(\mathcal{H})$ and transferred to $\mathfrak{u}^*(\mathcal{H})$ via the isomorphism ζ. On the other hand, the tensor Λ is the tensor defining the Lie-Poisson structure on $\mathfrak{u}^*(\mathcal{H})$. Notice that these two tensors are the geometric objects which directly encode Heisenberg formalism, which is defined on $\mathfrak{u}(\mathcal{H})$ in a natural way, or, via the isomorphism ζ, on $\mathfrak{u}^*(\mathcal{H})$.

Having defined contravariant tensors on M_Q to encode in a Kähler structure the Hermitian product of the Hilbert space, it makes sense to consider the action of those objects on the set of functions. It is immediate to verify that the tensors allow us to implement, at the level of quadratic functions, the three structures above

Lemma 2. *Consider two functions $f_A, f_B \in \mathcal{F}(M_Q)$. Then, the action of the tensors G and Ω define inner operations which encode the algebraic structures of the set of linear operators on the Hilbert space $\mathcal{H}$:*

$$G(df_A, df_B) = \{f_A, f_B\}_+ = f_{A\circ B} \qquad \Omega(df_A, df_B) = \{f_A, f_B\} = f_{[A,B]} \tag{17}$$

If we combine both tensors, we are able to reproduce, at the level of $\mathcal{F}(M_Q)$, the identity:

$$AB = \frac{1}{2}(AB + BA) + \frac{1}{2}(AB - BA) = \frac{1}{2}A \circ B + \frac{i}{2}[A, B],$$

which becomes a new binary operation on $\star : \mathcal{F}(M_Q) \times \mathcal{F}(M_Q) \to \mathcal{F}(M_Q)$:

$$f_A \star f_B := f_{AB} = \frac{1}{2}\{f_A, f_B\}_+ + \frac{i}{2}\{f_A, f_B\}. \tag{18}$$

Considering the three operations introduced so far, we can reproduce completely the algebraic structures of the space of operators on $\mathcal{H}$. We can summarize them in the following result:

Theorem 1. *The set of quadratic functions $\mathcal{F}(M_Q)$ endowed with the product $\star$ and the complex conjugation turns out to be a $\mathbb{C}^*$–algebra. The construction is tensorial since it is built on the pair of tensors G and Ω defined on M_Q.*

The conclusion thus is that we are able to reconstruct, at the level of $\mathcal{F}(M_Q)$, all the structures necessary to implement Heisenberg formalism. From that point of view, $\mathcal{F}(M_Q)$ can be considered to be the geometrical framework of Heisenberg's formalism, and the tensors G and Λ the geometrical structures to encode the dynamics and the indetermination relations.

2.3.2 Example II: the algebraic structures for a two level quantum system

Let us continue the analysis of the case of a two level quantum system that we began in Example 2.1.1. By using the Pauli matrices

$$\left\{\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}$$

as Hermitian operators to construct functions $\langle\psi|A|\psi\rangle$, we obtain the real quadratic functions

$$(q^1)^2 + p_1^2 + (q^2)^2 + p_2^2, \quad q^1q^2 + p_1p_2, \quad q^1p_2 - p_1q^2, \quad (q^1)^2 + p_1^2 - ((q^2)^2 + p_2^2).$$

It is not difficult now to compute the Poisson brackets of these quadratic functions to find that they are the Hamiltonian for the infinitesimal generators of the $\mathfrak{u}(2)$ algebra. We may also compute explicitly the Jordan brackets, as for instance

$$\{(q^1)^2 + p_1^2 + (q^2)^2 + p_2^2, q^1q^2 + p_1p_2\}_+ = 4(q^1q^2 + p_1p_2).$$

Similar results are obtained with the other functions. The result we want to point out is

Lemma 3. *The function* $(q^1)^2 + p_1^2 + (q^2)^2 + p_2^2$ *acts, with respect to the Jordan bracket, as the identity operator except for a normalization factor.*

We also find

$$\{q^1q^2 + p_1p_2, q^1q^2 + p_1p_2\}_+ = 4((q^1)^2 + p_1^2 + (q^2)^2 + p_2^2).$$

And analogously for the other quadratic functions. We have

Lemma 4. *The product of all functions (in the family above) with themselves produce a multiple of the quadratic isotropic function.*

We also can obtain easily

$$\{q^1q^2 + p_1p_2, q^1p_2 - p_1q^2\}_+ = 0 = \{q^1q^2 + p_1p_2, (q^1)^2 + p_1^2 - ((q^1)^2 + p_1^2)\}_+$$

The additional relevant property is that the Hamiltonian vector field are Killing vectors. In terms of brackets this amounts to:

$$\{f, \{g, h\}_+\} = \{\{f, g\}, h\}_+ + \{g, \{f, h\}\}_+$$

This condition, plus the compatibility between the Jordan and the Poisson brackets

$$\{\{f, g\}_+, h\}_+ - \{f, \{g, h\}_+\}_+ = \hbar^2\{g, \{h, f\}\}$$

where $\hbar \in \mathbb{R}$ represents the Planck constant, imply that the two brackets combined define a Lie-Jordan algebra.

In particular, by considering generic quadratic functions of two complex coordinates, we find a complex valued quadratic function whose real and imaginary parts are quadratic functions of the previous type. All in all, the result is:

Lemma 5. *Complex valued quadratic functions close on a* $\mathbb{C}^*$*–algebra with respect to the Hermitian bracket.*

Thus we have found that Hermitian operators are associated with Hamiltonian vector fields which are also Killing. As a matter of fact, this property characterizes functions on $\mathbb{C}^2$ which are associated with Hermitian operators.

2.3.3 Functions on the projective space and their algebraic structures

It is important to notice that the functions defined by Eq. (10) correspond to expectation values of physical observables when restricted to the suitable set of points. But in order to represent true physical magnitudes, they must correspond to functions which are constant

along the fibers of the fibration $\pi : M_Q \to \mathcal{P}$. Those functions, meaningful from a physical point of view, correspond to

$$e_A = \frac{\langle\psi|A\psi\rangle}{\langle\psi|\psi\rangle} \tag{19}$$

These are thus functions on M_Q which are in one-to-one correspondence with the functions on the projective space $\mathcal{P}$. Obviously, they are no longer quadratic; but this is a natural property taking into account that the projective space $\mathcal{P}$ has lost the linear structure of M_Q to become just a differentiable manifold.

Nonetheless, it is still possible to reconstruct the algebraic structures we introduced above by defining a pair of suitable tensors. Consider then the action of the tensors Ω and G on the set of functions of the form given by Eq. (69). We know that the functions are projectable under $\pi : M_Q \to \mathcal{P}$, but it is simple to understand that the product is not, since the tensors are derivations of degree 2, i.e., the Lie derivative of the tensors with respect to the dilation vector field Δ defined in Eq. (5) is

$$\mathcal{L}_\Delta G = -2G; \qquad \mathcal{L}_\Delta \Omega = -2\Omega.$$

Thus, in order to make it projectable, we must rescale it by a factor of degree two, and define for instance:

$$\{e_A, e_B\}_\mathcal{P}(\psi) := G_\mathcal{P}(de_A, de_B)(\psi) = \langle\psi|\psi\rangle\{e_A, e_B\}_+ \tag{20}$$

$$\{e_A, e_B\}_\mathcal{P} := \Omega_\mathcal{P}(de_A, de_B) = \langle\psi|\psi\rangle\{e_A, e_B\} \tag{21}$$

2.3.4 Example III: the projective space for a two level quantum system

Extending the example presented in Sections 2.1.1 and 2.3.2, we can consider now the corresponding projective space and the corresponding tensors. It is important to remark that while forms can not be projected, contravariant tensor fields can. This is the reason why we introduced the contravariant tensors Λ and G. Thus by considering

$$G = \frac{\partial}{\partial q^1} \otimes \frac{\partial}{\partial q^1} + \frac{\partial}{\partial p_1} \otimes \frac{\partial}{\partial p_1} + \frac{\partial}{\partial q^2} \otimes \frac{\partial}{\partial q^2} + \frac{\partial}{\partial p_2} \otimes \frac{\partial}{\partial p_2},$$

we can define a projectable tensor as:

$$\begin{aligned} G_\mathcal{P} &= \langle\psi|\psi\rangle G - \Gamma \otimes \Gamma - \Delta \otimes \Delta = \\ &= ((q^1)^2 + (q^2)^2 + p_1^2 + p_2^2)\left(\frac{\partial}{\partial q^1} \otimes \frac{\partial}{\partial q^1} + \frac{\partial}{\partial p_1} \otimes \frac{\partial}{\partial p_1} + \frac{\partial}{\partial q^2} \otimes \frac{\partial}{\partial q^2} + \frac{\partial}{\partial p_2} \otimes \frac{\partial}{\partial p_2}\right) - \\ &\sum_{lm}\left(p_l\frac{\partial}{\partial q^l} - q^l\frac{\partial}{\partial p_l}\right) \otimes \left(p_m\frac{\partial}{\partial q^m} - q^m\frac{\partial}{\partial p_m}\right) - \sum_{lm}\left(q^l q^m \frac{\partial}{\partial q^l} \otimes \frac{\partial}{\partial q^m} + p_l p_m \frac{\partial}{\partial p_l} \otimes \frac{\partial}{\partial p_m}\right) \end{aligned} \tag{22}$$

Analogously we can introduce

$$\Omega_{\mathcal{P}} = \langle\psi|\psi\rangle\Omega - \Gamma\otimes\Delta - \Delta\otimes\Gamma = ((q^1)^2 + (q^2)^2 + p_1^2 + p_2^2)\left(\frac{\partial}{\partial q^1}\wedge\frac{\partial}{\partial p^1} + \frac{\partial}{\partial q^2}\wedge\frac{\partial}{\partial p^2}\right) -$$
$$-\sum_{lm}\left(p_l\frac{\partial}{\partial p_l} + q^l\frac{\partial}{\partial q^l}\right)\otimes\left(p_m\frac{\partial}{\partial q^m} - q^m\frac{\partial}{\partial p_m}\right) - \sum_{lm}\left(p_l\frac{\partial}{\partial q^l} - q^l\frac{\partial}{\partial p_l}\right)\otimes\left(p_l\frac{\partial}{\partial p_l} + q^l\frac{\partial}{\partial q^l}\right) = \tag{23}$$

The next step is to consider the projectable quadratic functions. If we consider the basis of the Hermitian operators given by the Pauli matrices, we find:

$$e_{\sigma_0} = 1 \qquad e_{\sigma_1} = \frac{q^1q^2 + p_1p_2}{(q^1)^2 + (q^2)^2 + p_1^2 + p_2^2}$$

$$e_{\sigma_2} = \frac{q^1p_2 - p_1q^2}{(q^1)^2 + (q^2)^2 + p_1^2 + p_2^2} \qquad e_{\sigma_3} = \frac{(q^1)^2 + p_1^2 - (q^2)^2 - p_2^2}{(q^1)^2 + (q^2)^2 + p_1^2 + p_2^2}$$

We find that only the functions associated with $\{\sigma_1, \sigma_2, \sigma_3\}$ define non-trivial functions on the complex projective space. Of course, their associated vector fields generate the algebra of $SU(2)$.

We can compute now the action of the tensor $G_{\mathcal{P}}$ on these functions and obtain:

$$G_{\mathcal{P}}(de_{\sigma_0}, df) = 0 \qquad \forall f$$

$$G_{\mathcal{P}}(de_{\sigma_1}, de_{\sigma_1}) = e_0 - 4e_{\sigma_1}^2$$

$$G_{\mathcal{P}}(de_{\sigma_2}, de_{\sigma_2}) = e_0 - 4e_{\sigma_2}^2$$

$$G_{\mathcal{P}}(de_{\sigma_3}, de_{\sigma_3}) = 4(e_0 - e_3^2)$$

$$G_{\mathcal{P}}(de_{\sigma_1}, de_{\sigma_2}) = -4(e_{\sigma_1}e_{\sigma_2})$$

In an analogous way, other products can be computed. We obtain thus:

Lemma 6. *The action of $G_{\mathcal{P}}$ on the set of projectable functions corresponds to*

$$G_{\mathcal{P}}(de_A, de_B) = e_{A\circ B} - e_A.e_B.$$

This implies that for $A = B$ we have

$$G_{\mathcal{P}}(e_A, e_B) = e_{A^2} - e_A^2,$$

i.e. we find the variance, the quadratic deviation from the mean value.

