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GEOMETRIC HAMILTONIAN FORMULATION OF
QUANTUM MECHANICS

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Dedicated to Chiara,
a true genius.

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List of symbols

A	linear operator
A^*	adjoint of A
\overline{A}	closure of A
A_v	self-adjoint operator corresponding to $v \in T_p\mathbf{P}(\mathbf{H})$
\mathfrak{A}	abstract C^* -algebra
$\mathfrak{B}(\mathbf{H})$	C^* -algebra of bounded operators on \mathbf{H}
$\mathfrak{B}_1(\mathbf{H})$	space of trace-class operators on \mathbf{H}
$\mathfrak{B}_2(\mathbf{H})$	space of Hilbert-Schmidt operators on \mathbf{H}
$\mathcal{B}(X)$	Borel σ -algebra on X
\mathbb{C}	set of complex numbers
\mathbb{C}^n	set of n -tuples of complex numbers
$\mathcal{C}(X)$	set of functions on X
$\mathcal{C}^\infty(X)$	set of smooth functions on X
CM	acronym of Classical Mechanics
$\gamma_t^{(H)}$	dynamical flow associated to H
$D(A)$	domain of operator A
D_n	faithful unitary representation of $U(n)$ on $L^2(\mathbb{S}^{2n-1}, \nu_n)$
df	total differential of f
dx	Lebesgue measure on \mathbb{R} (or \mathbb{R}^n)
$d(\cdot, \cdot)$	distance function
$d_1(\cdot, \cdot)$	distance induced by $\ \cdot\ _1$
$d_2(\cdot, \cdot)$	distance induced by $\ \cdot\ _2$
Δ	Laplacian
ΔA	standard deviation of A
δ	Dirac delta
δ_{ij}	Kronecker delta
e	Euler's number (electric charge of electron in section 1.1)
E	Borel set
exp	exponential function
f	scalar function
f_A	classical-like observable associated to quantum observable A
$f_{\mathbf{H}}$	partial integral of $f : \mathbf{P}(\mathbf{H} \otimes \mathbf{K}) \rightarrow \mathbb{R}$ w.r.t. $\mathbf{P}(\mathbf{H})$

F^j	generalized zonal spherical harmonic of order j
$\mathcal{F}^2(\mathbf{H})$	set of square-integrable frame functions on \mathbf{H}
$\Phi^* f$	pullback of f by Φ
G	Lie group
G_p	isotropy group of $p \in \mathbf{P}(\mathbf{H})$
$G(df, dg)$	scalar product of one-forms induced by Fubini-Study metric
g	Fubini-Study metric
H	Hamiltonian
H_0	free Hamiltonian
\mathbf{H}	Hilbert space
\mathbf{H}_n	n -dimensional Hilbert space
$\mathbf{H}_{(p,q)}^n$	subspace of the orthogonal decomposition of $L^2(\mathbb{S}^{2n-1}, \nu_n)$
\hbar	reduced Planck constant
\mathbb{I}	identity operator
i	imaginary unit (or index as subscript/superscript)
j_p	almost complex form acting on $T_p\mathbf{P}(\mathbf{H})$
$\text{Ker}(A)$	kernel of A
κ	free parameter of inverse quantization prescription
$\mathcal{L}^2(\Omega, \mu)$	set of μ -square-integrable functions on the measure space Ω
$L^2(\Omega, \mu)$	Hilbert space of μ -square-integrable functions on the measure space Ω
\mathcal{M}	symplectic manifold (classical phase space in particular)
m_e	mass of the electron
$\tilde{\mu}$	Haar measure on $U(n)$
μ_n	Liouville measure on $\mathbf{P}(\mathbf{H}_n)$
μ_G	Gaussian measure
N	basis of $\mathbf{P}(\mathbf{H})$
\mathbb{N}	set of natural numbers
ν_n	$U(n)$ -invariant Borel measure on \mathbb{S}^{2n-1}
QM	acronym of Quantum Mechanics
\mathcal{O}	inverse quantization map for observables
\mathfrak{D}	re-quantization distribution for observables
P	orthogonal projector
P_E	orthogonal projector individuated by $E \in \mathcal{B}(\mathbb{R})$
$P_l(u)$	Legendre polynomials
P_k	momentum operators
$\{P_E\}_{E \in \mathcal{B}(\mathbb{R})}$	spectral measure
$\mathfrak{P}(\mathbf{H})$	lattice of orthogonal projectors on \mathbf{H}
$\mathbf{P}(\mathbf{H})$	projective space on \mathbf{H}
ψ	unit vector in \mathbf{H}
$[\psi]$	ray of ψ

\mathbb{R}	set of real numbers
\mathbb{R}^n	set of n -tuples of real numbers
ρ	Liouville density
ρ_σ	Liouville density associated to σ
$s\text{-lim}$	strong limit
$s\text{-}\Sigma$	sum calculated in strong operator topology
\mathbb{S}^{2n-1}	unit sphere in \mathbb{C}^n
$\mathbb{S}(\mathbb{H})$	unit sphere in \mathbb{H}
$\mathbb{S}(\mathbb{H})$	set of quantum states on \mathbb{H}
$\mathbb{S}_p(\mathbb{H})$	set of quantum pure states on \mathbb{H}
$\mathbb{S}^{sep}(\mathbb{H} \otimes \mathbb{K})$	set of separable states
$\mathbb{S}_p^{sep}(\mathbb{H} \otimes \mathbb{K})$	set of separable pure states
$\mathcal{E}(\mathbb{H} \otimes \mathbb{K})$	set of entangled states
$sp(A)$	spectrum of A
$sp_p(A)$	point spectrum of A
$\Sigma(X)$	σ -algebra on X
σ	density operator
σ_ψ	pure state associated to ψ
\mathcal{S}	inverse quantization map for states
\mathfrak{S}	re-quantization distribution for states
$tr(A)$	trace of operator A
$tr_{\mathbb{H}}(A)$	partial trace of A
$T_p\mathcal{M}$	tangent space of \mathcal{M} in $p \in \mathcal{M}$
$T_p^*\mathcal{M}$	cotangent space of \mathcal{M} in $p \in \mathcal{M}$
$\mathcal{T}(X)$	topology on X
U	unitary operator
$U(n)$	unitary group of degree n
$U(\mathbb{H})$	group of unitary operators in \mathbb{H}
$\{U_t\}_{t \in \mathbb{R}}$	one-parameter group of unitary operators
$U(t_0, t)$	time evolutor
$\mathfrak{u}(n)$	Lie algebra of $U(n)$
$iu(n)$	real vector space of self-adjoint operators on \mathbb{H}_n
V	vector space
v_A	vector in $T_p\mathbb{P}(\mathbb{H})$ individuated by $A \in iu(n)$
W_f	weight of the frame function f
ω	symplectic form (algebraic state in section 1.3)
$(\mathbb{H}_\omega, \pi_\omega, \Psi_\omega)$	GNS triple of algebraic state ω
X	non-empty set
$X(\cdot)$	vector field on a manifold
$X_H(\cdot)$	Hamiltonian vector field

X_i	position operators
\bar{z}	complex conjugate of $z \in \mathbb{C}$
\bigoplus	direct sum
\times	cartesian product
\otimes	tensor product of Hilbert spaces
\diamond	tensor product of frame functions
\star	C^* -product on $\mathcal{F}^2(\mathbf{H})$ (quantum star-product)
\wedge	wedge product
\bigwedge	logical conjunction
\bigvee	logical disjunction
\neg	negation
$[\cdot, \cdot]$	commutator
$\{\cdot, \cdot\}$	Poisson bracket
$\langle \cdot \cdot \rangle$	inner product
$ \psi\rangle\langle\psi $	rank-1 orthogonal projector
$\langle A \rangle_\sigma$	expectation value of A on σ
$(\cdot \cdot)_2$	Hilbert-Schmidt product
$\ \cdot \ $	norm
$\ \cdot \ _1$	trace norm
$\ \cdot \ _2$	norm induced by $(\cdot \cdot)_2$
$\ \cdot \ _\infty$	uniform norm
$ \cdot $	C^* -norm on $\mathcal{F}^2(\mathbf{H})$

Introduction

Motivations

The motivation of any scientific work is improving the human knowledge of this Universe as far as possible. It is a more than enough motivation to set up a scientific work, this one in particular! More precisely, this Ph.D dissertation summarizes the results of my research activity on the mathematical structure of Quantum Mechanics as a Hamiltonian theory within a geometric framework. The research on these topics during my Ph.D program originates from a result first presented in my Master thesis and edited in [33] in a developed version. Such result involves mathematical objects, so-called *frame functions*, introduced by A.M. Gleason in [21], as technical tools, to prove his celebrated theorem, a milestone in the mathematics of Quantum Mechanics. This theorem is crucial for the following reasons: within an axiomatic-constructive approach to QM, physical states of a quantum system can be represented by *generalized probability measures* on the lattice of orthogonal projectors in a Hilbert space, the statement of Gleason's theorem gives a complete characterization of states in terms of density matrices establishing a formal connection between *Von Neumann formulation* and *Dirac formulation* of QM. Moreover Gleason's theorem has an outstanding physical implication: The non-existence of quantum states described by probability measures assuming values 0 or 1, i.e. deterministic states in the classical sense. This fact has deep aftermaths in hypothetic extensions of QM with hidden variables.