As a conclusion we obtain the physical origin of the construction:

Corollary 1. *$G_{\mathcal{P}}$ is directly related to the indetermination relations.*

2.3.5 Characterizing the physical magnitudes

The final issue is to be able to identify which quadratic functions are actually related to physical magnitudes. In principle, there may exist quadratic functions on M_Q which are not associated to any physical magnitude. The complete characterization requires to take into account both tensorial objects. Indeed, the fact that the two algebraic structures (Jordan and Poisson) of the set $\mathrm{End}(\mathcal{H})$ are compatible and define a Lie-Jordan structure, ensures that the Hamiltonian vector fields, besides preserving the Poisson structure, preserve also the symmetric structure and therefore are Killing vector fields. We can characterize completely those vector field associated to physical magnitudes, precisely because of that property:

Proposition 1 ([27]). *The Hamiltonian vector field X_f (defined as $X_f = \hat{\Omega}(df)$) is a Killing vector field for the Riemannian tensor G if and only if f is a quadratic function associated with an Hermitian operator A, i.e. there exists $A = A^\dagger$ such that $f = f_A$.*

2.3.6 The spectral information

Finally, we can consider the problem of how to recover the eigenvalues and eigenvectors of the operators at the level of the functions of M_Q. We consider the expectation value functions associated to the operators as:

$$A \mapsto e_A(\psi) = \frac{\langle \psi | A\psi \rangle}{\langle \psi | \psi \rangle}.$$

Then,

- eigenvectors correspond to the critical points of functions e_A, i.e.

  $$de_A(\psi_a) = 0 \text{ if and only if } \psi_a \text{ is an eigenvector of } A.$$

  We notice that the invariance of e_A under multiplication by a phase $U(1)$ implies that critical points form a circle on the sphere of normalized vectors if the eigenvalue is not degenerate.

- the corresponding eigenvalue is recovered by the value $e_A(\psi_a)$

Thus we can conclude that the Kähler manifold (M_Q, J, ω, g) contains all the information of the usual formulation of Quantum Mechanics on a complex Hilbert space.

Up to now we have concentrated our attention on states and observables. If we consider observables as generators of transformations, i.e. we consider the Hamiltonian flows associated to the corresponding functions, the invariance of the tensor G implies that the evolution is actually unitary. It is, therefore, natural, to consider the action of the unitary group on the realification of the complex vector space.

2.4 The momentum map: geometrical structures on $\mathfrak{u}^*(\mathcal{H})$

The unitary action of $U(\mathcal{H})$ on $\mathcal{H}$ induces a symplectic action on the symplectic manifold (M_Q, ω). By using the association

$$F : M_Q \times \mathfrak{u}(\mathcal{H}) \to \mathbb{R} \quad (\psi, A) \mapsto \frac{1}{2}\langle\psi|iA\psi\rangle = f_{iA}(\psi),$$

we find, with $F_A := f_{iA} : M_Q \to \mathbb{R}$, that

$$\{F(A), F(B)\} = iF([A, B]).$$

Thus if we fix ψ, we have a mapping $F(\psi) : \mathfrak{u}(\mathcal{H}) \to \mathbb{R}$. With any element $\psi \in \mathcal{H}$ we associate an element in $\mathfrak{u}^*(\mathcal{H})$. The previous map defines a momentum map (see [43])

$$\mu : \mathcal{H} \to \mathfrak{u}^*(\mathcal{H}) \qquad \mu(\psi) = |\psi\rangle\langle\psi|, \tag{24}$$

which provides us with a symplectic realization of the natural Poisson manifold structure available in $\mathfrak{u}^*(\mathcal{H})$.

Analogously, we can consider the projected action:

$$F_{\mathcal{P}} : \mathcal{P} \times \mathfrak{u}(\mathcal{H}) \to \mathbb{R} \qquad ([\psi], A) \mapsto e_{iA}(\pi^{-1}([\psi])). \tag{25}$$

In the following we will omit the imaginary unit when referring to the function unless it is necessary.

Again,

$$F_{\mathcal{P}}([\psi]) : \mathfrak{u}(\mathcal{H}) \to \mathbb{R},$$

associates an element of the dual space $\mathfrak{u}^*(\mathcal{H})$ with any point $[\psi] \in \mathcal{P}$. This yields the momentum map corresponding to the action (25) that we can write:

$$\mu_{\mathcal{P}} : \mathcal{P} \to \mathfrak{u}^*(\mathcal{H}) \qquad \mu_{\mathcal{P}}([\psi]) = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} := \rho_\psi \tag{26}$$

Therefore, we have proved:

Lemma 7. *The projective space* $\mathcal{P}$ *is in one-to-one correspondence with the subset* $\mathcal{D}^1(\mathcal{H}) \subset \mathfrak{u}^*(\mathcal{H})$ *of elements which are rank-one projectors, i.e., with the subset of elements* $\{\rho_k\}$ *which satisfy*

$$\rho_k^2 = \rho_k \qquad \mathrm{Tr}\rho_k = 1 \tag{27}$$

If we denote the linear function on $\mathfrak{u}^*(\mathcal{H})$ associated with the element $iA \in \mathfrak{u}(\mathcal{H})$ by $\hat{A}$, we have

$$\mu^*(\hat{A}) = f_A. \tag{28}$$

Analogously, for the projected action we have

$$\mu^*_{\mathcal{P}}(\hat{A}) = e_A. \tag{29}$$

It is possible to show that the contravariant tensor fields on M_Q associated with the Hermitian structure are μ–related with a complex tensor on $\mathfrak{u}^*(\mathcal{H})$:

$$\mu_*(G + i\Omega) = R + i\Lambda.$$

Clearly the tensors representing the algebraic structures on each set are related by:

$$G(\mu^*\hat{A}, \mu^*\hat{B}) + i\Omega(\mu^*\hat{A}, \mu^*\hat{B}) = \mu^*(R(\hat{A}, \hat{B}) + i\Lambda(\hat{A}, \hat{B})),$$

and analogously

$$G_{\mathcal{P}}(\mu^*_{\mathcal{P}}\hat{A}, \mu^*_{\mathcal{P}}\hat{B}) + i\Omega_{\mathcal{P}}(\mu^*_{\mathcal{P}}\hat{A}, \mu^*_{\mathcal{P}}\hat{B}) + \mu^*_{\mathcal{P}}\hat{A} \circ \mu^*_{\mathcal{P}}\hat{B} = \mu^*_{\mathcal{P}}(R(\hat{A}, \hat{B}) + i\Lambda(\hat{A}, \hat{B})).$$

2.5 The dynamics

At this stage, we can incorporate dynamics into the picture. Although several approaches are possible, we will consider just the simplest one. Thus, we will consider the definition of a dynamical system on M_Q instead of on $\mathcal{P}$, aiming to construct the geometrical analogue of Schrödinger equation. In a similar way, we will discuss the analogue of Heisenberg equation by using the tensors which we have constructed on $\mathfrak{u}^*(\mathcal{H})$.

Consider then the Poisson structures defined by the tensor Ω (defined by Eq. (17)) on the set of quadratic functions and the tensor Λ defined by Equation and the function associated to the Hamiltonian operator:

$$f_H(\psi) = \frac{1}{2}\langle\psi|H\psi\rangle.$$

- We can consider now the one-parameter family of diffeomorphisms associated with the corresponding Hamiltonian vector field:

  $$X_H = \hbar^{-1}\Omega(df_H, \cdot). \tag{30}$$

  This object is, by construction, a vector field defined on the manifold M_Q. This vector field encodes Schrödinger equation in our geometric language, as we can see immediately.

  Let us consider again the simplest quantum situation defined on $\mathbb{C}^n$. As a real manifold, $M_Q \sim \mathbb{R}^{2n}$. Consider then a Hamiltonian $H : \mathbb{C}^n \to \mathbb{C}^n$ which is usually written as a matrix:

  $$H = \begin{pmatrix} H_{11} & H_{12} & \dots & H_{1n} \\ \vdots & \vdots & \dots & \vdots \\ H_{n1} & H_{n2} & \dots & H_{nn} \end{pmatrix}.$$

If we consider it as a matrix on the real vector space M_Q, it reads:

$$H = \begin{pmatrix} H_{q^1q^1} & H_{q^1p_1} & H_{q^1q^2} & H_{q^1p_2} & \dots & H_{q^1q^n} & H_{q^1p_n} \\ H_{p_1q^1} & H_{p_1p_1} & H_{p_1q^2} & H_{p_1p_2} & \dots & H_{p_1q^n} & H_{p_1p_n} \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots \\ H_{q^nq^1} & H_{q^np_1} & H_{q^nq^2} & H_{q^np_2} & \dots & H_{q^nq^n} & H_{q^np_n} \\ H_{p_nq^1} & H_{p_np_1} & H_{p_nq^2} & H_{p_np_2} & \dots & H_{p_nq^n} & H_{p_np_n} \end{pmatrix}.$$

The function f_H in $\mathcal{F}(M_Q)$ becomes thus:

$$f_H = \frac{1}{2}\left(q^1, p_1, q^2, p_2, \dots, q^n, p_n\right) \begin{pmatrix} H_{q^1q^1} & H_{q^1p_1} & H_{q^1q^2} & H_{q^1p_2} & \dots & H_{q^1q^n} & H_{q^1p_n} \\ H_{p_1q^1} & H_{p_1p_1} & H_{p_1q^2} & H_{p_1p_2} & \dots & H_{p_1q^n} & H_{p_1p_n} \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots \\ H_{q^nq^1} & H_{q^np_1} & H_{q^nq^2} & H_{q^np_2} & \dots & H_{q^nq^n} & H_{q^np_n} \\ H_{p_nq^1} & H_{p_np_1} & H_{p_nq^2} & H_{p_np_2} & \dots & H_{p_nq^n} & H_{p_np_n} \end{pmatrix} \begin{pmatrix} q^1 \\ p_1 \\ q^2 \\ p_2 \\ \vdots \\ q^n \\ p_n \end{pmatrix},$$

where the matrix above is symmetric because H is Hermitian, since we have:

$$\begin{aligned} H_{q^kq^k} &= H_{kk} = H_{p_kp_k}, \\ H_{q^kp_k} &= 0 = H_{p_kq^k}, \\ H_{q^jq^k} &= \mathrm{Re}(H_{jk}) = H_{p_jp_k}, \\ H_{q^jp_k} &= -\mathrm{Im}(H_{jk}) = -H_{p_jq^k}. \end{aligned}$$

Then, the Hamiltonian vector field turns out to be:

$$X_H = \hbar^{-1} \sum_k \left(\frac{\partial f_H}{\partial p_k}\frac{\partial}{\partial q^k} - \frac{\partial f_H}{\partial q^k}\frac{\partial}{\partial p_k} \right).$$

And its integral curves are precisely the expression of Schrödinger equation when we write it back in complex terms:

$$\begin{aligned} \dot{q}^1 &= \hbar^{-1}(H_{p_1q^1}q^1 + H_{p_1p_1}p_1 + \ldots + H_{p_1q^n}q^n + H_{p_1p_n}p_n), \\ \dot{p}_1 &= -\hbar^{-1}H_{q^1q^1}q^1 + H_{q^1p_1}p_1 + \ldots + H_{q^1q^n}q^n + H_{q^1p_n}p_n), \\ &\vdots \\ \dot{q}^n &= \hbar^{-1}(H_{p_nq^1}q^1 + H_{p_np_1}p_1 + \ldots + H_{p_nq^n}q^n + H_{p_np_n}p_n), \\ \dot{p}_n &= -\hbar^{-1}(H_{q^nq^1}q^1 + H_{q^np_1}p_1 + \ldots + H_{q^nq^n}q^n + H_{q^np_n}p_n). \end{aligned}$$

We can write these equations as:

$$\frac{d}{dt}\begin{pmatrix} q^1 \\ p_1 \\ q^2 \\ p_2 \\ \vdots \\ q^n \\ p_n \end{pmatrix} = -\hbar^{-1}\mathbf{J}\begin{pmatrix} H_{q^1q^1} & H_{q^1p_1} & H_{q^1q^2} & H_{q^1p_2} & \dots & H_{q^1q^n} & H_{q^1p_n} \\ H_{p_1q^1} & H_{p_1p_1} & H_{p_1q^2} & H_{p_1p_2} & \dots & H_{p_1q^n} & H_{p_1p_n} \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots \\ H_{q^nq^1} & H_{q^np_1} & H_{q^nq^2} & H_{q^np_2} & \dots & H_{q^nq^n} & H_{q^np_n} \\ H_{p_nq^1} & H_{p_np_1} & H_{p_nq^2} & H_{p_np_2} & \dots & H_{p_nq^n} & H_{p_np_n} \end{pmatrix}\begin{pmatrix} q^1 \\ p_1 \\ q^2 \\ p_2 \\ \vdots \\ q^n \\ p_n \end{pmatrix},$$

where

$$\mathbf{J} = \begin{pmatrix} 0 & -1 & 0 & 0 & \dots & 0 & 0 \\ 1 & 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & -1 \\ 0 & 0 & 0 & 0 & \dots & 1 & 0 \end{pmatrix};$$

or, equivalently,

$$\dot{\psi}(q,p) = -\hbar^{-1}\mathbf{J}H\psi(q,p),$$

where

$$\psi(q,p) = \begin{pmatrix} q^1 \\ p_1 \\ q^2 \\ p_2 \\ \vdots \\ q^n \\ p_n \end{pmatrix} \tag{31}$$

is the real space representation of the state vector and $\mathbf{J}$ the complex structure. This is precisely the real space expression of Schrödinger equation.

The most significative result is then:

Theorem 2. *Schrödinger equation defines a Hamiltonian vector field on M_Q.*

- On the set $\mathfrak{u}^*(\mathcal{H})$, dynamics is introduced directly as the Hamiltonian vector field associated to the operator H, or, isomorphically, as the derivation

$$\hat{X}_H = \hbar^{-1}\{\hat{H}, \cdot\} = \Lambda(d\hat{H}, \cdot)$$

where $\hat{H}$ is the linear function on $u^*(\mathcal{H})$ which corresponds to the operator $H \in \mathfrak{u}(\mathcal{H})$. This vector field is representing Heisenberg formalism of quantum dynamics. If we write the expression of the corresponding flow we obtain:

$$\frac{d\hat{A}(t)}{dt} = \hbar^{-1}\{\hat{H}, \hat{A}\}. \tag{32}$$

We could also see that the integral curve above can be represented, isomorphically, on the set $\mathcal{F}(M_Q)$, as

$$\hbar \frac{d}{dt} f_A(t) = \{f_H, f_A\} = \Omega(df_H, df_A). \tag{33}$$

The most significative result is then:

Theorem 3. *Heisenberg equation defines a Hamiltonian vector field on* $\mathfrak{u}^*(\mathcal{H})$.

- By our geometric construction is possible to prove, easily, that both formalisms are equivalent. Indeed, by direct computation, we can prove that the momentum map μ is equivariant with respect to the unitary action $U(\mathcal{H}) \times \mathcal{H} \to \mathcal{H}$ (as it is $\mu_{\mathcal{P}}$ with respect to $U(\mathcal{H}) \times \mathcal{P} \to \mathcal{P}$) and the co-adjoint action of $U(\mathcal{H})$ on $\mathfrak{u}^*(\mathcal{H})$. Both vector fields are therefore related via the momentum mapping given by Eq. (24), i.e.,

$$\mu_*(X_H) = \hat{X}_H \tag{34}$$

The conclusion is then:

Theorem 4. *The dynamics of a closed quantum system is Hamiltonian with respect to the canonical Poisson tensors defined on* M_Q *or* $\mathfrak{u}^*(\mathcal{H})$. *Besides, both Hamiltonian vector fields are related by the momentum mapping* μ *associated to the canonical action of the unitary group* $U(\mathcal{H})$.

3 The space of density states

3.1 General considerations

We know that the manifold $\mathcal{P}$ is not enough to represent all the possible physical states of a system. Given one point $\psi_k \in \mathcal{H} - \{0\}$ which is associated to a point $[\psi_k] \in \mathcal{P}$ and corresponds then via the momentum mapping $\mu_{\mathcal{P}}$ to the rank-one projector ρ_{ψ_k}, we know that

$$\rho_{\psi_k}(A) := \langle A \rangle = \mathrm{Tr}(\rho_{\psi_k} A) \qquad \forall A \in i\mathfrak{u}(\mathcal{H}) \tag{35}$$

This implies that the action on the physical magnitude can be written as

$$\rho_{\psi_k}(A) = \frac{\langle \psi_k | A \psi_k \rangle}{\langle \psi_k | \psi_k \rangle} = e_A(\psi_k). \tag{36}$$

But, as we know, arbitrary convex combinations of rank-one projectors also define admissible physical states.

Definition 6. *The **set of density states** $\mathcal{D}(\mathcal{H})$ of the system corresponds to the subset of $\mathfrak{u}^*(\mathcal{H})$ obtained by convex combinations of rank-one projectors, i.e.,*

$$\mathcal{D}(\mathcal{H}) = \left\{ \rho = \sum_k p_k \rho_k |\ \ p_k \geq 0, \sum_j p_j = 1, \rho_k \in \mathcal{D}^1(\mathcal{H}) \right\} \tag{37}$$

Equivalently, we can consider the following definition: an element $\rho \in \mathfrak{u}^*(\mathcal{H})$ is a density operator if and only if

$$\mathrm{Tr}\rho = 1, \qquad \rho \geq 0. \tag{38}$$

This is the most general set containing the possible states of a quantum system defined on a Hilbert space $\mathcal{H}$, even if it can be presented in different ways (see [12, 34]).

We can also construct the set following the second characterization, following [35]. First, we introduce the space of all non-negatively defined operators, i.e. the space of all those $\rho \in \mathfrak{gl}(\mathcal{H})$ which can be written in the form

$$\rho = T^\dagger T \quad T \in \mathfrak{gl}(\mathcal{H}).$$

We will denote by $\mathcal{PH}$ this space of operators, which is a convex cone in $\mathfrak{u}^*(\mathcal{H})$. By imposing the condition $\mathrm{Tr}\rho = 1$ we select in $\mathcal{PH}$ the convex body of density states $\mathcal{D}(\mathcal{H})$. We have then the sequence

$$\mathcal{D}(\mathcal{H}) \subset \mathcal{PH} \subset \mathfrak{u}^*(\mathcal{H}).$$

We will also consider non-negative Hermitian operators and density states of rank k (defined as those operators which have k non-vanishing eigenvalues) and denote the corresponding spaces as $\mathcal{P}^k(\mathcal{H})$ and $\mathcal{D}^k(\mathcal{H})$ respectively. The complex projective space is in one-to-one correspondence with $\mathcal{D}^1(\mathcal{H})$. Indeed, any state in $\mathcal{D}(\mathcal{H})$ can be written as a convex combination of distinct states $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$, with $0 \leq \lambda \leq 1$. We will call **extremal states** those which can not be written in this form (i.e. as convex combination of two ρ_1 and ρ_2). The extremal states are thus given by $\mathcal{D}^1(\mathcal{H})$.

Under this framework, it is natural to consider the following $\mathrm{GL}(\mathcal{H})$–action:

$$\mathrm{GL}(\mathcal{H}) \times \mathfrak{u}^*(\mathcal{H}) \to \mathfrak{u}^*(\mathcal{H}) \quad (T, \xi) \mapsto T\xi T^\dagger.$$

Then:

1. The Hermitian operators ξ_1 and ξ_2 belong to the same GL–orbit if and only if they have the same number K_+ of positive eigenvalues and the same number K_- of negative eigenvalues (counted with multiplicities).

2. Any GL–orbit intersecting the positive cone $\mathcal{PH}$ is contained in $\mathcal{PH}$; so that $\mathcal{PH}$ is stratified by the GL–orbits. These GL–orbits in $\mathcal{PH}$ are determined by the rank of the operator, i.e. they are exactly $\mathcal{P}^k(\mathcal{H})$.

3. When we restrict to the space of density states by imposing the condition $\mathrm{Tr}\rho = 1$, this GL–action will not preserve the states. It is however possible to define a new action that maps $\mathcal{D}(\mathcal{H})$ into itself by setting

$$\mathrm{GL}(\mathcal{H}) \times \mathcal{D}(\mathcal{H}) \to \mathcal{D}(\mathcal{H}) \quad (T, \rho) \mapsto \frac{T\rho T^\dagger}{\mathrm{Tr}(T\rho T^\dagger)}.$$

This action does preserve the rank of ρ and then the following proposition holds true:

Proposition 2. *The decomposition of the convex body of density states $\mathcal{D}(\mathcal{H})$ into orbits of the $\mathrm{GL}(\mathcal{H})$–action $\rho \mapsto \frac{T\rho T^\dagger}{\mathrm{Tr}(T\rho T^\dagger)}$ is exactly the stratification*

$$\mathcal{D}(\mathcal{H}) = \bigcup_{k=1}^{n} \mathcal{D}^k(\mathcal{H}),$$

into states of a given rank.

The boundary of the convex body of density states consists of states of rank lower than n, i.e. $\partial\mathcal{D}(\mathcal{H}) = \bigcup_{k=1}^{n-1} \mathcal{D}^k(\mathcal{H})$, and each stratum is a smooth submanifold in $\mathfrak{u}^*(\mathcal{H})$. However, the boundary $\partial\mathcal{D}(\mathcal{H})$ is not smooth (for $n > 2$). For $n = 2$, the set of density states is diffeomorphic to a 3-dimensional ball, as we will see later, while its boundary corresponds to the set of rank-one projectors $\mathcal{D}^1(\mathbb{C}^2)$, which are represented on the 3-dimensional ball by the surface 2-dimensional sphere, which is, of course, a smooth manifold.

From a dynamical point of view, we can summarize the geometrical picture of the evolution in the following theorem:

Theorem 5. *Every smooth curve $\gamma : \mathbb{R} \to \mathfrak{u}^*(\mathcal{H})$ through the convex body of density states is tangent, at every point, to the stratum to which it belongs, i.e.*

$$\gamma(t) \in \mathcal{D}^k(\mathcal{H}) \Rightarrow T\gamma(t) \in T_{\gamma(t)}\mathcal{D}^k(\mathcal{H}).$$

Once this property is known, we can use the fact that the set is contained in the set $\mathfrak{u}^*(\mathcal{H})$, and restrict the geometrical objects to it. In particular, we can consider the restriction of the Poisson tensor Λ and this allows to define a Hamiltonian vector field by

$$\frac{d\hat{\rho}(t)}{dt} = \hbar^{-1}\{\hat{H}, \hat{\rho}\} = \hbar^{-1}\Lambda(d\hat{H}, d\hat{\rho}), \tag{39}$$

or analogously as

$$\hbar\frac{df_\rho(t)}{dt} = \{f_H, f_\rho\} = \Omega(df_H, df_\rho) \tag{40}$$

if we use the tensor Ω defined on M_Q. This unitary dynamics associated with a Hermitian Hamiltonian H is known as **von Neumann equation**.

3.2 Example: States of a two level system

3.2.1 The geometrical objects

We will consider in some detail two examples. The first one is the two level system with carrier space $\mathcal{H} = \mathbb{C}^2$. We consider $\mathfrak{u}(2)$ and $\mathfrak{u}^*(2)$ and choose again as a basis the Pauli matrices:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_1 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We can introduce coordinate functions with respect to them:

$$y_\mu(A) = \frac{1}{2}\mathrm{Tr}\sigma_\mu A.$$

In these coordinates, a generic Hermitian matrix A can be written as

$$A = y_0\sigma_0 + y_r\sigma_r$$

The corresponding Poisson brackets for the canonical Lie-Poisson structure on the dual of the Lie algebra read:

$$\{y_0, y_a\} = 0 \quad \{y_a, y_b\} = 2\epsilon_{abc}y_c.$$

The expression of the Poisson tensor thus becomes:

$$\Lambda = 2\left(y_1\frac{\partial}{\partial y_2}\wedge\frac{\partial}{\partial y_3} + y_2\frac{\partial}{\partial y_3}\wedge\frac{\partial}{\partial y_1} + y_3\frac{\partial}{\partial y_1}\wedge\frac{\partial}{\partial y_2}\right)$$

It is also possible to construct the Riemann-Jordan tensor in the form:

$$R = \frac{\partial}{\partial y_0}\otimes_s\left(y_1\frac{\partial}{\partial y_1} + y_2\frac{\partial}{\partial y_2} + y_3\frac{\partial}{\partial y_3}\right) + y_0\left(\frac{\partial}{\partial y_0}\otimes\frac{\partial}{\partial y_0} + \frac{\partial}{\partial y_1}\otimes\frac{\partial}{\partial y_1} + \frac{\partial}{\partial y_2}\otimes\frac{\partial}{\partial y_2} + \frac{\partial}{\partial y_3}\otimes\frac{\partial}{\partial y_3}\right)$$

where $\otimes_s$ means the symmetrized tensor product.