In [33] we proved that linear operators in a finite-dimensional Hilbert space are in bijective correspondence with a class of functions given by \mathcal{L}^2 -frame functions defined on the Hilbert projective space. This result can be used to prove Gleason's theorem (even in infinite dimension), in this sense it supplies a mathematical machinery. However the bijective correspondence between operators and frame functions can be used to characterize quantum states and quantum observables of a finite-dimensional quantum theory as real scalar functions on the projective space of the Hilbert space of considered quantum theory. Within the quantum geometric framework introduced and discussed in [27, 6, 9, 10], QM can be formulated as a classical-like Hamiltonian theory where quantum dynamics is

described by a Hamiltonian vector field on the phase space given by a projective Hilbert space.

If \mathbf{H} is a finite-dimensional Hilbert space then its projective space $\mathbf{P}(\mathbf{H})$ can be equipped with a structure of Kähler manifold, in particular a symplectic form can be defined on $\mathbf{P}(\mathbf{H})$ (then a notion of Poisson bracket can be introduced). The machinery of frame functions has been applied in [34] to give a complete characterization of states and observables in terms of classical-like objects on the quantum phase space: All the prescriptions to associate a real function to each quantum observable and a probability density to each quantum state, in order to obtain a self-consistent Hamiltonian theory, are classified. This kind of symplectic-geometrization of finite-dimensional QM (and its eventual extension to infinite dimension) offers a remarkable description of a quantum system in a classical fashion, so it has the epistemological dignity of a point of view approaching Quantum Mechanics and Classical Mechanics.

Geometric Hamiltonian formulation of finite-dimensional QM, in particular description of quantum states as classical-like *Liouville densities*, can be applied to study alternative approaches to quantum entanglement, for instance how quantum entanglement can be defined (and measured) describing a quantum system within the classical-like formalism with possible applications to quantum information theory.

The description of finite-dimensional quantum systems is relevant in the *quantum control theory*. In this context the geometric Hamiltonian formulation can be crucial to exploit the huge machinery of classical control theory to investigate controllability of quantum systems.

Synopsis

This section represents an abstract of the main part of this work about the formulation of finite-dimensional QM as an Hamiltonian theory on projective space.

Finite dimensional QM can be formulated as a classical-like Hamiltonian theory where the phase space is given by the projective space $\mathbf{P}(\mathbf{H}) = U(n)/U(n-1)U(1)$ on the n -dimensional Hilbert space \mathbf{H} of considered quantum theory (e.g. [6]). $\mathbf{P}(\mathbf{H})$ has a structure of $(2n-2)$ -dimensional real manifold which can be equipped with a *Kähler structure*. In particular the symplectic form is given by the *Konstant-Kirillov* form considering $\mathbf{P}(\mathbf{H})$ as a rank-1 orbit of the unitary group $U(n)$. To define explicitly the symplectic form let us introduce the following characterization of the tangent space $T_p\mathbf{P}(\mathbf{H})$. In the following $iu(n)$ denotes the real vector space of self-adjoint operators.

The tangent vectors v at $p \in \mathbf{P}(\mathbf{H})$ are all the linear operators on \mathbf{H} of the form: $v = -i[A_v, p]$, for some $A_v \in iu(n)$. Consequently, $A_1, A_2 \in iu(n)$ define the same vector in $T_p\mathbf{P}(\mathbf{H}_n)$ iff $[A_1 - A_2, p] = 0$. A symplectic form on $\mathbf{P}(\mathbf{H})$ can be defined for any $\kappa > 0$ as:

$$\omega_p(u, v) := -i\kappa \text{tr}(p[A_v, A_u]) \quad u, v \in T_p\mathbf{P}(\mathbf{H}), \quad (1)$$

the symplectic structure is compatible with a Riemannian metric on $\mathbf{P}(\mathbf{H})$, the *Fubini-Study metric*, w.r.t. to an almost complex form ([6]). The idea of geometric Hamiltonian formulation of QM is associating a quantum observable $A \in i\mathfrak{u}(n)$ to a real scalar function f_A on $\mathbf{P}(\mathbf{H})$ (a classical-like function) in order to obtain a classical description of a quantum system on the projective space, in particular the description of the quantum dynamics via a Hamiltonian vector field w.r.t. the symplectic form (1).

Imposing several physical requirements (see [34] and chapter 4 of this work) the unique (up to a factor κ) prescription to set up a meaningful classical-like formulation of a quantum theory is given by the so-called *inverse quantization maps* \mathcal{O} and \mathcal{S} :

$$\mathcal{O} : i\mathfrak{u}(n) \ni A \mapsto f_A, \quad (2)$$

with

$$f_A(p) = \kappa \operatorname{tr}(Ap) + \frac{1-\kappa}{n} \operatorname{tr}(A) \quad \kappa > 0, \quad (3)$$

for observables. And about states:

$$\mathcal{S} : \mathfrak{D}(\mathbf{H}) \ni \sigma \mapsto \rho_\sigma \quad (4)$$

with

$$\rho_\sigma(p) = \kappa' \operatorname{tr}(\sigma p) + \frac{\kappa - (n+1)}{\kappa} \quad \kappa > 0 \quad (5)$$

where $\kappa' = \frac{n(n+1)}{\kappa}$ and $\mathfrak{D}(\mathbf{H})$ denotes the set of density matrices on \mathbf{H} . In other words, varying κ we have the all prescriptions to translate a quantum theory from the standard language of operators to the classical-like language of functions. For $\kappa = 1$, the observable A is represented by the expectation value function $f_A(p) = \operatorname{tr}(Ap)$ as in the Ashtekar-Schilling picture ([6]). Using the maps \mathcal{O} and \mathcal{S} to obtain classical-like observables and states we can compute quantum expectation values as classical expectation values:

$$\langle A \rangle_\sigma = \operatorname{tr}(A\sigma) = \int_{\mathbf{P}(\mathbf{H}_n)} f_A \rho_\sigma d\mu \quad (6)$$

where μ is the suitably normalized Liouville measure w.r.t. the symplectic form ω ([34]). Furthermore the Hamiltonian vector field associated to $f_A = \mathcal{O}(A)$ is:

$$X_{f_A}(p) = -i[A, p] \quad \forall p \in \mathbf{P}(\mathbf{H}), \quad (7)$$

if $A = H$ is the Hamiltonian operator, the Hamilton dynamics given by the field X_{f_H} is equivalent to the Schrödinger dynamics given by H , i.e. a curve $t \mapsto p(t) \in \mathbf{P}(\mathbf{H})$ satisfies the Schrödinger equation ($\hbar = 1$):

$$\dot{p}(t) = -i[H, p(t)], \quad (8)$$

if and only if it satisfies the Hamilton equation:

$$\dot{p}(t) = X_{f_H}(p(t)). \quad (9)$$

Classification of all inverse quantization prescriptions is based on the notion of *frame function* [21, 33, 34] acting on projective space $\mathbf{P}(\mathbf{H})$ (see definition 50). Defining $\mathcal{F}^2(\mathbf{H})$ as the space of frame functions in $\mathcal{L}^2(\mathbf{P}(\mathbf{H}), \mu)$, we prove that there is an isomorphism of vector spaces between $\mathcal{F}^2(\mathbf{H})$ and $\mathfrak{B}(\mathbf{H})$; since $\mathcal{F}^2(\mathbf{H})$ can be equipped with an involution (given by complex conjugation), a norm and a star-product, we can construct the observable C^* -algebra in terms of classical-like observables of a quantum theory. In particular the quantum product on $\mathcal{F}^2(\mathbf{H})$ is made by the contribution of three parts: Poisson bracket (Lie product), scalar product induced by the Fubini-Study metric (Jordan product), pointwise product (commutative product).

Even quantum states can be completely defined in terms of functions on phase space with a classical-like interpretation of probability densities (Liouville densities). A composite system, with phase space given by a projective space $\mathbf{P}(\mathbf{H}_1 \otimes \mathbf{H}_2)$ can be described in this framework exploiting the action of *Segre embedding* to characterize quantum entanglement.

Structure of dissertation

The core of this dissertation is given by the results presented in the papers [33, 34, 36]. In my opinion an article is a deeply different format from a chapter of a PhD thesis, thus the results have been re-arranged and inserted in a quite cohesive context. Obviously some parts, passages, proofs are almost identical to those appearing in the papers; however I tried to construct a solid presentation to explain in what spirit these results have been reached. The spirit of an investigation about mathematical foundations of Quantum Mechanics.

Chapter 1 is devoted to the introduction of some foundational aspects and mathematical concepts of Quantum Mechanics (QM). After a short introduction to the standard quantum formalism of operators on Hilbert spaces, there are two sections about foundations of QM: In the first one, the axiomatic approach is adopted, quantum states are defined as *generalized probability measures* on the lattice of orthogonal projectors in a separable Hilbert space and quantum observables are defined as *projective valued measures* on the Borel σ -algebra of \mathbb{R} . Gleason's theorem and its several implications are discussed to characterize quantum states as density matrices. In the last section of the chapter there are some fundamentals of the *algebraic formulation* of a quantum theory. In the first chapter there are many well-known results, thus several proofs are omitted.

The second chapter is based on the paper [33] and it is quite technical. Frame functions are introduced as a tool to prove Gleason's theorem. These functions are defined on the

unit sphere in a separable Hilbert space but in chapter 3 they are re-defined on the projective Hilbert space. In finite dimension (but larger than 2) the set of frame functions which are square-integrable w.r.t. a certain Borel measure on the sphere turns out to be in bijective correspondence with linear operators on the finite-dimensional Hilbert space. This result (theorem 21) is crucial to relate quantum observables to functions in the studied geometric formulation.