In order to characterize the rank of the tensors, we can consider the distributions associated by them to the coordinate functions, i.e., the distributions generated as

$$\mathfrak{h} = \mathrm{span}\left(\Lambda(dy_j)\right) \qquad \mathfrak{r} = \mathrm{span}\left(R(dy_j)\right) \quad j = 0, 1, 2, 3 \tag{41}$$

It is easy to see that the Hamiltonian distribution is generated by

$$H_1 = y_3\frac{\partial}{\partial y_2} - y_2\frac{\partial}{\partial y_3}, \quad H_2 = y_1\frac{\partial}{\partial y_3} - y_3\frac{\partial}{\partial y_1}, \quad H_3 = y_2\frac{\partial}{\partial y_1} - y_1\frac{\partial}{\partial y_2},$$

while the distribution associated with the Riemann-Jordan tensor is

$$X_0 = y^a\frac{\partial}{\partial y^a} + y^0\frac{\partial}{\partial y^0} \quad X_a = y^a\frac{\partial}{\partial y^0} + y^0\frac{\partial}{\partial y^a}$$

It is clear that X_0 is central and $\{X_a\}$ are boosts of a four dimensional Lorentz group, therefore their commutator will provide us with the Lie algebra of the rotation group:

$$[X_a, X_b] = y^a \frac{\partial}{\partial y^b} - y^b \frac{\partial}{\partial y^a}.$$

From the analysis of the dimension of these distributions at each point, we find that:

Lemma 8. *The rank of Λ is zero if $y_1^2 + y_2^2 + y_3^2 = 0$ and the rank is equal to 2 if $y_1^2 + y_2^2 + y_3^2 > 0$.*

The situation is richer with R:

Lemma 9. *The rank of R is*

- *zero if $y_0^2 + y_1^2 + y_2^2 + y_3^2 = 0$*
- *two if $y_0 = 0$ and $y_1^2 + y_2^2 + y_3^2 > 0$.*
- *three for $y_0^2 = y_1^2 + y_2^2 + y_3^2$*
- *four if $y_0^2 \neq y_1^2 + y_2^2 + y_3^2$*

3.2.2 The space of density states in two dimensions

As we have already seen in the previous sections the set of states is identified with a subset of $\mathfrak{u}^*(\mathcal{H})$ satisfying a positivity condition and a normalization condition. In the specific situation we are considering, a generic Hermitian matrix $A = y^0\sigma_0 + y^a\sigma_a$

$$A = \begin{pmatrix} y_0 + y_3 & y_1 - iy_2 \\ y_1 + iy_2 & y_0 - y_3 \end{pmatrix}.$$

We know that A will define a state if and only if

$$\mathrm{Tr}A = 1; \qquad \mu_\pm = y_0 \pm \sqrt{(y_1^2 + y_2^2 + y_3^2)} \geq 0,$$

where $\mu_\pm$ are the two eigenvalues.

Explicitly we have

$$y^0 = \frac{1}{2}, \quad (y_1)^2 + (y_2)^2 + (y_3)^2 \leq \frac{1}{4}.$$

Thus in our parametrization states are determined by points in $\mathbb{R}^4$ on the hyperplane $y^0 = \frac{1}{2}$, and on this three dimensional space are identified by the points in the ball of radius $\frac{1}{2}$. When referring to states we replace A with ρ and write:

$$\rho = \begin{pmatrix} \frac{1}{2} + y_3 & y_2 + iy_1 \\ y_2 - iy_1 & \frac{1}{2} - y_3 \end{pmatrix}. \tag{42}$$

Then,

$$\mathcal{D}(\mathbb{C}^2) = \left\{ \mathfrak{u}(2) \ni \rho = \begin{pmatrix} \frac{1}{2} + y_3 & y_2 + iy_1 \\ y_2 - iy_1 & \frac{1}{2} - y_3 \end{pmatrix} \Big| \ (y_1)^2 + (y_2)^2 + (y_3)^2 \leq \frac{1}{4} \right\} \qquad (43)$$

The pure states corresponding to the vector $(z_1, z_2) \in \mathbb{C}^2$ with unit norm $z_1\bar{z}_1 + z_2\bar{z}_2 = 1$ has a density state

$$\rho = \begin{pmatrix} \bar{z}_1 \\ \bar{z}_2 \end{pmatrix} \otimes (z_1, z_2) = \begin{pmatrix} z_1\bar{z}_1 & \bar{z}_1 z_2 \\ \bar{z}_2 z_1 & z_2\bar{z}_2 \end{pmatrix}.$$

Within the previous parametrization we find

$$y_3 = \frac{1}{2}(z_1\bar{z}_1 - z_2\bar{z}_2), \quad y_1 = \mathrm{Im}(\bar{z}_1 z_2), \quad y_2 = \mathrm{Re}(\bar{z}_1 z_2),$$

and for these points the inequality is saturated thus implying that they lie on the surface of the ball of radius $\frac{1}{2}$. These points on the surface sphere, are in one-to-one correspondence with the unit rays in $\mathbb{C}^2$ and the map is given by the momentum map associated with the symplectic action of $U(2)$ on $\mathcal{P} \sim \mathbb{CP}^1$.

For any generic $\rho \in \mathcal{D}$ there exist pure states ρ_1 and ρ_2 and a positive number $0 \leq \lambda \leq 1$ such that $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$. The decomposition of an arbitrary density state ρ corresponding to some point in the ball, as a convex sum of two pure states

$$\xi_1 = \frac{|\psi_1\rangle\langle\psi_1|}{\langle\psi_1, \psi_1\rangle}$$

and

$$\xi_2 = \frac{|\psi_2\rangle\langle\psi_2|}{\langle\psi_2, \psi_2\rangle},$$

is given geometrically by drawing a straight line through ρ: the states ξ_1 and ξ_2 are the intersections of the line with the sphere. Evidently this decomposition may be done in a two parameter family of ways, filling the disc which has as boundary the yellow circle in Figure 1.

As a subset of $\mathfrak{u}^*(2)$, the ball of the density states is foliated by symplectic leaves associated with the coadjoint action of $U(2)$, which coincide also with the orbits of the $SU(2)$ group. As we know that the rank of the matrices will be preserved, the analysis of these orbits may also be done by considering the orbits passing through diagonal matrices, in other terms

$$\rho = S \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} S^\dagger \quad a + b = 1 \quad a \geq 0, \quad b \geq 0 \qquad S \in SU(2).$$

We should keep in mind that these orbits will also correspond to the corresponding dynamical evolution for unitary dynamics, and therefore is physically meaningful.

We visualize the situation with the help of Figure 2. The red segment connecting $(\frac{1}{2}, \frac{1}{2})$ with $(1, 0)$ (or equivalently the dashed green one, connecting with $(0, 1)$) parametrizes the

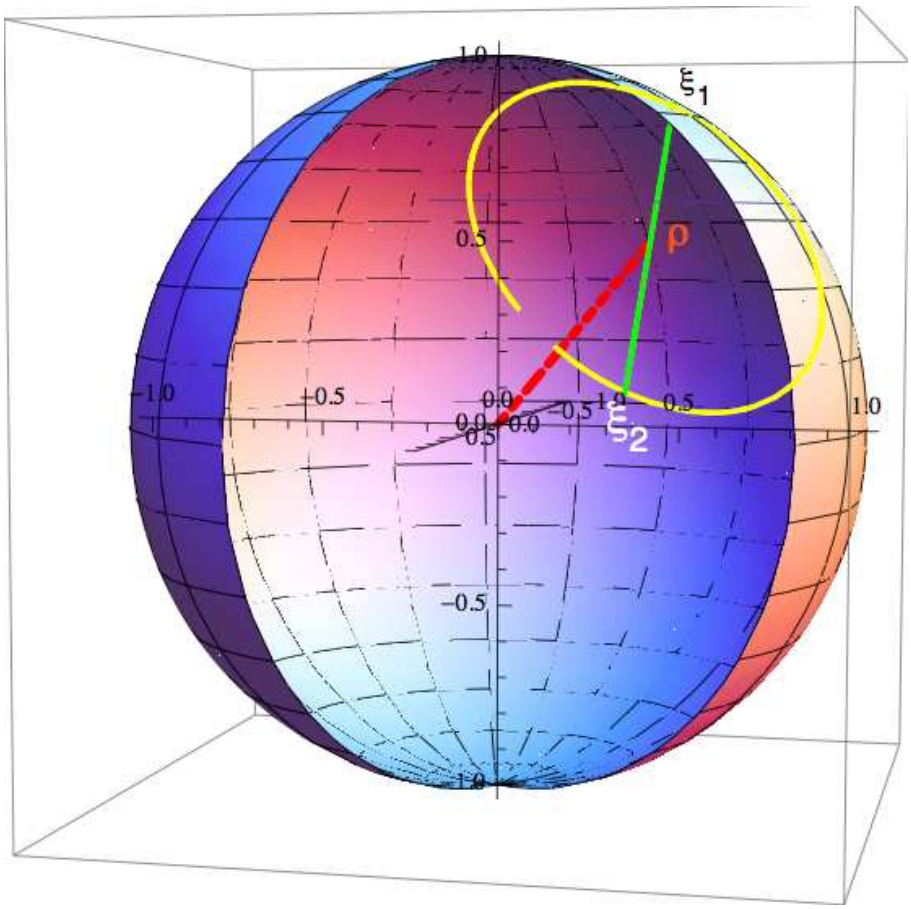


Figure 1.— Bloch sphere and state ρ corresponding to the point $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. This state can be written as the sum of the two extremal states in infinitely many ways, each one corresponding to the diameters of the yellow circle. The diameter corresponding to the pair of states ξ_1 and ξ_2 is depicted in green.

family of two dimensional spheres. The point $(\frac{1}{2}, \frac{1}{2})$ coincides with the center of the Bloch sphere (Figure 1) and represents the maximally mixed state and $(1, 0)$ (or $(0, 1)$) belongs to the outmost sphere of pure states.

3.3 Example: States of a three level system

Now $\mathcal{H} = \mathbb{C}^3$. The states are normalized positive 3×3 matrices inside $\mathfrak{u}^*(3)$. We first consider the geometrical tensors defined by means of the momentum map construction.

3.3.1 The choice of the basis

We choose a basis for $\mathfrak{u}(3)$ given by the Gell-Mann matrices

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

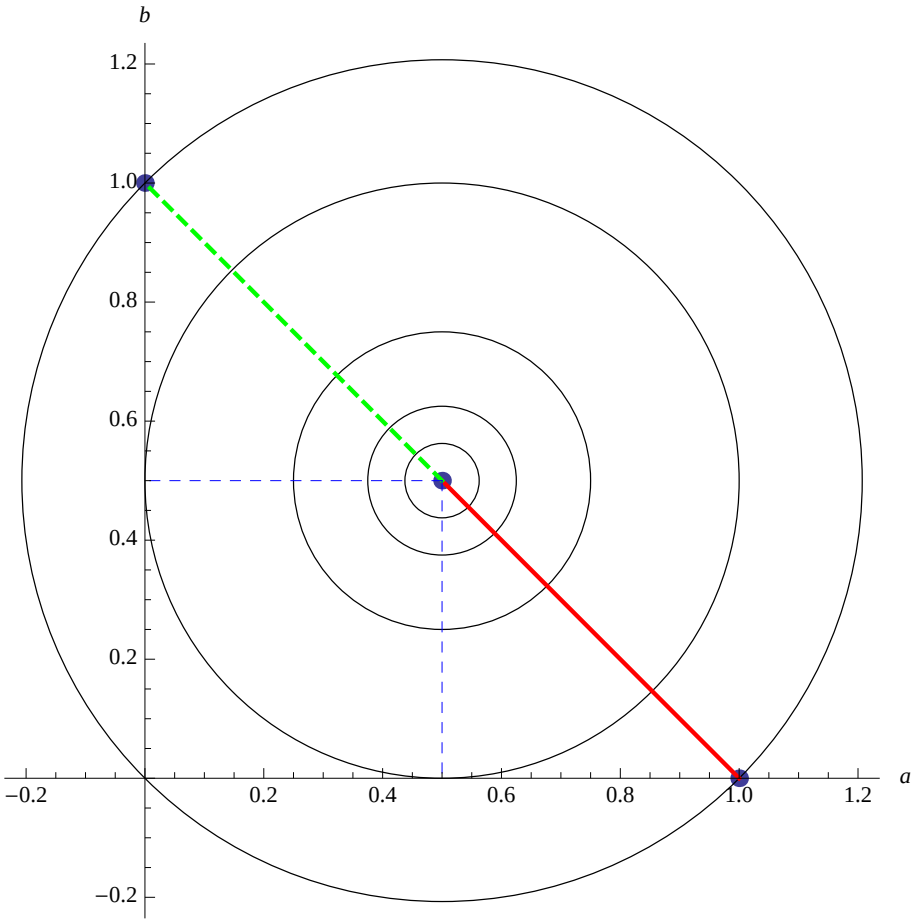


Figure 2.— Set of orbits of the group $SU(2)$ acting on the (a, b) plane

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \quad \lambda_0 = \sqrt{\frac{2}{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

These matrices satisfy the scalar product relation

$$\mathrm{Tr}\lambda_\mu \lambda_\nu = 2\delta_{\mu\nu}.$$

Their commutation and anti-commutation relations are written in terms of the anti-symmetric structure constants and symmetric d–symbols $d_{\mu\nu\rho}$. We find

$$[\lambda_\mu, \lambda_\nu] = 2iC_{\mu\nu\rho}\lambda_\rho \quad [\lambda_\mu, \lambda_\rho]_+ = 2\sqrt{\frac{2}{3}}\lambda_0\delta_{\mu\nu} + 2d_{\mu\nu\rho}\lambda_\rho.$$

The numerical values turn out to be

$$C_{123} = 1, \qquad C_{458} = C_{678} = \frac{\sqrt{3}}{2}, \quad C_{147} = -C_{156} = C_{246} = C_{257} = C_{345} = -C_{367} = \frac{1}{2}$$

The values of these symbols show the different embeddings of $SU(2)$ into $SU(3) \subset U(3)$. For the other coefficients we have

$$d_{jj0} = -d_{0jj} = -d_{j0j} = \sqrt{\frac{2}{3}} \quad j = 1, \cdots, 8$$

$$-d_{888} = d_{8jj} = d_{jj8} = d_{j8j} = \frac{1}{\sqrt{3}} \quad j = 1, 2, 3$$

$$d_{8jj} = d_{jj8} = d_{j8j} = -\frac{1}{2\sqrt{3}} \quad j = 4, 5, 6, 7$$

$$d_{3jj} = d_{jj3} = d_{j3j} = \frac{1}{2} \quad j = 4, 5 \qquad d_{3jj} = d_{jj3} = d_{j3j} = -\frac{1}{2} \quad j = 6, 7$$

$$d_{146} = d_{157} = d_{164} = d_{175} = -d_{247} = d_{256} = d_{265} = -d_{274} = \frac{1}{2}$$

$$d_{416} = -d_{427} = d_{461} = -d_{472} = d_{517} = d_{526} = d_{562} = d_{571} = \frac{1}{2}$$

$$d_{614} = d_{625} = d_{641} = d_{652} = d_{715} = -d_{724} = d_{751} = -d_{742} = \frac{1}{2}$$

3.3.2 The tensors

The scalar product induced on vectors on $\mathbb{R}^8$ will be invariant under the action of $SO(8)$. It is now possible to write the Poisson tensor

$$\Lambda = 2C_{\mu\nu\rho} y^\rho \frac{\partial}{\partial y^\mu} \wedge \frac{\partial}{\partial y^\nu}$$

and the Riemann-Jordan tensor

$$R = \frac{\partial}{\partial y^0} \otimes_s y^\mu \frac{\partial}{\partial y^\mu} + y^0 \frac{\partial}{\partial y^r} \otimes \frac{\partial}{\partial y^r} + d_{\mu\nu\rho} y^\mu \frac{\partial}{\partial y^\nu} \otimes_s \frac{\partial}{\partial y^\rho}.$$

Now the analysis of the various distributions is more cumbersome, however it is easy to identify a few elements:

$$R(dy^0) = y^\mu \frac{\partial}{\partial y^\mu},$$

which is the dilation vector field on $\mathbb{R}^9$; while $R(dy^r) = y^r \frac{\partial}{\partial y^0} + y^0 \frac{\partial}{\partial y^r} + d_{\mu\nu r} y^\mu \frac{\partial}{\partial y^\nu}$, where it is possible to identify a boost structure plus a correction due to the d–symbols. In any case the union of the Hamiltonian distribution and the Riemannian-Jordan distribution generates $\mathrm{GL}(3, \mathbb{C})$.

3.3.3 Describing the density matrices

The indices appearing in the non-null structure constants are identifying the corresponding λ–matrices whose pairwise commutators define $SU(2)$–subgroups. It is now possible to introduce coordinate functions

$$y^\mu(A) = \frac{1}{2} \mathrm{Tr} \lambda_\mu A.$$

In these coordinates, a generic Hermitian matrix A can be written as

$$A = y^0\lambda_0 + y^r\lambda_r$$

The trace condition

$$\mathrm{Tr}\rho = 1 \Leftrightarrow y_0 = \frac{1}{\sqrt{6}}$$

allows to identify this subset as a subset of the vector space of $\mathbb{R}^8$ corresponding to the dual space of the Lie algebra of $SU(3)$. To identify the set of density matrices, we can consider those points satisfying

$$\mathrm{Tr}\rho^2 \leq \mathrm{Tr}\rho = 1.$$

If we write the states in terms of the λ–matrices, we have

$$\rho = \frac{1}{3}\mathbb{I}_3 + \sum_{j=1}^{8} y_j\lambda_j,$$

with

$$\sum_{j=1}^{8} y_j^2 \leq \frac{1}{2}$$

Extremal states (pure states) are in one-to-one correspondence with the minimal symplectic orbit of the unitary group according to the coadjoint action and corresponds to $\mathbb{CP}^2$, the complex projective space of $\mathbb{C}^3$. They are defined from vectors $(z_1, z_2, z_3) \in \mathbb{C}^3$ with the normalization condition $z_1\bar{z}_1 + z_2\bar{z}_2 + z_3\bar{z}_3 = 1$ as

$$\begin{pmatrix} z_1\bar{z}_1 & \bar{z}_1 z_2 & \bar{z}_1 z_3 \\ \bar{z}_2 z_1 & z_2\bar{z}_2 & \bar{z}_2 z_3 \\ \bar{z}_3 z_1 & z_3\bar{z}_2 & \bar{z}_3 z_3 \end{pmatrix}$$

Previous inequalities are saturated by these matrices.

Under conjugation with $S \in SU(3)$, any matrix A can be written as

$$A = S \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} S^\dagger \quad a \geq 0, b \geq 0, c \geq 0, \;\; a+b+c = 1, \quad s \in SU(3).$$

By using this "radial-angular" parametrization of states, we may study the structure of this union of symplectic orbits by considering the family of diagonal matrices with the positivity condition (elements of a positive Weyl chamber in the Abelian Cartan subalgebra). The hyperplane $\mathrm{Tr}\rho = 1$ identifies a triangle (the blue one in Figure 3) with the intersection with positive axes (Oa, Ob, Oc); i.e. in the positive octant.

Each internal point of the triangle corresponds to a 6–dimensional symplectic orbit, out of which we may consider convex combinations, excepting the vertices of the triangle where

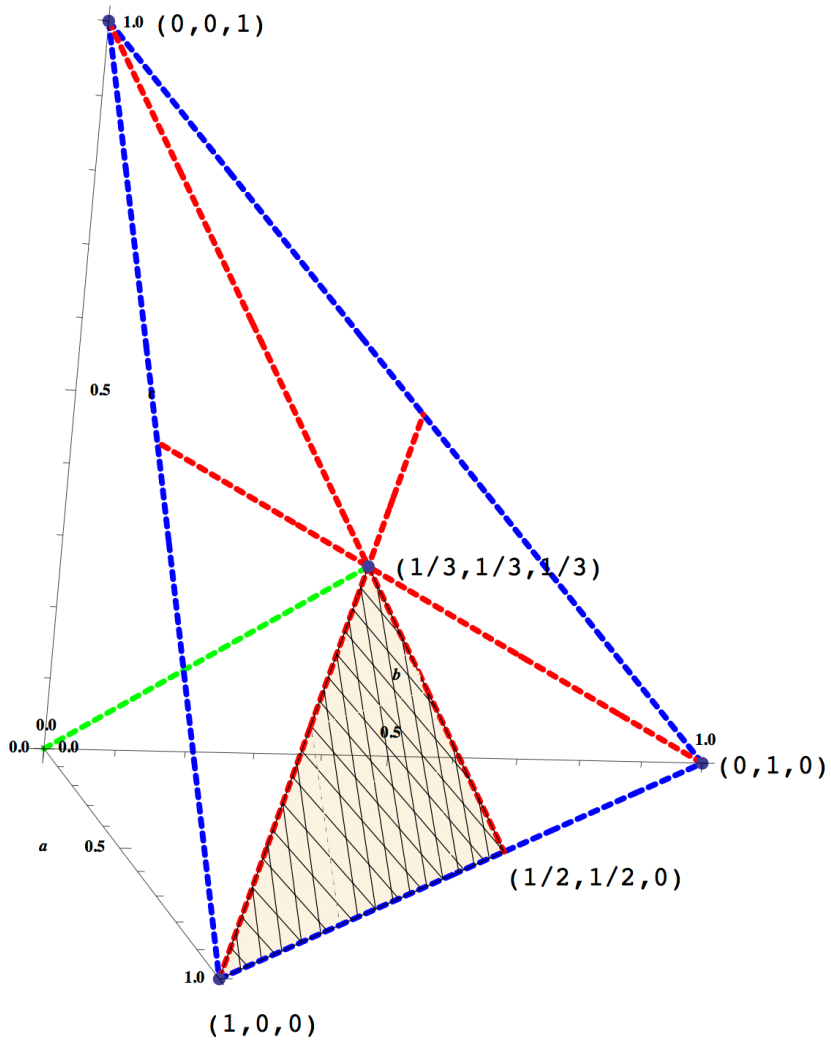


Figure 3.— Representaton of the orbits of $SU(3)$ on the simplex of diagonal density matrices in three dimensions

it is 4–dimensional. Due to the action of $SU(3)$ containing the action of the discrete Weyl group, the symplectic orbits are actually parametrized by the smaller triangle (colored in Figure 3). When $a = b = c = \frac{1}{3}$ we have the "maximally mixed state" which play a crucial role when we consider composite systems and entangled states (the orbit passing through this point degenerates to a zero dimensional orbit). On the boundary of the blue triangle the rank of ρ is either 1 (in the vertex, which represent the pure states) or 2 (on the segment, which represent the mixtures of two of the three levels). For a generic point, the orbits are diffeomorphic to $SU(3)/U(1) \times U(1)$. It appears quite clearly that the set of states is a stratified manifold characterized by the rank of the state.

4 Application I: Describing entanglement

4.1 Generalities

Entanglement is a property of composite physical systems which plays a very important role in many different phenomena, but in particular, it has become a crucial issue of quantum computation and quantum information theory. Despite the growing interest in recent years, it was already discussed by Schrödinger and the "founding fathers" of quantum theory in the early years (see [44, 45]).

Roughly speaking, entanglement is the concept dual to separability.

Definition 7. *Let $|\psi\rangle$ be state of a Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ of a bipartite system. Then, $|\psi\rangle$ is said to be* **separable** *if there exists a pair of states $|\psi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle \in \mathcal{H}_2$ satisfying that $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$. A system which is not separable, it is said to be* ***entangled****.*

But entanglement exhibits many interesting properties, for instance the fact that there is a gradation in the level of entanglement of the different states. Thus we can measure the entanglement of a state by using physical magnitudes. These different observables are called **entanglement witnesses**.

It is known that the set of pure states is completely clasified, from the point of view of entanglement, with just one observable. The usual choices are the **concurrence** of the state, the **von Neumann entropy** of one of its partial traces (i.e. the entropy of the density state $\rho_1 = \mathrm{Tr}_2\rho_\psi$ or of $\rho_2 = \mathrm{Tr}_1\rho_\psi$, where $\rho_\psi = |\psi\rangle\langle\psi|$).

Definition 8. *The concurrence of a density matrix $\rho \in \mathcal{D}(\mathcal{H})$ is defined as*

$$C(\rho) = \max(0, 2\lambda_{max}(\hat{\rho}) - \mathrm{Tr}(\hat{\rho}))$$

where $\hat{\rho}$ corresponds to

$$\hat{\rho} = \sqrt{(\sigma_2 \otimes \sigma_2)\rho^*(\sigma_2 \otimes \sigma_2)\rho}$$

and $\lambda_{max}(\hat{\rho})$ stands for its largest eigenvalue.

Definition 9. *The von Neumann entropy of a density matrix $\rho \in \mathcal{D}(\mathcal{H})$ is defined as*

$$S(\rho) = \mathrm{Tr}\rho\log(\rho). \tag{44}$$

When the density matrix corresponds to a pure state the function above vanishes. Thus we define the corresponding entropy as the value of the function on the partial trace over one of the subsystems:

$$S(\rho_\psi) = \mathrm{Tr}\rho_1\log(\rho_1) \qquad \rho_1 = \mathrm{Tr}_1\rho_\psi \tag{45}$$

If the state ρ_ψ is separable and we can find $\rho_{\psi_a} \in \mathcal{D}^1(\mathcal{H}_1)$ and $\rho_{\psi_b} \in \mathcal{D}^1(\mathcal{H}_2)$ such that

$$\rho_\psi = \rho_{\psi_a} \otimes \rho_{\psi_b};$$

the corresponding partial traces satisfy:

$$\begin{cases} \rho_1 = \rho_{\psi_a} \Rightarrow S(\rho_1) = S(\rho_{\psi_a}) = 0 \\ \rho_2 = \rho_{\psi_b} \Rightarrow S(\rho_2) = S(\rho_{\psi_b}) = 0 \end{cases},$$

because both partial states are pure. If the state ρ is entangled, though, the partial trace yields a density state for the subsystem which is a mixed state. Therefore, the corresponding von Neumann entropy is different from zero. But it is simple to verify that, in the case of pure states, both functions provide the same information, since they are functionally dependent.