In chapter 3 the interplay of standard formalism of QM with the Hamiltonian formalism is discussed, stressing the choice of the projective Hilbert space as a quantum phase space. Definition and properties of frame functions are revisited on the projective space presenting the so-called *trace-integral formulas* which generalize a result of [20]. Geometry of the projective space and the machinery of frame functions allow to set up a complete Hamiltonian formulation of finite-dimensional QM.

Such formulation is described in chapter 4. A prescription to associate a classical-like observable to every quantum observable and a Liouville density to every density matrix is constructed exploiting the fact that the classical-like objects must be frame functions. By means of a complete characterization of quantum observables in the geometric-Hamiltonian formalism, the algebra of observables is concretely realized as a C^* -algebra of functions with a non-commutative quantum product.

In the last chapter there is a general description of composite systems in terms of the geometric Hamiltonian formalism. In particular a notion of separability for a Liouville density is defined, in order to introduce the concept of entanglement in this classical-like fashion. An entanglement measure is proposed exploiting the description of quantum states as classical-like Liouville densities.

Chapter 1

Mathematical foundations of Quantum Mechanics

1.1 Preliminaries

1.1.1 *In Nature there are quantum systems*

Quantum Mechanics (QM) is a theory (nowdays a cluster of theories) describing a huge class of phenomena observed in Atomic Physics, Optics, Chemistry, Nuclear and Subnuclear Physics. From the beginning of XX century several experimental evidences showed that Classical Mechanics (CM) does not work as a good theory at the atomic and subatomic length scales.

Let us introduce the general (and informal) concept of *quantum system* through a simple example. Once fixed a frame of reference consider a free electron moving in \hat{x} -direction. The position x and the momentum p_x are not simultaneously measurable by an experiment. Another phenomenological evidence about this system is that two orthogonal components of spin cannot be simultaneously measured. In the first pair of physical quantities (x and p_x), standard deviations satisfy the so-called Heisemberg uncertainty relation (1.8). Experimental Physics gives a rich phenomenology about *incompatible quantities*, i.e. non-simultaneously measurable quantities. Thus a very general observation is the following: *In nature, there exist systems for which some physical quantities are not simultaneously measurable by an experiment.* We call those systems **quantum systems**.

From the 20's, the formalism of Quantum Mechanics was developed and now it is familiar to every physicist and mathematician. The physical quantities, *observables*, related to a quantum system are described by selfadjoint operators in a complex Hilbert space and the real spectrum of an observable represents the experimentally measurable values of the correspondent physical quantity. The compatibility between two observables is mathematically represented by the commutation of operators. The state at time t of a quantum system is given by a positive trace-class operator, called **density matrix**. QM associates a complex Hilbert space to every quantum system, for example a free quantum particle moving in \mathbb{R}^d is decribed in the Hilbert space $L^2(\mathbb{R}^d, dx)$, where dx is the Lebesgue

measure on \mathbb{R}^d .

The expectation value of the observable O evaluated on the state σ is given by:

$$\langle O \rangle_\sigma = \text{tr}(\sigma O), \quad (1.1)$$

where tr denotes the trace. The set of the states of a quantum system, that is the set of positive trace-class operators with unit trace in the Hilbert space \mathbf{H} associated to the system, is convex and its extremal elements have this form:

$$\sigma_\psi(\cdot) = \psi(\psi|\cdot) \quad \text{with} \quad \|\psi\| = 1, \quad (1.2)$$

where $(|\cdot\rangle)$ denotes the hermitean scalar product on \mathbf{H} and $\|\cdot\|$ the induced norm. The extremal elements (1.2), individuated by unit vectors are in bijective correspondence with rays in \mathbf{H} , they are called **pure states**. According to Krein-Millman theorem, any state can be obtained by a convex combination of pure states, the non-pure states are called **mixed states**. Consider two pure states σ_ψ and σ_ϕ , the positive real number:

$$\text{tr}(\sigma_\phi \sigma_\psi) = |\langle \psi | \phi \rangle|^2, \quad (1.3)$$

is interpreted as the probability that a transition of the system occurs from the state σ_ϕ to the state σ_ψ . Using Dirac formalism the hermitian product is denoted by $\langle \cdot | \cdot \rangle$, and a pure state is written as $\sigma_\psi = |\psi\rangle\langle\psi|$. Of course, we can denote the pure state ρ_ψ as ψ without ambiguity. In this notation the pure state ψ is typically named *wave function* or *state vector*; within Dirac formalism the redundant symbol $|\psi\rangle$ is often adopted.

Time evolution of a quantum system is given by a one parameter group of unitary operators $\{U_t\}_{t \in \mathbb{R}}$, its infinitesimal generator is the *Hamiltonian operator* H that is essentially self-adjoint and its associated physical quantity is the total energy of the system. Time evolution of the state vector $\psi(t)$ is given by the following differential equation:

$$i\hbar \frac{d}{dt} \psi(t) = H\psi(t), \quad (1.4)$$

called **Schrödinger equation**. The constant \hbar is the reduced *Planck constant*, its experimental value is:

$$\hbar = 1,054\,571\,726(47) \times 10^{-34} \text{ Joule} \cdot \text{second}.$$

One can derive the equation for the time evolution of a general density matrix:

$$i\hbar \frac{d}{dt} \sigma(t) = [H, \sigma],$$

where $[H, \sigma]$ is the standard commutator of operators H and σ .

In QM a crucial rôle is played by *canonical commutation relations* (CCR) between canonical conjugate quantities. Let us recall a fundamental example: The Hilbert space

of a non-relativistic particle with mass $m > 0$ and spin 0 is $\mathbf{H} = L^2(\mathbb{R}^3, dx)$ where \mathbb{R}^3 is identified as the rest space in a fixed frame of reference with coordinates x_1, x_2, x_3 and dx is the Lebesgue measure on \mathbb{R}^3 . The **position operators** are defined as follows:

$$X_i \psi(x_1, x_2, x_3) = x_i \psi(x_1, x_2, x_3) \quad i = 1, 2, 3 \quad \forall \psi \in D(X_i), \quad (1.5)$$

where the domains are given by:

$$D(X_i) := \left\{ \psi \in \mathbf{H} : \int_{\mathbb{R}^3} |x_i \psi(x_1, x_2, x_3)|^2 dx < +\infty \right\}.$$

Momentum operators are defined as:

$$P_k = -i\hbar \frac{\partial}{\partial x_k}. \quad (1.6)$$

Operators X_i and P_k satisfies the **canonical commutation relations**:

$$[X_i, P_k] = i\hbar \delta_{ik} \mathbb{I}, \quad (1.7)$$

where \mathbb{I} is the identity operator and the domain of $[X_i, P_k]$ is given by $D(X_i P_k) \cap D(P_k X_i)$. A consequence of CCR is the **Heisemberg principle** as a formal resut:

$$(\Delta X_i)_\rho (\Delta P_i)_\rho \geq \frac{\hbar}{2} \quad i = 1, 2, 3, \quad (1.8)$$

where $(\Delta X_i)_\rho = \sqrt{\langle X_i^2 \rangle_\rho - \langle X_i \rangle_\rho^2}$ and $(\Delta P_i)_\rho = \sqrt{\langle P_i^2 \rangle_\rho - \langle P_i \rangle_\rho^2}$. A direct consequence of (1.8) is the positivity of the differential opeartor $-\Delta - \frac{1}{4|x|^2}$ on $L^2(\mathbb{R}^3, dx)$, where $\Delta = \sum_{i=1}^3 \frac{\partial}{\partial x_i}$ is the standard Laplacian operator. So we can apply this fact to prove that hydrogen atom is stable, one of the first hisorical successes of QM. The Hamiltonian describing the system is given by the operator:

$$H = -\frac{\hbar^2}{2m_e} \Delta - \frac{e^2}{|x|}$$

where m_e and e are respectively mass and electric charge of electron. The Coulomb attractive potential $V(x) = -e^2/|x|$ is a multiplicative operator and it is selfadjoint as a consequence of Kato's theorem. Since $-\Delta \geq \frac{1}{4|x|^2}$, H satisfies the operator inequality:

$$H \geq \frac{\hbar^2}{8m_e|x|^2} - \frac{e^2}{|x|}.$$

The function $f : \mathbb{R}^3 \rightarrow \mathbb{R} : x \mapsto \frac{\hbar^2}{8m_e|x|^2} - \frac{e^2}{|x|}$ has a minimum at $|x|^{-1} = \frac{4m_e e^2}{\hbar^2}$, thus:

$$H \geq -\frac{2m_e e^4}{\hbar^2},$$

so the spectrum of H is bounded from below, i.e. the energy cannot decrease under this bound and the electron does not collapse. Classical Physics provides electron radiates away energy falling onto the nucleus. While QM gives a good model to explain the stability of hydrogen.

1.1.2 In Mathematics there are operators in Hilbert spaces

Adopting a slightly more formal approach we can characterize the *standard formulation* of Quantum Mechanics with the following statement: Bounded observables, i.e. physical quantities which only take bounded sets of values, are described by self-adjoint elements of the C^* -algebra $\mathfrak{B}(\mathbf{H})$ of bounded operators in a Hilbert space \mathbf{H} . Unbounded observables can be constructed out of the bounded ones through limit procedures in the strong operator topology.

In $\mathfrak{B}(\mathbf{H})$, there are two remarkable two-sided $*$ -ideals of compact operators: The space of *Hilbert-Schmidt operators* $\mathfrak{B}_2(\mathbf{H})$ and the space of *trace-class operators* $\mathfrak{B}_1(\mathbf{H})$, with the inclusions $\mathfrak{B}_1(\mathbf{H}) \subset \mathfrak{B}_2(\mathbf{H}) \subset \mathfrak{B}(\mathbf{H})$. The standard norm on the C^* -algebra $\mathfrak{B}(\mathbf{H})$ is defined as:

$$\| A \| := \sup_{\psi \neq 0} \frac{|\langle \psi | A \psi \rangle|}{\| \psi \|_{\mathbf{H}}} \quad \text{for } A \in \mathfrak{B}(\mathbf{H}) \quad (1.9)$$

and it induces the distance $d(A, B) := \| A - B \|$ for $A, B \in \mathfrak{B}(\mathbf{H})$.

$\mathfrak{B}_1(\mathbf{H})$ is a Banach space w.r.t. the norm:

$$\| A \|_1 := \text{tr}(|A|) \quad \text{for } A \in \mathfrak{B}_1(\mathbf{H}) \quad (1.10)$$

inducing the distance $d_1(\cdot, \cdot)$. The Hilbert-Schmidt product on $\mathfrak{B}_2(\mathbf{H})$ is defined as

$$(A|B)_2 := \text{tr}(A^*B) \quad \text{for } A, B \in \mathfrak{B}_2(\mathbf{H})$$

inducing a structure of Hilbert space on $\mathfrak{B}_2(\mathbf{H})$ with norm $\| \cdot \|_2$ and distance $d_2(\cdot, \cdot)$. The three norms are related with each other as: $\| A \| \leq \| A \|_2 \leq \| A \|_1$ when $A \in \mathfrak{B}_2(\mathbf{H})$.

From the general algebraic point of view, a quantum system is described in an abstract C^* -algebra whose self-adjoint elements represent the observables, so $\mathfrak{B}(\mathbf{H})$ turns out to be a concrete representation of such abstract object, we discuss algebraic QM in section 1.3. The space $\mathfrak{B}_1(\mathbf{H})$ of trace-class operators plays a crucial rôle in the definition of quantum states, in fact the well-definition of trace is necessary for the computation of expectation values.

Definition 1 *Let \mathbf{H} be a complex Hilbert space. The **quantum states** on \mathbf{H} are the operators $\sigma \in \mathfrak{B}_1(\mathbf{H})$ with $\text{tr}(\sigma) = 1$ which are positive. The set of states (convex in $\mathfrak{B}_1(\mathbf{H})$) is denoted by $\mathfrak{S}(\mathbf{H})$, its extremal elements are called **pure states**, the set of pure*

states are denoted by $S_p(\mathbf{H})$. The operators belonging to $S(\mathbf{H}) \setminus S_p(\mathbf{H})$ are called **mixed states**.

Pure states can be represented by points of complex projective space $P(\mathbf{H})$ on \mathbf{H} . Once defined the equivalence relation \sim on \mathbf{H} in this way: for $\psi, \varphi \in \mathbf{H}$, $\psi \sim \varphi$ iff $\psi = \alpha\varphi$ with $\alpha \in U(1)$, the complex projective space $P(\mathbf{H})$ is defined as the quotient \mathbf{H}/\sim deprived of $[0]$. On $P(\mathbf{H})$ there is the quotient topology. Considering the unit sphere $S(\mathbf{H}) := \{\psi \in \mathbf{H} : \|\psi\| = 1\}$, as a topological subspace of \mathbf{H} it is connected, Hausdorff and also compact only if the Hilbert space is finite dimensional. The projection $\pi : S(\mathbf{H}) \ni \psi \mapsto [\psi] \in P(\mathbf{H})$ is surjective, continuous and open thus $P(\mathbf{H})$ is a connected Hausdorff space. The statements of following proposition characterize the set of quantum states, represented by density operators. In the third statement the projective space is introduced to describe the set of pure quantum states, by a rough analogy with Classical Mechanics one can compare the representation of pure states as points of $P(\mathbf{H})$ with the representation of *classical deterministic states* as single points of the phase space: This comparison can be considered an informal hint to the construction of a classical-like Hamiltonian theory in $P(\mathbf{H})$.

Proposition 2 *If \mathbf{H} is a separable complex Hilbert space, the following facts hold:*

1. $S(\mathbf{H})$ and $S_p(\mathbf{H})$ are closed in $\mathfrak{B}_1(\mathbf{H})$ and are complete d_1 -metric spaces.
2. If $\sigma \in S(\mathbf{H})$, then: $\sigma^2 \leq \sigma$ and $\text{tr}(\sigma^2) \leq 1$, and the following facts are equivalent:
 - (i) $\sigma \in S_p(\mathbf{H})$;
 - (ii) $\sigma^2 = \sigma$;
 - (iii) $\text{tr}(\sigma^2) = 1$;
 - (iv) $\|\sigma\| = 1$;
 - (v) $\|\sigma\|_2 = 1$;
 - (vi) $\sigma = \psi\langle\psi|\cdot\rangle$ for some $\psi \in S(\mathbf{H})$.
3. The homeomorphism exists $P(\mathbf{H}) \ni p \mapsto \psi\langle\psi|\cdot\rangle \in S_p(\mathbf{H})$ for $\psi \in S(\mathbf{H})$ with $[\psi] = p$, the topology assumed on $S_p(\mathbf{H})$ being equivalently induced by $\|\cdot\|$ or $\|\cdot\|_1$ or $\|\cdot\|_2$, since $d_1(p, p') = 2d(p, p') = \sqrt{2}d_2(p, p')$ if $p, p' \in S_p(\mathbf{H})$.
4. If $\sigma \in S(\mathbf{H})$, then $sp(\sigma) \setminus \{0\} \subset sp_p(\sigma)$ is finite or countable with 0 as uniquely possible limit point. If $q \in sp_p(\sigma)$ then $0 \leq q \leq 1$; the associated eigenspace H_q has finite dimension if $q \neq 0$ and the sum of all eigenvalues, taking the geometric multiplicities into account, equals 1. If K is a Hilbert basis of $\text{Ker}(\sigma)$ and $\{\psi_i^{(q)}\}_{i=1, \dots, \dim(H_q)}$ a Hilbert basis of H_q , then $K \cup \{\psi_i^{(q)} \mid i = 1, \dots, \dim(H_q), q \in sp_p(\sigma)\}$ is a Hilbert basis of \mathbf{H} .

5. Every $\sigma \in \mathbf{S}(\mathbf{H})$ is a finite or countable convex combination of pure states, referring to the operator strong topology for infinite combinations. The spectral decomposition of σ is an example of such convex decomposition.

Let us omit the proof of the above proposition whose statements are well-known. The spectrum $sp(A) \subset \mathbb{R}$ of the bounded observable $A \in \mathfrak{B}(\mathbf{H})$ is the set of the possible results of a measurement of A . If $\sigma \in \mathbf{S}(\mathbf{H})$, $E \subset sp(A)$ is a Borel set and P_E is the orthogonal projector of the spectral measure of A corresponding to E , then $tr(\sigma P_E)$ is the probability of finding the outcome of the measurement of A in E when the system is in the state σ . Thus $tr(\sigma A)$ is the expectation value of A on σ . The notion of spectral measure to representing quantum observable is briefly discussed in the next section.

In this dissertation a remarkable part concerns the finite-dimensional QM, which is important for the quantum information theory in particular. A n -dimensional Hilbert space is denoted by \mathbf{H}_n when it is necessary. The following proposition shows some interesting topological properties of $\mathfrak{B}(\mathbf{H}_n)$ and $\mathbf{S}(\mathbf{H}_n)$.

Proposition 3 *Let \mathbf{H}_n be a n -dimensional Hilbert space with $1 < n < +\infty$. The following facts hold:*

1. *The topologies induced by $\|\cdot\|$, $\|\cdot\|_1$ and $\|\cdot\|_2$ on $\mathfrak{B}(\mathbf{H}_n) = \mathfrak{B}_2(\mathbf{H}_n) = \mathfrak{B}_1(\mathbf{H}_n)$ coincide.*
2. *$\mathbf{S}(\mathbf{H}_n)$ and $\mathbf{S}_p(\mathbf{H}_n)$ are compact and, if $\sigma \in \mathbf{S}(\mathbf{H}_n)$, the following inequalities hold: $n^{-1/2} \leq \|\sigma\|_2 \leq 1$ and $n^{-1} \leq \|\sigma\| \leq 1$. In both cases, the least values of the norms are attained at $\sigma = n^{-1}I$.*
3. *Equip the set T of operators $A = A^* \in \mathfrak{B}(\mathbf{H}_n)$ such that $tr(A) = 1$ with the topology induced by $\mathfrak{B}(\mathbf{H}_n)$. As a subset of the topological space T , $\mathbf{S}(\mathbf{H}_n)$ fulfils:*

$$\partial\mathbf{S}(\mathbf{H}_n) = \{\sigma \in \mathbf{S}(\mathbf{H}_n) | \dim(\text{Ran}(\sigma)) < n\}, \text{Int}(\mathbf{S}(\mathbf{H}_n)) = \{\sigma \in \mathbf{S}(\mathbf{H}_n) | \dim(\text{Ran}(\sigma)) = n\}.$$

In particular: $\mathbf{S}_p(\mathbf{H}_n) = \{\sigma \in \mathbf{S}(\mathbf{H}_n) | \dim(\text{Ran}(\sigma)) = 1\} \subset \partial\mathbf{S}(\mathbf{H}_n)$, and $\mathbf{S}_p(\mathbf{H}_n) = \partial\mathbf{S}(\mathbf{H}_n)$ if and only if $n = 2$.