Analogously, we can define a simpler operator containing similar information:

Definition 10. *The linear entropy of a density matrix $\rho \in \mathcal{D}(\mathcal{H})$ is defined as*

$$S_L(\rho) = \frac{4}{3}\left(1 - \mathrm{Tr}\rho^2\right). \tag{46}$$

4.2 Entanglement of pure states

For pure states, the three functions provide the same information, as we can simply verify in a simple case:

Example 1. *Let us consider a simple example. Assume $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ and consider a family of pure states in the form:*

$$|\psi\rangle = \cos(\alpha)\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} + \sin(\alpha)\begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} \tag{47}$$

We can evaluate the concurrence for this state and obtain:

$$C(|\psi\rangle) = \sin(2\alpha).$$

On the other hand, we can construct the density state associated to $|\psi\rangle$ and evaluate the corresponding partial trace:

$$\rho_\psi = |\psi\rangle\langle\psi| = \begin{pmatrix} \cos^2\alpha & 0 & 0 & \cos\alpha\sin\alpha \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \cos\alpha\sin\alpha & 0 & 0 & \sin^2\alpha \end{pmatrix} \Rightarrow \rho_1 = \mathrm{Tr}_2\rho_\psi = \begin{pmatrix} \cos^2\alpha & 0 \\ 0 & \sin^2\alpha \end{pmatrix}.$$

Thus, the corresponding von Neumann entropy reads:

$$S(\rho_1) = \cos^2\alpha\log(\cos^2\alpha) + \sin^2\alpha + \log(\sin^2\alpha) \tag{48}$$

But it is simple to verify that both quantities are functionally dependent, since a direct representation as that of Figure 4 of the three functions prove that, excepting the normalization, both entropy functions and the square of the concurrence behave exactly in the same way.

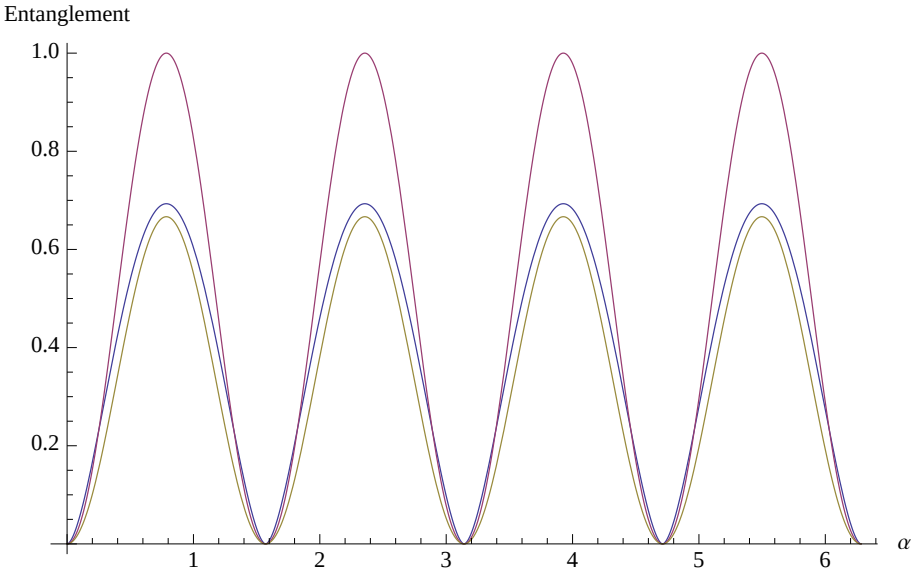


Figure 4.— Representation of the square of the concurrence, the linear entropy and the von Neumann entropy for a pure state

The reason for this is the following result:

Theorem 6. *Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ of dimensions $n_1 \leq n_2$. Given any state $|\psi\rangle \in \mathcal{H}$, there exists orthonormal sets $\{|v_j\rangle\}$ for $\mathcal{H}_1$ and a basis $\{|w_k\rangle\}$ for $\mathcal{H}_2$ such that*

$$|\psi\rangle = \sum_{j=1}^{n_1} \alpha_j |v_j\rangle \otimes |w_j\rangle \qquad \alpha_j > 0. \tag{49}$$

*This is the **Schmidt decomposition of the pure state** $|\psi\rangle$. The number of non-vanishing coefficients in the decomposition is called the **Schmidt rank**.*

Therefore, it is trivial to prove from here that the Schmidt coefficient encodes completely the degree of entanglement of pure states:

Theorem 7. *A pure state $|\psi\rangle \in \mathcal{H}$ is separable if and only if its Schmidt rank is equal to one.*

Thus, we can easily understand the system of the previous example, since the family of states defined in Equation (47) has Schmidt rank equal to 2.

4.3 Entanglement of mixed states

On the other hand, if we consider the case of mixed states, the situation is not that simple. In general, it is necessary to consider more than one entanglement witness in order to completely characterize the state of the system. One interesting question arises thus: how can we characterize the independence of the different observables we use?

In the framework of classical mechanics this question is simple to answer. Given two physical magnitudes, which are represented by two functions f_1, f_2 on phase-space, they are said to be independent at a point $p \in M$ if their exterior differentials satisfy

$$(df_1 \wedge df_2)(p) \neq 0$$

The usual approach to Quantum Mechanics, in terms of Hilbert spaces or $\mathbb{C}^*$–algebras does not allow a similar treatment of the analogous quantum problem. We lack of a noncommutative differential calculus allowing to define a "noncommutative" exterior differential translating the previous definition to the quantum setting.

But the geometrical formalism we introduced in the previous sections allows us to look at the problem from a different perspective. Treating the quantum state space as a real differential manifold, we do have a differential calculus at our disposal: the usual differential calculus of real manifolds.

Consider the Hilbert space $\mathcal{H}$ and an operator A. We know that we can associate with A the quadratic function

$$A \to f_A(\psi) = \frac{1}{2}\langle\psi|A|\psi\rangle \qquad \psi \in \mathcal{H}.$$

In the geometric description of Quantum Mechanics we read from the set of quadratic functions the algebraic structures the set of operators is endowed with:

- the associative product of operators is translated into the nonlocal product $\star$,
- the Lie algebra defined by the commutator is translated into the Poisson algebra defined by the tensor Λ
- the Jordan algebra given by the anticommutator is translated into the Jordan algebra defined by the tensor G

But the geometric description also includes a pointwise algebra $(f_A.f_B)(\psi) = f_A(\psi)f_B(\psi)$, which is commutative, and whose differential calculus is the standard one. This is the algebraic structure with respect to which we define the differential algebra we are interested in:

Definition 11. *Two observables A and B are said to be* **independent** *if their associated functions satisfy*

$$df_A \wedge df_B \neq 0 \text{ on a dense submanifold of } \mathcal{H}$$

Example 2. *Now we will test this formalism with a particular example. Consider for instance the family of density states defined by the matrices:*

$$\rho_t = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & a & \frac{1}{2}ce^{i\phi}, 0 & \\ 0 & \frac{1}{2}ce^{-i\phi} & b & 0 \\ 0 & 0 & 0 & 1-a-b \end{pmatrix}$$

Such a matrix represents a density state provided that

$$0 \leq a+b \leq 1 \quad 0 \leq c \leq 1 \quad 4ab \geq c$$

This is clearly a 4–dimensional submanifold $\mathcal{S}$ of $\mathcal{D}(\mathbb{C}^4)$ and therefore much simpler to handle than the full space. We can take an adapted basis for it, considering the matrices

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

We can use the four real numbers $\{a, b, c, \phi\}$ as adapted coordinates on that submanifold.

Now we can evaluate the three functions above on these states. As we already know the expression of the Jordan and the Poisson bracket we can also obtain the corresponding Hamiltonian and gradient vector fields. And besides, we can also study the independence of the functions by evaluating the expressions of

$$dS \wedge dC \quad dS_L \wedge dC,$$

where d represents the exterior differential of the differentiable structure defined on $\mathfrak{u}^*(\mathcal{H})$.

Let us thus proceed:

- *The value of the different functions is easy to obtain. We have*

  Von neumann entropy reads,

$$\begin{aligned} 2S(\rho_t) = &-2(-1+a+b)\log[1-a-b]+ \\ &\left(a+b-\sqrt{(a-b)^2+c^2}\right)\log\left[\frac{1}{2}\left(a+b-\sqrt{(a-b)^2+c^2}\right)\right]+ \\ &\left(a+b+\sqrt{(a-b)^2+c^2}\right)\log\left[\frac{1}{2}\left(a+b+\sqrt{(a-b)^2+c^2}\right)\right]. \end{aligned}$$

  The linear entropy S_L corresponds to

$$S_L(\rho_t) = -\frac{2}{3}\left(4\left(a^2+a(-1+b)+(-1+b)b\right)+c^2\right) \tag{50}$$

  Finally, the value of the concurrence is very simple:

$$C(\rho_t) = c \tag{51}$$

- *We can study now the Poisson brackets corresponding to them. It is simple to prove that all three functions commute, i.e.*

$$\{S, S_L\} = \{S, C\} = \{S_L, C\} = 0 \tag{52}$$

This implies that the local transformations generated by them are independent.

- *Finally, we can study the independence of the different functions. This is an important issue, in particular the independence of the von Neumann entropy and the concurrence, because it affects the description of entanglement of general quantum density states. We can prove the following:*

Lemma 10. *The concurrence and the von Neumann entropy of the family of states ρ_t are not indepent in all the space of density states but are independent as observables.*

Proof. We are considering the submanifold of $\mathfrak{u}(\mathcal{H})$ corresponding to the family of density states ρ_t. On this set, the differential of the concurrence is trivial to obtain:

$$dC(\rho_t) = dc. \tag{53}$$

The computation of the differential of the von Neumann entropy is quite more involved. It is evident from the expression above that the functions $\mathcal{S}$ depends on the three variables. But as C depends only on c, we have to consider only the a and b dependence in what regards the computation of $dS \wedge dC$. We compute thus $\frac{\partial S}{\partial a}$ and $\frac{\partial S}{\partial b}$. Now, the condition for (53) to be equal to zero corresponds to

$$\frac{\partial S}{\partial a} = 0 = \frac{\partial S}{\partial b}$$

And these conditions become

$$2\mathrm{Log}[1 - a - b] + \mathrm{Log}\left[ab - \frac{c^2}{4}\right] = 0$$

These equations have a solution on

$$\frac{1}{3} < a < \frac{1}{2}; \qquad b = a; \qquad c = \sqrt{-1 + 4a - 3a^2}$$

Figure 5 presents these functions and the subset where they functionally dependent.

Thus we conclude that there is a nonempty subset of $\mathfrak{u}^*(4)$ where the von Neumann entropy functions and the concurrence function introduced above are not independent. On any point outside this submanifold the two functions are indeed independent, as it can be verified easily from the different behavior in different regions. As the submanifold where the functions are functionally-dependent is clearly not dense in M_Q, we can conclude that the two entanglement witnesses S and C are indeed independent. □

The main advantage of this approach is that, as the dimensions are finite, it is simple to identify what is the number of functions (or observables) which are necessary to unambiguously describe the entanglement of the of density states.