Proof. 1. The norms $\|\cdot\|$, $\|\cdot\|_1$, $\|\cdot\|_2$ are topologically equivalent since $\mathfrak{B}(\mathbf{H}_n) = \mathfrak{B}_1(\mathbf{H}_n) = \mathfrak{B}_2(\mathbf{H}_n)$ are finite dimensional normed spaces with respect to the corresponding norms.
 2. $\mathbf{S}(\mathbf{H}_n)$ is compact since it is closed and bounded, with respect to the norm $\|\cdot\|_1$, in a finite dimensional normed space. Since $\mathbf{S}(\mathbf{H}_n)$ is compact and the zero operator $0 \notin \mathbf{S}(\mathbf{H}_n)$, the continuous functions $\mathbf{S}(\mathbf{H}_n) \ni \sigma \mapsto d(0, \sigma) = \|\sigma\|$, $\mathbf{S}(\mathbf{H}_n) \ni \sigma \mapsto d_1(0, \sigma) = \|\sigma\|_1$,

$\mathbf{S}(\mathbf{H}_n) \ni \sigma \mapsto d_2(0, \sigma) = \|\sigma\|_2$ must have strictly positive minima (and maxima). For d_1 everything is trivial. Let us pass to consider d and d_2 . Using the fact that the n eigenvalues q_k of $\sigma \in \mathbf{S}(\mathbf{H}_n)$ verify both $q_k \in [0, 1]$ and $\sum_{k=1}^n q_k = 1$ one sees that $\sum_{k=1}^n q_k^2 \geq \frac{n}{n^2}$, and $1/n$ is indeed the least possible value. All that is equivalent to say that $\|\frac{1}{n}I\|_2 \leq \|\sigma\|_2$ where $\frac{1}{n}I$ is an admitted state. Again with the constraints $q_k \in [0, 1]$ and $\sum_{k=1}^n q_k = 1$, the maximum of the eigenvalues $q_k = |q_k|$ must be greater than $1/n$, that is equivalent to say $\|\sigma\| \geq \|\frac{1}{n}I\|$. Concerning maxima, $q_k \in [0, 1]$ and $\sum_{k=1}^n q_k = 1$ imply, varying $\sigma \in \mathbf{S}(\mathbf{H}_n)$: $1 \geq \sum_{k=1}^n q(\sigma)_k^2$ and $\max\{q(\sigma)_k \mid k = 1, \dots, n, \sigma \in \mathbf{S}(\mathbf{H}_n)\} = 1$ determining the maximum of both $\sigma \mapsto \|\sigma\|_2$ and $\sigma \mapsto \|\sigma\|$ since the value 1 of the norms is attained on pure states.

3. We view $\mathbf{S}(\mathbf{H}_n)$ a subset of the topological space T of self-adjoint operators A on \mathbf{H}_n with $tr(A) = 1$ endowed with the topology induced by $\mathfrak{B}(\mathbf{H}_n)$.

First of all, notice that $\mathbf{S}(\mathbf{H}_n) \supset \partial\mathbf{S}(\mathbf{H}_n)$ because the former is closed with respect to the said topology, so $\mathbf{S}(\mathbf{H}_n)$ is the disjoint union of $\partial\mathbf{S}(\mathbf{H}_n)$ and $Int(\mathbf{S}(\mathbf{H}_n))$. Let σ be an element of $\mathbf{S}(\mathbf{H}_n)$. First suppose that $dim(Ran(\sigma)) = n$ we want to show that $\sigma \in Int(\mathbf{S}(\mathbf{H}_n))$, that is, there is an open set $O \subset T$ containing σ and such that $\sigma' \in O$ entails $\sigma' \in \mathbf{S}(\mathbf{H}_n)$. To this end, let us define $m := \min\{\langle \psi | \sigma \psi \rangle \mid \|\psi\| = 1\}$. m is real since $\sigma = \sigma^*$ and $m > 0$, because: (1) all eigenvalues of σ are strictly positive (since $\sigma \geq 0$ and $dim(Ran(\sigma)) = n$), (2) $\psi \mapsto \langle \psi | \sigma \psi \rangle$ is continuous and (3) the set of vectors ψ with $\|\psi\| = 1$ is compact because $dim(\mathbf{H}_n) = n < +\infty$. Next, if $\sigma' = \sigma'^* \in \mathfrak{B}(\mathbf{H}_n)$ verifies $\|\sigma - \sigma'\| < m/2$, one has:

$$\frac{m}{2} \leq \|\sigma - \sigma'\| = \sup\{|\langle \psi | (\sigma - \sigma') \psi \rangle| \mid \|\psi\| = 1\}$$

so that: $\langle \psi | \sigma' \psi \rangle = \langle \psi | \sigma' \psi \rangle - \langle \psi | \sigma \psi \rangle + \langle \psi | \sigma \psi \rangle \geq -\frac{m}{2} + m = \frac{m}{2} > 0$ for $\|\psi\| = 1$. Consequently: $\sigma' \geq 0$. Summarizing, if $B_{m/2}(\sigma)$ denotes the open ball in $\mathfrak{B}(\mathbf{H}_n)$ centred on σ with radius $m/2$, $O := T \cap B_{m/2}(\sigma)$ is open in T by definition and $\sigma' \in O$ verifies $\sigma' = \sigma'^*$, $tr \sigma' = 1$ and, as we have proved, $\sigma' \geq 0$. In other words, for $\sigma \in \mathbf{S}(\mathbf{H}_n)$, $dim(Ran(\sigma)) = n$ implies $\sigma \in Int(\mathbf{S}(\mathbf{H}_n))$.

We pass to the other case for $\sigma \in \mathbf{S}(\mathbf{H}_n)$. We suppose that $dim(Ran(\sigma)) < n$ and we want to show that $\sigma \in \partial\mathbf{S}(\mathbf{H}_n)$. $dim(Ran(\sigma)) < n$ implies $det(\sigma) = 0$. Thus all eigenvalues are non-negative and one at least vanishes. Let $\psi \in Ker(\sigma)$. The operators, for $n = 1, 2, \dots$:

$$\sigma_n := \left(1 + \frac{1}{n}\right) \sigma - \frac{1}{n} \psi \langle \psi | \cdot \rangle,$$

are self-adjoint with $tr(\sigma_n) = 1$ so that they stay in T . Furthermore they verify $\sigma_n \rightarrow \sigma$ for $n \rightarrow +\infty$, but $\sigma_n \notin \mathbf{S}(\mathbf{H}_n)$ because σ_n has the negative eigenvalue $-\frac{1}{n}$. So $\sigma \in \partial\mathbf{S}(\mathbf{H}_n)$. In particular, since a pure state is a one-dimensional orthogonal projector, it verifies $dim(Ran(\sigma)) = 1 < n$ and thus $\sigma \in \partial\mathbf{S}(\mathbf{H}_n)$. If $n = 2$ this is the only possible case for an element $\sigma \in \partial\mathbf{S}(\mathbf{H}_n)$. However, if $n > 2$, also elements of $\mathbf{S}(\mathbf{H}_n)$ with $dim(Ran(\sigma)) \leq n - 1$ belong to $\partial\mathbf{S}(\mathbf{H}_n)$. \square

1.2 A set of axioms for QM

1.2.1 Quantum states from quantum logic

From the point of view of the mathematical structure, for any scientific theory there is a set of fundamental statements or axioms from which the whole theory can be derived in a very general manner. Nonrelativistic QM has an accepted axiomatic formulation that we briefly discuss in this section in order to introduce the Gleason theorem and its physical implications.

One of the first experimental evidences of quantum phenomenology is the production of *probabilistic outcomes*, so it is not possible to deterministically predict a measurement outcome but only the probability of each possible outcome. After this operative achievement the first question can be: Is Quantum Mechanics complete? In this regards there are the celebrated extensions via so-called *hidden variables*, one of the consequences of Gleason's theorem is establishing a relevant constraint on a possible extension of QM to a deterministic theory.

A general theory of probability is based on two main definitions: The set of possible events and the probability measure defined on such set. If we found QM as a probability theory the set of events is made by the possible outcomes of an experimental measurement performed on a quantum system or, equivalently, by the *propositions* that describe the outcomes like the following proposition referred to a measurement of a physical quantity performed at time t : «The measured value of the physical quantity A , at time t , belongs to $[a, b] \subset \mathbb{R}$ ». Thus the existence of incompatible quantities¹ implies the existence of incompatible propositions, so we need a mathematical structure on the event space taking into account this fact. If two quantum propositions are incompatible then the simultaneous assignement of their truth value has not a physical meaning, then a Boolean σ -algebra where conjunction and disjunction are always possible is not a suitable model to describe quantum propositions.

In their 1936 outstanding paper about quantum logic [7], Birkhoff and von Neumann identified a good model to describe the set of quantum events in the algebra of closed subspaces of a Hilbert space. Within a modern approach we can describe quantum propositions by means of orthogonal projectors in a Hilbert space \mathbf{H} . Orthogonal projectors are bounded operators that are self-adjoint and idempotent, so their set is defined as:

$$\mathfrak{P}(\mathbf{H}) := \{P \in \mathfrak{B}(\mathbf{H}) | PP = P, P^* = P\}. \quad (1.11)$$

In order to discuss the interesting structure of $\mathfrak{P}(\mathbf{H})$, let us recall the definition of a lattice as a partially ordered set.

Definition 4 Let (X, \geq) be a poset. It is called **lattice** if for any pair $x, y \in X$ the

¹We choose the existence of incompatible quantities as the heuristic definition of a quantum system or, in other words, the phenomenological definition of the quantumness of a physical system.

subset $\{x, y\}$ admits infimum and supremum.

We denote $\sup\{x, y\}$ as $x \vee y$ and $\inf\{x, y\}$ as $x \wedge y$. The following theorem shows that $\mathfrak{P}(\mathbf{H})$, equipped with the standard order relation \geq between linear operators² has the structure of a lattice with some crucial properties.

Theorem 5 *Let \mathbf{H} be a Hilbert space. The set $\mathfrak{P}(\mathbf{H})$ of orthogonal projectors in \mathbf{H} equipped with the standard operator order relation \geq is a lattice with the following properties:*

- i) Maximum and minimum in $\mathfrak{P}(\mathbf{H})$ are respectively the identity operator \mathbb{I} and the null operator 0 , i.e. $\mathfrak{P}(\mathbf{H})$ is a bounded lattice;*
- ii) If $\dim \mathbf{H} \geq 2$ then $\mathfrak{P}(\mathbf{H})$ is not distributive;*
- iii) If $P, Q \in \mathfrak{P}(\mathbf{H})$ satisfy $[P, Q] = PQ - QP = 0$ then:*

$$P \wedge Q = PQ,$$

$$P \vee Q = P + Q - PQ;$$

- iv) A set $\mathfrak{P}_0(\mathbf{H})$ of pairwise commuting elements of $\mathfrak{P}(\mathbf{H})$ which is maximal w.r.t. the commutation condition is a Boolean σ -algebra, i.e. $\mathfrak{P}_0(\mathbf{H})$ is a bounded distributive lattice that is orthocomplemented³ and σ -complete⁴.*

Even the lattice $\mathfrak{P}(\mathbf{H})$ is orthocomplemented (the orthocomplement of $P \in \mathfrak{P}(\mathbf{H})$ is given by $\neg P = \mathbb{I} - P$) and σ -complete but not distributive (ii), thus it does not carry the structure of a Boolean algebra which can be restored in any set of commuting projectors. In $\mathfrak{P}_0(\mathbf{H})$, \vee and \wedge can be interpreted as logical connectives *or* and *and* respectively, \neg as a negation *not* and \leq as the logical implication \Rightarrow . Thus we can summarize these assumptions in the statement of an axiom-zero which requires that quantum propositions, i.e. elementary propositions about a quantum system (whose truth value is assigned after an experimental measurement), are represented by orthogonal projectors in a Hilbert space and the compatibility corresponds to commutativity.

² \geq is defined as $A \geq B$ iff $\langle \psi | A - B \psi \rangle \geq 0$ for all $\psi \in \mathbf{H}$, where $\langle |, \rangle$ denotes the inner product in \mathbf{H} .

³A lattice (X, \geq) is orthocomplemented if there exists a map $\neg : X \ni a \mapsto \neg a$ such that: $a \vee \neg a = 1$, $a \wedge \neg a = 0$, $\neg(\neg a) = a$, if $a \geq b$ then $\neg b \geq \neg a$ for any $a, b \in X$.

⁴A lattice (X, \geq) is σ -complete if each countable set $\{a_n\}_{n \in \mathbb{N}} \subset X$ admits supremum.

Axiom 0 Quantum propositions are in bijective correspondence with the lattice of orthogonal projectors in a Hilbert space with the following identifications:

- i) Compatible propositions correspond to commuting projectors;
- ii) Logical implication (\Rightarrow) correspond with order relation \leq ;
- iii) Always true proposition corresponds to identity \mathbb{I} and always false proposition corresponds to null operator 0 ;
- iv) The negation of the proposition given by the projector P corresponds to $\mathbb{I} - P$;
- v) If two propositions are compatible then their logical conjunction (disjunction) makes sense and corresponds to \wedge (\vee).

If two orthogonal projectors do not commute then operations \wedge and \vee do not produce orthogonal projectors, i.e. quantum propositions, this is consistent with the notion of incompatibility as a non-commutativity. At the beginning of this chapter, we gave the operative definition of quantumness of a physical system as the existence of incompatible physical quantities, now we can characterize the quantum nature of a system by means of the notion of *non-commutativity* in a mathematical structure: This notion is recurrent in every quantization prescription and ubiquitous in Quantum Physics.

Let us introduce the following general definition:

Definition 6 Let S be a quantum system and H be a Hilbert space. We say S is **described in H** if the quantum propositions about S are in bijective correspondence with the elements of $\mathfrak{P}(H)$ in the sense of Axiom 0.

If one consider a quantum system described in H , then a very abstract notion of physical state of the system, a *quantum state*, at time t is given by a map acting on $\mathfrak{P}(H)$ and valued in $[0, 1]$ whose action on any proposition is the assignment of the probability that it turns out to be true after an experimental measurement performed at time t . In other words we can require that quantum states are represented by *generalized probability measures* on $\mathfrak{P}(H)$ as an axiom:

Axiom 1 A state at time t of a quantum system is a map $\mu : \mathfrak{P}(H) \rightarrow [0, 1]$ satisfying the following properties:

- i) Normalization: $\mu(\mathbb{I}) = 1$;
- ii) If $\{P_i\}_{i \in \mathbb{N}} \subset \mathfrak{P}(H)$ satisfies $P_i P_j = 0$, for $i \neq j$, then:

$$\mu \left(s - \sum_{i=0}^{\infty} P_i \right) = \sum_{i=0}^{\infty} \mu(P_i).$$

Requirement ii) is a generalization of σ -additivity. One can prove the existence of a class of functions provided by the axiom 1 [32]. For a fixed state μ of a quantum system, propositions about the system are divided into classes: There is a class of propositions

$\{P\}$ such that $\mu(P) = 1$ and a class of propositions $\{Q\}$ such that $\mu(Q) < 1$. We can assume that propositions of the first kind correspond to the *properties* of the system in that state, the so-called *good quantum numbers*. A concrete characterization of quantum states is given by the statement of Gleason's theorem.

Theorem 7 (Gleason's theorem) *Let \mathbf{H} be a complex separable Hilbert space with $\dim \mathbf{H} > 2$. For each function $\mu : \mathfrak{P}(\mathbf{H}) \rightarrow [0, 1]$ satisfying the properties required by Axiom 1, there exists a unique positive trace-class operator T with trace equal to 1 such that:*

$$\mu(P) = \text{tr}(TP) \quad \forall P \in \mathfrak{P}(\mathbf{H}).$$

The converse is true: Every $T \in \mathfrak{B}_1(\mathbf{H})$ which is positive with $\text{tr}(T) = 1$ defines a generalized probability measure (Axiom 1) as $P \mapsto \text{tr}(TP)$.

By means of Gleason's theorem, we can introduce the notion of quantum state as a positive normalized trace-class operator, i.e. a *density matrix*. The first version of the complicated proof of this theorem is presented in [21], but an alternative proof based on the machinery of frame functions is sketched in the next chapter.

A remarkable corollary of Gleason's theorem is given by the Kochen-Specker theorem, whose physical interpretation is crucial to establish a constraint on a hidden variables extension of QM, more precisely the statement of the theorem is a negative result: a map as in Axiom 1 cannot describe a deterministic state. As a probability measure, a deterministic state should be represented by a Dirac measure which has values 0 or 1, for example in Classical Mechanics a deterministic state can be defined as a Dirac measure whose support is a single point of phase space.

Theorem 8 (Kochen-Specker) *Let \mathbf{H} be a complex separable Hilbert space with $\dim \mathbf{H} > 2$. There is no (bi-valued) function $\mu : \mathfrak{P}(\mathbf{H}) \rightarrow \{0, 1\}$ satisfying the properties required by Axiom 1.*

Proof. By the application of Gleason's theorem one has that a $\mu : \mathfrak{P}(\mathbf{H}) \rightarrow \{0, 1\}$ defines a function on the unit sphere $\mathbb{S}(\mathbf{H})$, given by $f : \psi \mapsto \mu(|\psi\rangle\langle\psi|) = \langle\psi|T\psi\rangle$ with $T \in \mathfrak{B}_1(\mathbf{H})$ positive and normalized, which is continuous w.r.t. the induced topology. Thus its range is connected as well as $\mathbb{S}(\mathbf{H})$. So $f(\psi) = 0$ for every $\psi \in \mathbb{S}(\mathbf{H})$ or $f(\psi) = 1$ for every $\psi \in \mathbb{S}(\mathbf{H})$. In the first case $T = 0$, then $\text{tr}(T) \neq 1$; in the second case $T = \mathbb{I}$, so $\text{tr}(T) \neq 1$ in finite dimension and it is not trace-class in infinite dimension. \square

Consider a quantum system described in the Hilbert space \mathbf{H} , the set of states is given by:

$$\mathbf{S}(\mathbf{H}) = \{\rho \in \mathfrak{B}_1(\mathbf{H}) | \rho \geq 0, \text{tr}(\rho) = 1\}, \quad (1.12)$$

an element $\rho \in \mathbf{S}(\mathbf{H})$ is historically called **density matrix**. In proposition 2 there is the well-known characterization of the convex set $\mathbf{S}(\mathbf{H})$ in $\mathfrak{B}_1(\mathbf{H})$. The extremal elements,

pure states, are given by the all rank-1 orthogonal projectors $\rho_\psi = |\psi\rangle\langle\psi|$ with $\|\psi\| = 1$. According to Krein-Millman theorem, every element of $\mathbf{S}(\mathbf{H})$ can be obtained as a convex combination of pure states and the coefficients of the combination can be interpreted as statistical weights in a mixed state. Moreover, using the statement of Gleason's theorem, we can observe that the notion of transition probability between pure states is encoded in the Axiom 1. Consider a quantum system S and the elementary proposition P_ψ : «The state of S at time t is the pure state identified by the normalized vector $\psi \in \mathbf{H}$ », if $\rho \in \mathbf{S}(\mathbf{H})$ then $\text{tr}(\rho P_\psi) = 1$ if and only if $\rho = |\psi\rangle\langle\psi|$. So the quantity $\text{tr}(\rho_\phi P_\psi) = |\langle\phi|\psi\rangle|^2$ can be interpreted as the probability that there is a transition from the pure state $|\psi\rangle\langle\psi|$ to the pure state $|\phi\rangle\langle\phi|$ after a measurement performed at time t .