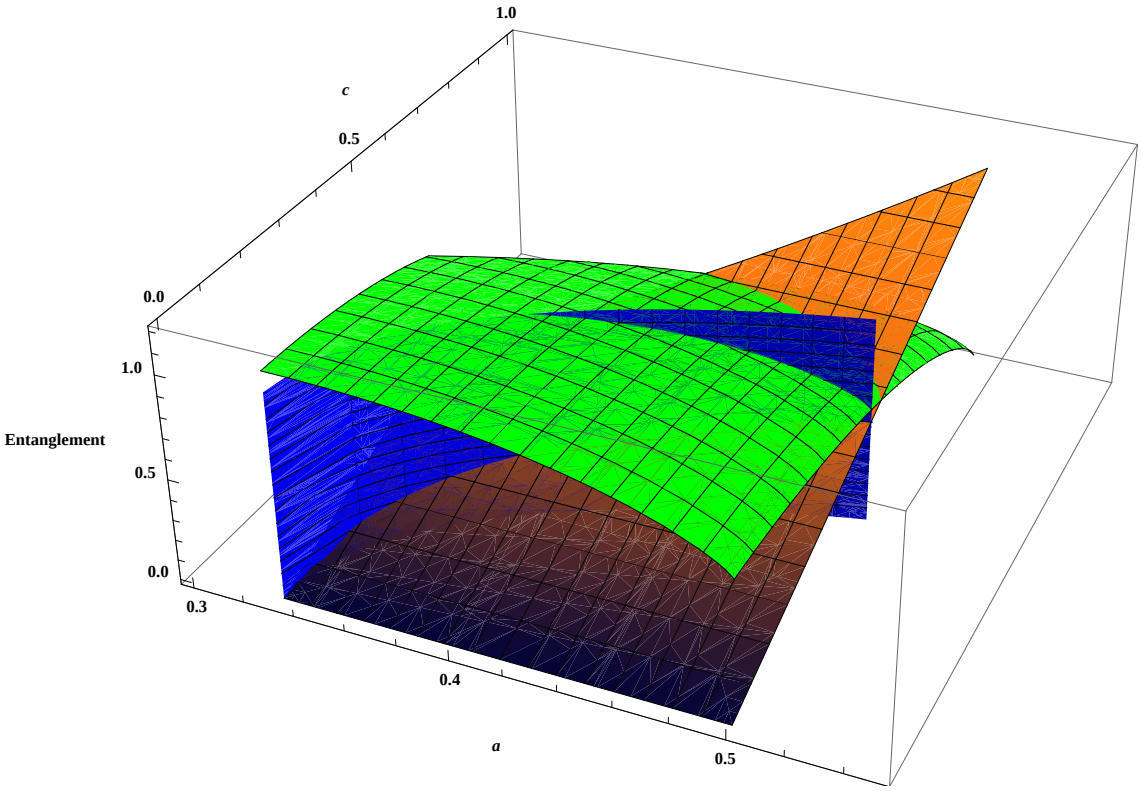


Figure 5.— Representations of the concurrence (in brown) and the von Neumann entropy (in green) in the space parametrized by (a, a, c). In blue, we show the line corresponding to the submanifold where both functions are functionally dependent even if they take different values

5 Application II: Ehrenfest dynamics as a Hamiltonian system

The goal of this section is to summarize some of the results which have been presented in [2, 4] concerning the mathematical description of Mixed Quantum Classical Dynamical (MQCD) systems. We will see how we can combine quantum and classical models by using the tensorial objects we have introduced in the first sections. The combination is possible because, from a formal point of view, those objects are completely analogous to those used in the geometrical description of classical mechanical systems.

5.1 Symplectic description of Classical Mechanics

Let us begin by recalling very quickly the Hamiltonian formulation of classical dynamics. We address the interested reader to a classical reference as [1] for a more detailed presentation.

Let us consider a classical system with phase space M_C. For the sake of simplicity, let us assume that this set is endowed with a vector space structure, i.e., $M_C \sim \mathbb{R}^{2n}$ for n the number of degrees of freedom of the system. In that manifold, there are two types of degrees of freedom: the states of the physical variables describing the position of the system (by "position" we mean any relevant degree of freedom one should consider), and their corresponding momenta. We will use $(\vec{R}, \vec{P})$ as notation to represent these variables.

In what regards the observables, Classical Mechanics uses the set of differentiable functions

$$f : M_C \to \mathbb{R}, \tag{54}$$

assigning the result of the measurement to every point in M_C.

On the set of functions $C^\infty(M_C)$ we introduce an operation, known as Poisson bracket, which allows us to study the effect of symmetry transformations and also the dynamical evolution. The precise definition is as follows:

Definition 12. *A **Poisson bracket**, $\{\cdot,\cdot\}$, is a bilinear operation*

$$\{\cdot,\cdot\} : C^\infty(M_C) \times C^\infty(M_C) \to C^\infty(M_C), \tag{55}$$

which:

- *It is antisymmetric,*

$$\{f, g\} = -\{g, f\}, \qquad \forall f, g \in C^\infty(M_C).$$

- *It satisfies the Jacobi identity, i.e. $\forall f, g, h \in C^\infty(M_C)$:*

$$\{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g, \{h, f\}\} = 0.$$

- *It satisfies the Leibniz rule i.e. $\forall f, g, h \in C^\infty(M_C)$:*

$$\{f, gh\} = \{f, g\}h + g\{f, h\}.$$

A Poisson bracket allows us to introduce the concept of Hamiltonian vector field:

Definition 13. *Given a function $f \in C^\infty(M_C)$ and a Poisson bracket $\{\cdot,\cdot\}$, a vector field, X_f is said to be its **Hamiltonian vector field** if*

$$X_f(g) = \{f, g\}, \qquad \forall g \in C^\infty(M_C).$$

The concept can also be given a tensorial flavor by using a tensor Π, which allows us to define

$$\Pi(df, dg) = \{f, g\} \qquad \forall f, g \in C^\infty(M_C). \tag{56}$$

See [1] for the expression of the conditions to be satisfied by the 2-vector Π.

Example 3. *Let $M_C = \mathbb{R}^2$ with coordinates (R, P). We consider as Poisson bracket*

$$\{f_1, f_2\} = \frac{\partial f_1}{\partial P}\frac{\partial f_2}{\partial R} - \frac{\partial f_1}{\partial R}\frac{\partial f_2}{\partial P}.$$

Then, given $f \in C^\infty(\mathbb{R}^2)$, we can write the corresponding Hamiltonian vector field X_f as

$$X_f = \frac{\partial f(R,P)}{\partial P}\frac{\partial}{\partial R} - \frac{\partial f(R,P)}{\partial R}\frac{\partial}{\partial P}.$$

The geometric formulation of Hamiltonian Mechanics is very often defined on Poisson manifolds, i.e. manifolds endowed with a Poisson bracket on the corresponding space of functions. We will call a **Hamiltonian system** to a triple $(M_C, \{\cdot,\cdot\}, H)$, where $\{\cdot,\cdot\}$ is a Poisson structure on M_C, and dynamics is introduced via the function $H \in C^\infty(M_C)$, that we call the Hamiltonian. One can consider two different formulations of the dynamics:

- One which defines the corresponding Hamiltonian vector field X_H obtained as above

  $$X_H(g) = \{H, g\}, \qquad \forall g \in C^\infty(M_C).$$

  The integral curves of the vector field X_H define the solution of the dynamics.

- An analogous formulation can be given in terms of the observables. If we consider now the set of functions of the system, i.e. the set of classical observables which contains, as elements, the functions 'position' and 'momenta' of each particle (i.e. $\vec{R}$ and $\vec{P}$), dynamics is written as the Poisson bracket of the Hamiltonian function H with any other function of the system, i.e.

  $$\frac{df}{dt} = \{H, f\}, \qquad \forall f \in C^\infty(M_C). \tag{57}$$

Both approaches are equivalent.

5.2 The set of states of our system

Let us now proceed to combine the geometrical description of Classical Mechanics and Quantum Mechanics. It is immediate to realize that, from a dynamical point of view, both approaches are closely related. Indeed, in both cases there is an intrinsic Poisson structure which allows us to interpret the solutions of the dynamics as the integral curves of Hamiltonian vector fields.

Besides, we know that if we have two classical particles, defined on symplectic manifolds (M_1, ω_1) and (M_2, ω_2), the dynamical description of the system of the two particles is achieved on the manifold $M_1 \times M_2$, with a symplectic structure which is obtained as the sum of both, i.e.,

$$\omega_{12} = \pi_1^*\omega_1 + \pi_2^*\omega_2,$$

where $\pi_1 : M_1 \times M_2 \to M_1$ and $\pi_2 : M_1 \times M_2 \to M_2$ are the canonical projections.

Our goal now is to provide a geometrical framework to represent Ehrenfest equations of a molecular system. Ehrenfest equations represent an approximation for the description of an atomic or molecular system where:

- the nuclei and the inner electrons, are represented as classical systems, called **cores**, coupled to
- the outer electrons which are considered to behave as quantum systems.

The approximation makes sense when the evolution of the degrees of freedom which are assumed to be classical is much slower than the quantum evolution. This implies that we are implicitly assuming that we can disregard the entanglement between the classical and the quantum degrees of freedom. But this fact implies that the complete set of states will be just the cartesian product of the sets of states of the classical and the quantum parts.

Thus, the set of states of the complete system contains:

- First, a Hilbert space $\mathcal{H}$ which contains the states of the set of objects of our system which are described quantum-mechanically. It is the vector space corresponding to the completely antisymmetric representation of the permutation group S_N (i.e. a set of Slater determinants), where N is the number of electrons of the system and each electron lives in a Hilbert space of dimension M. Thus, the dimension of $\mathcal{H}$ will be $N_Q = \binom{M}{N}$. We know that it is a complex vector space, but we choose to consider it as a real vector space with the double of degrees of freedom and denote it as M_Q. Also, in correspondence with the Hilbert space vectors in the usual formalism of quantum mechanics, several states in M_Q represent the same physical state. To consider true physical states one should extract only those corresponding to the projective space, which can be identified with a submanifold of M_Q. A more general approach is to consider the sphere of states with norm equal to one, S_Q, and take into account the phase transformations generated by Eq (4) in a proper way. We will discuss this in the following sections.

- Second, a differentiable manifold M_C (for simplicity we can just consider it to be a vector space), which contains the classical degrees of freedom. We will assume it to be a phase space, and thus it will have an even number of degrees of freedom and it will be endowed with a canonical symplectic structure. Therefore we can also consider a Poisson structure on the set of functions of the manifold M_C.

- Third, we let our state space S be the Cartesian product of both manifolds,

$$\mathcal{S} = M_C \times M_Q.$$

Such a description has important implications: it is possible to consider each subsystem separately in a proper way but it is not possible to entangle the subsystems one with the other. As long as Ehrenfest dynamics disregards this possibility, the choice of the Cartesian product is the most natural one.

Example 4. *If we consider a simple case, where we have one nucleus moving in a three dimensional domain and the electron state is considered to belong to a two-level system, the situation would be:*

$$\Psi = (\vec{R}, \vec{P}, q^1, q^2, p_1, p_2), \qquad (q^1, q^2, p_1, p_2) \in \mathbb{R}^4,$$

where $\vec{R}$ represents the position of the nucleus, and $\vec{P}$ represents its linear momentum. The tetrad (q^1, q^2, p_1, p_2) represents the set of four real coordinates which correspond to the representation of the state of the two-level system on a real vector space (of four 'real' dimensions which corresponds to a two 'complex'-dimensional vector space).

As a conclusion from the example above, we use as coordinates for our states:

- The positions and momenta of the nuclei and electrons of the cores:

$$(\vec{R}, \vec{P}) \in M_C. \tag{58}$$

  We will have $3N_C + 3N_C$ of these, for N_C the number of classical particles of the system.

- The real and imaginary parts of the coordinates of the Hilbert space elements with respect to some basis:

$$(\vec{q}, \vec{p}) \in M_Q. \tag{59}$$

  We will have $N_Q + N_Q$ of these, for N_Q the complex dimension of the Hilbert space $\mathcal{H}$.

5.3 The observables

To represent the physical magnitudes we must consider also the classical-quantum observables from a new perspective. Our observables must be functions defined on the state space $S = M_C \times M_Q$. We can consider also the projections:

$$\pi_C : M_C \times M_Q \to M_C, \quad \pi_C(\vec{R}, \vec{P}, \vec{q}, \vec{p}) = (\vec{R}, \vec{P}) \tag{60}$$

and

$$\pi_Q : M_C \times M_Q \to M_Q, \quad \pi_Q(\vec{R}, \vec{P}, \vec{q}, \vec{p}) = (\vec{q}, \vec{p}). \tag{61}$$

We know from our discussion in the case of a purely quantum system that any function of the form (38) produces an evolution, via the Poisson bracket, which preserves the norm. In the MQCD case, we can easily write the analogue of the vector field (4) by writting:

$$\Gamma_Q = \mathbb{I} \otimes \Gamma. \tag{62}$$

It is simple to see that this object is completely determined by the pullback of the projections π_C and π_Q:

$$\pi_{C*}\Gamma_Q = 0, \qquad \pi_{Q*}\Gamma_Q = \Gamma.$$

This is again the infinitesimal generator of phase transformations for the quantum subsystem, but written at the level of the global state space $M_C \times M_Q$. A reasonable property to be asked to the functions chosen to represent our observables is to be constant under this transformation. From a mathematical point of view we can write such a condition as follows:

Definition 14. *We will define the set of possible physical observables, $\mathcal{O}$, as the set of all C^∞–functions on the set $M_C \times M_Q$ which are constant under phase changes on the quantum degrees i.e.*

$$\mathcal{O} = \{f \in C^\infty(M_C \times M_Q) |\ \Gamma_Q f = 0\}. \tag{63}$$

As we will see later, this choice reflects the fact that, when considered coupled together, the nonlinearity of Classical Mechanics expands also to MQCD.