1.2.2 Measurement processes and quantum observables

In order to state an axiom about quantum measurement, we start from an evidence of quantum phenomenology: *If a measurement of a physical quantity performed on a quantum system gives a certain result, then an immediately following measurement of the same quantity produces the same result.* This fact is historically called *collapse of the wavefunction*, it is fundamental to *prepare* a quantum system in a given state. Now we need an axiom whose requirements imply the observed collapse of wavefunction.

Axiom 2 Let S be a quantum system. If the state S at time t is $\rho \in \mathbf{S}(\mathbf{H})$ and the proposition represented by $P \in \mathfrak{P}(\mathbf{H})$ is verified by a measurement process at time t , after this measurement the state of S is:

$$\rho_P = \frac{P\rho P}{\text{tr}(\rho P)}.$$

The content of Axiom 2 seems to be an almost instantaneous non-unitary evolution from a state to another one (unitary evolution of a quantum system is an axiom of QM, see next section). This apparent contradiction originates by the following fact: measurement apparatus is external to the observed system thus we have not the evolution of a closed system; in this regard the theory of open quantum systems can be used to study quantum measurements beyond the basic description provided in Axiom 2.

In this section we briefly describe how all physical quantities (quantum observables) can be represented in the set of axioms. Consider an observable A (i.e. a physical quantity whose value can be known by means an experimental measurement, thus its value should be a real number) and a Borel set $E \in \mathcal{B}(\mathbb{R})$, we can formulate the proposition $P_E^{(A)}$: «the value of A measured at time t belong to E ». Thus a general notion of observable can be given in the following terms: An observable is a map from the Borel σ -algebra of \mathbb{R} to the lattice of orthogonal projectors in a Hilbert space. According to Axiom 0 which establishes the model for propositions and logical connectives, a quantum observable can be represented by a *projective valued measure* (PVM or spectral measure).

Axiom 3 Each observable which can be measured by an experiment on the system S described in the Hilbert space \mathbf{H} is represented by a map $A : \mathcal{B}(\mathbb{R}) \rightarrow \mathfrak{P}(\mathbf{H}) : E \mapsto P_E^{(A)}$ such that:

- i) $[P_E^{(A)}, P_{E'}^{(A)}] = 0$ for any pair $E, E' \in \mathcal{B}(\mathbb{R})$;
- ii) $P_E^{(A)} \wedge P_{E'}^{(A)} = P_{E \cap E'}^{(A)}$ for any pair $E, E' \in \mathcal{B}(\mathbb{R})$;
- iii) $P_{\mathbb{R}}^{(A)} = \mathbb{I}$;
- iv) If $\{E_n\}_{n \in \mathbb{N}}$ is a countable family of Borel sets then: $\bigvee_{n \in \mathbb{N}} P_{E_n}^{(A)} = P_{\bigcup_{n \in \mathbb{N}} E_n}^{(A)}$

The first requirement implies that every quantum observable is compatible with itself, ii) and iv) are imposed by consistency with Axiom 0 and iii) is the requirement that a measurement outcome be a real number. In the standard formulation of QM, observables are represented by self-adjoint operators in a Hilbert space, this picture can be recovered via the spectral theory, in particular with the notion of integration w.r.t. a PVM⁵, where the bijective correspondence between spectral measures on \mathbb{R} and self-adjoint operators can be proved. The general spectral decomposition of a (bounded or unbounded) self-adjoint operator A has the celebrated form:

$$A = \int_{sp(A)} \lambda dP^{(A)}(\lambda), \quad (1.13)$$

where $sp(A)$ is the spectrum of A which corresponds with the support of $P^{(A)}$.

1.2.3 Quantum dynamics

In chapter 4 and chapter 5, we will discuss how time evolution of a quantum system can be described by a Hamiltonian vector field as well as a classical system. Here, we simply recall how quantum dynamics is described in the standard formulation of quantum mechanics, the following axiom states the unitarity of time evolution in QM.

Axiom 4 Let S be a quantum system described in the Hilbert space \mathbf{H} and J be an inertial frame of reference. There exists a self-adjoint operator H on \mathbf{H} corresponding to the observable *total mechanical energy of S* and a one-parameter family $\{\sigma_t\}_{t \in \mathbb{R}^+} \subset \mathfrak{S}(\mathbf{H})$ such that:

- i) $\sigma(H)$ is lower bounded;
- ii) For a fixed $\tau \in \mathbb{R}$: $\sigma_{t+\tau} = e^{-i\frac{\tau}{\hbar}H} \sigma_t e^{i\frac{\tau}{\hbar}H}$, for all $t \in \mathbb{R}^+$.

Let us define some basic concepts in view of the above axiom:

⁵The integral w.r.t. a spectral measure P is defined on a simple function $s = \sum_i a_i \chi_{E_i}$ as $\int s dP := \sum_i a_i P(E_i)$. There is a unique extension of the defined integral operator to the Banach space of bounded Borel-measurable functions.

Definition 9 The self-adjoint operator H , introduced in Axiom 4, is called **Hamiltonian of the system**. The family $\{\sigma_t\}_{t \in \mathbb{R}^+}$ of quantum states is called **time evolution of the system S (or quantum dynamics)**. The strongly continuous one-parameter group $\{U_\tau\}_{\tau \in \mathbb{R}} = \{e^{-i\frac{\tau}{\hbar}H}\}_{\tau \in \mathbb{R}}$ is called **time evolver** of the system S with respect to the frame of reference J .

The first requirement of Axiom 4 avoids the existence of a quantum system which can radiate an infinite amount of energy, while the second one implements the following principle, known since the pioneering times of QM: *The motion of a quantum system with energy E is periodic and its frequency ω is given by the law $E = \hbar\omega$.*

If σ_t is a pure state, then $\sigma_{t+\tau}$ is pure as well by definition of quantum dynamics. Writing these states as projectors $\sigma_t = |\psi_t\rangle\langle\psi_t|$ and $\sigma_{t+\tau} = |\psi_{t+\tau}\rangle\langle\psi_{t+\tau}|$, Axiom 4 gives the equation of motion for pure states:

$$\psi_{t+\tau} = e^{-i\frac{\tau}{\hbar}H}\psi_t. \quad (1.14)$$

Denoting the domain of H as $D(H)$, $\psi_t \in D(H)$ implies $\psi_{t+\tau} \in D(H)$ as one can prove applying the spectral theorem for unbounded self-adjoint operators. Moreover Stone theorem on one-parameter unitary groups ensures the existence of the limit:

$$\left(\frac{dU_t}{dt}\right)_{t=0} \psi := \lim_{t \rightarrow 0} \frac{U_t\psi - \psi}{t} \quad \forall \psi \in D(H), \quad (1.15)$$

and the relation:

$$\left(\frac{dU_t}{dt}\right)_{t=0} \psi = iH\psi \quad \forall \psi \in D(H). \quad (1.16)$$

Using (1.14) and (1.16), one has the **Schrödinger equation**:

$$i\hbar \frac{d}{dt} \psi_t = H\psi_t. \quad (1.17)$$

Suppose the quantum dynamics (in a frame of reference J) of the system S is given by the time evolver $\{U_\tau\}_{\tau \in \mathbb{R}}$, one can define the map $\gamma_\tau^{(H)}(\sigma) := U_\tau\sigma U_\tau^{-1}$. The continuous projective representation of the abelian group \mathbb{R} induced by U_τ in this way $\mathbb{R} \ni \tau \mapsto \gamma_\tau^{(H)}$ is called **dynamical flow** of S w.r.t. J . If A is a quantum observable, its **Heisenberg representation** at time t is defined as:

$$A_H(t) := \gamma_t^{(H)*}(A) = e^{itH} A e^{-itH} \quad \hbar = 1, \quad (1.18)$$

where $\mathbb{R} \ni t \mapsto \gamma_t^{(H)*}$ is the contragradient representation of $\mathbb{R} \ni t \mapsto \gamma_t^{(H)}$. In this dual picture quantum states do not evolve in time and dynamics is represented in terms of observables.

A constant of motion is a physical quantity for which the probabilities of measuring its values are independent of time in all states of the system. Thus a good mathematical definition is the following: The observable A is a **constant of motion** if its Heisenberg representation satisfies:

$$A_H(t) = A_H(0) \quad \forall t \in \mathbb{R}. \quad (1.19)$$

Neglecting the issues about the domain of the operators we have that (1.19) is true if and only if A commutes with H , in particular this equivalence is true in finite dimension where the notion of domain of linear operators is superfluous.

1.2.4 Composite quantum systems

The last item of the present axiomatic setting is focused on composite quantum systems. Chapter 5 of the dissertation is devoted to the application of geometric Hamiltonian formulation to describe composite quantum systems made by two subsystems.

Axiom 5 If a quantum system S is composed of subsystems S_1 and S_2 that are described in Hilbert spaces \mathbf{H}_1 and \mathbf{H}_2 , then S is described in the Hilbert space given by the tensor product $\mathbf{H}_1 \otimes \mathbf{H}_2$.