We would like to remark that because of the choice of the set of states as a Cartesian product of the classical states and the quantum states, we can consider as subsets of the set of observables:

- The set of classical functions: these are functions which depend only on the classical degrees of freedom. Mathematically, they can be written as those functions $f \in \mathcal{O}$ such that there exists a function $f_C \in C^\infty(M_C)$ such that

  $$f = \pi_C^*(f_C);\ \text{i.e. } f(\vec{R}, \vec{P}, \vec{q}, \vec{p}) = f_C(\vec{R}, \vec{P}),$$

  for π_C^* the pullback of the projection π_C. We denote this subset as $\mathcal{O}_C$. An example of a function belonging to this set is the linear momentum of the nuclei.

- The set of **generalized quantum functions**: functions which depend only on the quantum degrees of freedom and which are constant under changes in the global phase. Mathematically, they can be written as those functions $f \in \mathcal{O}$ such that there exists a function $f_Q \in C^\infty(M_Q)$ for which $f = \pi_Q^*(f_Q)$, i.e.

  $$f(\vec{R}, \vec{P}, \vec{q}, \vec{p}) = f_Q(\vec{q}, \vec{p}); \quad \Gamma(f_Q) = 0, \tag{64}$$

for π_Q^* the pullback of the projection π_Q. We denote these functions as $\mathcal{O}_Q$. We have added the adjective "generalized" because this set is too large to represent the set of pure quantum observables. These later functions, should be considered, when necessary, as a smaller subset, which corresponds to the set of functions defined in Eq. (38). We denote this smaller subset as $\mathcal{O}_Q^s$. An example of a function belonging to $\mathcal{O}_Q^s$ is the linear momentum of the electrons.

- A third interesting subset is the set of arbitrary linear combinations of the subsets above, i.e. those functions which may be written as the sum of a purely classical function and a purely quantum one: $f = \pi_Q^*(f_Q) + \pi_C^*(f_C)$, i.e.

$$f(\vec{R}, \vec{P}, \vec{q}, \vec{p}) = f_C(\vec{R}, \vec{P}) + f_Q(\vec{q}, \vec{p}). \tag{65}$$

  We will denote this set as $\mathcal{O}_{C+Q}$. An element of this set of functions is the total linear momentum of the composed system.

We would like to make a final but very important remark. We have not chosen the set of observables as

$$\left\{ f \in C^\infty(M_C \times M_Q) | f = \langle \psi(\vec{q}, \vec{p}), A(\vec{R}, \vec{P}) \psi(\vec{q}, \vec{p}) \rangle \right\}, \tag{66}$$

for $A(\vec{R}, \vec{P})$ a linear operator on the Hilbert space $\mathcal{H}$ depending on the classical degrees of freedom because of two reasons:

- It is evident that the set above is a subset of (63) and thus we are not loosing any of these operators. But it is a well known property that Ehrenfest dynamics is not linear and then if we consider the operator describing the evolution of the system, it can not belong to the set above. We must thus enlarge the set (66).

- We are going to introduce in the next section a Poisson bracket on the space of operators. For that bracket to close a Poisson algebra, we need to consider the whole set (63).

It is important to notice that in the set (63) there are operators which are not representing linear operators for the quantum part of the system and hence the set of properties listed above for the pure quantum case are meaningless for them. But this is a natural feature of the dynamics we are considering, because of its nonlinear nature.

5.4 Geometry and the Poisson bracket on the classical-quantum world

Finally, we must combine the quantum and the classical description in order to provide a unified description of our system of interest. As we assume that both the classical and the quantum subsystems are endowed with Poisson structures, we face the same problem

we have when combining, from a classical mechanics perspective, two classical systems. Therefore it is immediate to conclude that the corresponding Poisson structures can be combined as:

$$\{\cdot,\cdot\} = \{\cdot,\cdot\}_C + \hbar^{-1}\{\cdot,\cdot\}_Q, \tag{67}$$

where the term $\{\cdot,\cdot\}_C$ acts on the degrees of freedom of the first manifold and $\{\cdot,\cdot\}_Q$ acts on the degrees of freedom of the second one.

From a more geometric point of view, this combination is equivalent to define a symplectic tensor on $M_C \times M_Q$ combining the corresponding symplectic structures, ω_C and ω_Q, in the form:

$$\omega = \omega_C + \hbar\omega_Q. \tag{68}$$

Remember that it is always possible to combine two symplectic forms in this way, because of the properties of differential algebra.

Lemma 11. *The tensor* (67) *defines a Poisson structure on* $C^\infty(M_C \times M_Q)$.

Proof It is completely straightforward if we realize that the Poisson tensor is directly related to the form ω which is trivally a symplectic form. □

Notice that the set of pure classical functions $\mathcal{O}_C$ and the set of quantum generalized functions $\mathcal{O}_Q$ are closed under the Poisson bracket. The same happens with the quantum functions $\mathcal{O}_Q^s$ and the set of linear combinations $\mathcal{O}_{C+Q}$. In mathematical terms, what we have is a family of Poisson subalgebras. This property ensures that the description of purely classical or purely quantum systems, or even both systems at once but uncoupled to each other, can be done within the formalism.

Once the Poisson bracket on $M_C \times M_Q$ has been introduced we can express again the constraint we introduced in the definition of the observables in Poisson terms. Thus we find that in a completely analogous way to the pure quantum case, we can prove that

Lemma 12. *The condition in Eq.*(63)

$$\Gamma_Q(f) = 0$$

is equivalent to ask the function f *to Poisson-commute with the function* $f_{\mathbb{I}} = \sum_k((q^k)^2 + p_k^2)$, *i.e.*

$$\Gamma_Q(f) = 0 \Leftrightarrow \{f_{\mathbb{I}}, f\} = 0.$$

5.5 The definition of the dynamics

From the previous sections we know that our formulation of MQCD can be implemented on:

- The manifold which represents the set of states by defining a vector field whose integral curves represent the solutions of the dynamics (equivalent to the Schrödinger picture of standard quantum mechanical systems).

- The set of functions (please note the differences between the classical and the quantum cases) defined on the set of states which represent the set of observables of the system. In this case the Poisson bracket of the functions with the Hamiltonian of the system defines the corresponding evolution (equivalent to the Heisenberg picture of standard quantum mechanical systems).

Remember that both approaches are not disconnected, since they can be easily related either by the momentum mapping or simply by the vector fields::

$$X_H = \{f_H, \cdot\}, \tag{69}$$

where we denote by X_H the vector field which represents the dynamics on the phase space and by f_H the function which corresponds to the Hamiltonian of the complete system.

We can now proceed to our first goal: to provide a Hamiltonian description of Ehrenfest dynamics in terms of a Poisson structure. We thus define the following Hamiltonian system:

- A state space corresponding to the Cartesian product $M_C \times M_Q$.

- A set of operators corresponding to the set of functions $\mathcal{O}$ defined in Eq. (17). On this set, we consider the Poisson bracket defined in Eq. (67) defined on the symplectic vector space $M_C \times M_Q$ with symplectic form (68).

- And finally, the dynamics introduced by the following Hamiltonian function:

$$f_H(\vec{R}, \vec{P}, \vec{q}, \vec{p}) = \sum_J \frac{\vec{P}_J^2}{2M_J} + \langle \psi(\vec{q}, \vec{p}), H_e(\vec{R})\psi(\vec{q}, \vec{p})\rangle, \tag{70}$$

  where H_e is the expression of the electronic Hamiltonian, M_J are the masses of the classical subsystem of the nuclei and $\psi(\vec{q}, \vec{p})$ is the real-space representation of the state ψ analogous to Eq. (31).

As a result, the dynamics of both subsystems are obtained easily. In the Schrödinger picture we obtain:

$$\dot{\vec{R}} = \frac{\partial f_H}{\partial \vec{P}} = M^{-1}\vec{P}, \tag{71}$$

$$\dot{\vec{P}} = -\frac{\partial f_H}{\partial \vec{R}} = -\text{grad}(\langle\psi(\vec{q},\vec{p}), H_e(\vec{R})\psi(\vec{q},\vec{p})\rangle), \tag{72}$$

$$\dot{q}^1 = \hbar^{-1}\frac{\partial f_H}{\partial p_1}, \tag{73}$$

$$\dot{p}_1 = -\hbar^{-1}\frac{\partial f_H}{\partial q^1}, \tag{74}$$

$$\vdots$$

$$\dot{q}^{N_Q} = \hbar^{-1}\frac{\partial f_H}{\partial p_{N_Q}}, \tag{75}$$

$$\dot{p}_{N_Q} = -\hbar^{-1}\frac{\partial f_H}{\partial q_{N_Q}}. \tag{76}$$

This set of equations corresponds exactly with Ehrenfest dynamics.

The final point is to prove the following lemma:

Lemma 13. *The dynamics preserves the set of observables $\mathcal{O}$.*

Proof An observable belongs to $\mathcal{O}$ if it Poisson-commutes with $f_{\mathbb{I}}$. Thus, as $f_H \in \mathcal{O}$, if we consider an observable $f \in \mathcal{O}$, by the Jacobi identity:

$$\{f_{\mathbb{I}}, \{f_H, f\}\} = -\{f, \{f_{\mathbb{I}}, f_H\}\} - \{f_H, \{f, f_{\mathbb{I}}\}\} = 0 \tag{77}$$

□

Example 5. *In the following example we will study a simple toy model in which the coupling of classical and quantum degrees of freedom gives rise to chaotic-like behavior. This behavior has been proven to be related with physical effects such as the change of the degree of purity of the quantum part of the system (see [4]).*

The system consists of a complex two dimensional Hilbert space $M_Q = \mathbb{C}^2$ and a classical 2-D phase space where we define a 1-D harmonic oscillator. Using coordinates (J_θ, θ) for the classical variables (action-angle coordinates for the oscillator) and $\Psi \in \mathbb{C}^2$ we define the following Hamiltonian

$$f_H = J_\theta + \frac{1}{2}\langle\Psi|\sigma_z + \epsilon\cos(\theta)\sigma_x|\Psi\rangle,$$

with σ_x, σ_z the Pauli sigma matrices.

We parametrize the normalized quantum state by

$$|\Psi\rangle = e^{i\alpha}\begin{pmatrix}\sqrt{J_\phi}\\ e^{i\phi}\sqrt{1-J_\phi}\end{pmatrix},$$

α *being the global phase.*

In these variables the Hamiltonian reads

$$f_H = J_\theta + J_\phi + \epsilon\sqrt{J_\phi}\sqrt{1 - J_\phi}\cos(\theta)cos(\phi), \tag{78}$$

where ϵ *measures the coupling of the classical and quantum systems.*

In the limit of vanishing ϵ *the system is integrable and actually linear in these coordinates. However for non vanishing* ϵ *the model becomes non linear and more complicated behavior appears. We can represent the trajectories of the corresponding Hamilton equations, which read:*

$$\begin{cases} \dot{\theta} = 1 \\ \dot{\phi} = \hbar^{-1}\left(1 + \left(-1 + \frac{1}{2\sqrt{J_\phi}}\right)\epsilon\cos(\theta)\cos(\phi)\right) \\ \dot{J}_\theta = -(-1 + \sqrt{J_\phi})\sqrt{J_\phi}\epsilon\cos(\phi)\sin(\theta) \\ \dot{J}_\phi = -\hbar^{-1}\left((-1 + \sqrt{J_\phi})\sqrt{J_\phi}\epsilon\sin(\phi)\cos(\theta)\right) \end{cases} \tag{79}$$

We can see then how the dynamics becomes more complex as the coupling ϵ *increases, the nonlinear effects becoming more and more important. For small values of* ϵ *the trajectory is almost planar and periodic while when it is increased, it becomes more and more complicated.*

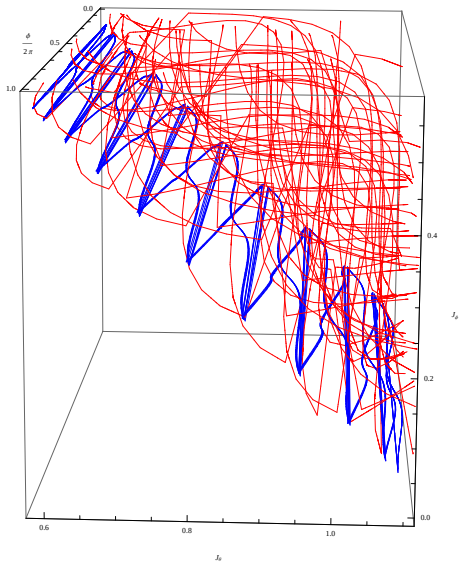


Figure 6.— The plot shows the trajectory with initial conditions $(\theta(0), \phi(0), J_\theta(0), J_\phi(0)) = (0.1, 0.32, 0.6, 0.55)$ on the hyperplane $(\phi/2\pi, J_\theta, J_\phi)$ for $\epsilon = 0.15$ (blue curve) and for $\epsilon = 1.55$ (red curve). For simplicity, we take $\hbar = 1$

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