Obviously the requirement of Axiom 5 can extend to quantum systems made by n subsystems. If the state at time t of subsystem S_1 is described by the density matrix σ_1 and the state at time t of S_2 is described by σ_2 then the state at time t of S is described by $\sigma_1 \otimes \sigma_2$. However not all the density matrices in $\mathbf{S}(\mathbf{H}_1 \otimes \mathbf{H}_2)$ are of product form $\sigma_1 \otimes \sigma_2$ by definition of quantum state; there are the so-called *entangled states* for which the quantum state of each subsystem *cannot* be described independently.

If A_1 is an observable for the subsystem S_1 then $A_1 \otimes \mathbb{I}_2$, where \mathbb{I}_2 is the identity operator in \mathbf{H}_2 , is the corresponding observable for the composite system S . Since the operators $A_1 \otimes \mathbb{I}_2$ and $\mathbb{I}_1 \otimes A_2$ always commute (i.e. describe compatible observables) then measurements on different subsystems can always be performed simultaneously. Some basic features of composite systems are defined and characterized in chapter 5 of the present dissertation.

1.3 Algebraic formulation

Algebraic approach to QM is a very general way to formulate quantum theories which is also adopted in QFT, it provides a generalization of the standard framework discussed above. In the section 4.3 of the present work the interplay of algebraic and geometric formulations of QM is discussed.

Definition 10 A linear associative algebra \mathfrak{A} over \mathbb{C} is a C^* -algebra if it has the following properties:

- i) \mathfrak{A} is a Banach algebra, i.e. a normed space such that its norm $\| \cdot \|$ satisfies:
 $\|AB\| \leq \|A\| \|B\|$ for all $A, B \in \mathfrak{A}$ and \mathfrak{A} is complete w.r.t. the topology induced by $\| \cdot \|$;
- ii) There is an involution $*$: $\mathfrak{A} \rightarrow \mathfrak{A}$,

$$(A + B)^* = A^* + B^* \quad (\lambda A)^* = \bar{\lambda}A^* \quad (AB)^* = B^*A^* \quad (A^*)^* = A;$$

for all $A, B \in \mathfrak{A}$ and $\lambda \in \mathbb{C}$;

- iii) $\|A^*A\| = \|A\|^2$ for all $A \in \mathfrak{A}$.

The algebraic approach to the general mathematical description of a physical system is based on the following assumptions:

Assumption 1 A physical system is completely characterized by an associated C^* -algebra \mathfrak{A} (with identity). The observables of the system are the self-adjoint elements $A^* = A$ of \mathfrak{A} .

Assumption 2 A state of the system is a normalized positive linear functional on \mathfrak{A} .

Some arguments to recognize the structure of a C^* -algebra in a set of physical quantities, justifying the above assumptions, are given in [41] for example. The action of a state ω on a $A \in \mathfrak{A}$ is interpreted as the expectation value of A on ω . The set of states turns out to be a convex set of the dual \mathfrak{A}' of \mathfrak{A} , so we can define the notion of *pure states* even in the algebraic formalism.

The observables of a quantum system generate a *non-abelian* C^* -algebra which is an absolutely abstract object. Thus finding concrete realizations of the C^* -algebra of observables is crucial to describe a physical system. From Gelfand-Naimark theory, we know that every abelian C^* -algebra (classical systems) is represented by an algebra of continuous functions on a compact space (given by the Gelfand spectrum). In order to study quantum systems, one must know the concrete realization of a general abstract C^* -algebra. An outstanding result in this way is given by *Gelfand-Naimark-Segal theorem* which establishes that every state ω on a C^* -algebra \mathfrak{A} defines a unique (up to unitaries) representation of \mathfrak{A} in a Hilbert space H_ω .

Theorem 11 (GNS) Let \mathfrak{A} be a C^* -algebra with identity and ω be a state on \mathfrak{A} . There is a Hilbert space H_ω , a representation $\pi_\omega : \mathfrak{A} \rightarrow \mathfrak{B}(H_\omega)$ and a cyclic vector $\Psi_\omega \in H_\omega$ such that:

$$\omega(A) = \langle \Psi_\omega | \pi_\omega(A) \Psi_\omega \rangle \quad \forall A \in \mathfrak{A}. \quad (1.20)$$

Every representation π of \mathfrak{A} in \mathbf{H}_ω with cyclic vector Ψ s.t. $\omega(A) = \langle \Psi | \pi(A) \Psi \rangle \forall A \in \mathfrak{A}$, is unitarily equivalent to π_ω .

GNS theorem shows that the abstract structure of the algebraic formulation can be concretely realized in terms of standard formulation in Hilbert spaces: Representation of observables as operators and expectation values as matrix elements. Thus the fundamental Hilbert space structure of QM postulated in the discussed axiomatic setting is a structural consequence of the first assumption of the algebraic approach. Another feature of the standard formulation arising from GNS theorem is the following: The cyclic vector Ψ_ω can be interpreted as the *state vector* associated to ω in fact the action of ω on the observable A , i.e. the expectation value, is the matrix element w.r.t. this vector. However also a mixed state can be represented by a state vector using the cyclic vector of its GNS representation. But one can prove that GNS representation of ω is irreducible if and only if ω is pure, thus a mixed state cannot be represented by a cyclic vector of an irreducible representation. In a irreducible representation, mixed states are obtained as convex combinations of pure states.

GNS representation defined by a state may not be faithful. A very important and celebrated result is the following.

Theorem 12 (Gelfand-Naimark) *A C^* -algebra \mathfrak{A} is isomorphic to an algebra of bounded operators in a Hilbert space.*

The C^* -isomorphism provided by Gelfand-Naimark theorem can be constructed as the direct sum $\bigoplus_\omega \pi_\omega$ where ω ranges over pure states and π_ω is the associated irreducible GNS representation [41]. In section 4.3 we construct explicitly the C^* -algebra of observables $\mathcal{F}^2(\mathbf{H})$ of a finite-dimensional quantum system in terms of classical-like observables exploiting the machinery of frame functions. The studied prescription to obtain classical-like observables in the geometric formulation from self-adjoint operators in a n -dimensional Hilbert space \mathbf{H}_n is extended by linearity to $\mathfrak{B}(\mathbf{H}_n)$ giving rise to the Gelfand-Naimark C^* -isomorphism. Definitions of a suitable product and a norm on $\mathcal{F}^2(\mathbf{H}_n)$ allow a geometric description of the C^* -algebraic structure of quantum observables in terms of the Kähler structure of the projective space $\mathbf{P}(\mathbf{H}_n)$.

Chapter 2

Machinery of frame functions

Content of this chapter is based on the paper [33].

2.1 Frame functions and quantum states

In the previous chapter Gleason's theorem (theorem 7) is introduced as a remarkable result to characterize quantum states of a system described in \mathbf{H} that are generalized probability measures (GPMs), according to Axiom 1, defined on the lattice of orthogonal projectors $\mathfrak{P}(\mathbf{H})$. Gleason's theorem establishes that GPMs are in bijective correspondence with density matrices. The key-tool exploited in Gleason's proof is the notion of *frame function* [21].

Definition 13 *Let \mathbf{H} be a complex separable Hilbert space and $\mathbb{S}(\mathbf{H}) := \{\psi \in \mathbf{H} \mid \|\psi\| = 1\}$. A map $f : \mathbb{S}(\mathbf{H}) \rightarrow \mathbb{C}$ is called **frame function** on \mathbf{H} if there is $W_f \in \mathbb{C}$, called **weight** of f , such that:*

$$\sum_{x \in N} f(x) = W_f \quad \text{for every Hilbertian basis } N \text{ of } \mathbf{H}. \quad (2.1)$$

As an hint about the importance of frame function in the characterization of quantum states: A GPM $\mu : \mathfrak{P}(\mathbf{H}) \rightarrow [0, 1]$ defines a frame function with unit weight taking the restriction of μ to the set of rank-1 orthogonal projectors:

$$f_\mu(x) = \mu(P_x) \quad \text{with} \quad P_x = |x\rangle\langle x|, \quad x \in \mathbb{S}(\mathbf{H}), \quad (2.2)$$

in fact, once fixed some Hilbertian basis $N \subset \mathbf{H}$:

$$\sum_{x \in N} f_\mu(x) = \mu \left(s - \sum_{x \in N} P_x \right) = \mu(I) = 1.$$

It is known that a real bounded frame function defined on a real Hilbert space with

dimension 3 is continuous and can be uniquely represented as a quadratic form [21, 15]. The key-point of the original proof by Gleason is establishing that there is a positive trace-class operator T_μ with $\text{tr}(T_\mu) = 1$ such that $f_\mu(x) = \langle x|T_\mu x \rangle$ for all $x \in \mathbb{S}(\mathbf{H})$, with $\dim \mathbf{H} \geq 3$. Hence, representing frame functions as quadratic forms is sufficient to prove Gleason's theorem. Let P_Q be the orthogonal projector onto the subspace $Q \subset \mathbf{H}$. Let $\{q_i\}_{i \in I}$ be an orthonormal basis of Q and $\{h_j\}_{j \in J}$ be the set of vectors which complete $\{q_i\}_{i \in I}$ to a basis of \mathbf{H} ; thus:

$$P_Q q_i = q_i \quad \text{and} \quad P_Q h_j = 0 \quad \forall i \in I, \forall j \in J.$$

If μ is a GPM on \mathbf{H} , f_μ is the frame function obtained from μ and T_μ is the associated operator, then we have:

$$\begin{aligned} \mu(P_Q) &= \mu \left(s - \sum_{i \in I} P_{q_i} \right) = \sum_{i \in I} f_\mu(q_i) = \sum_{i \in I} f_\mu(q_i) = \sum_{i \in I} \langle q_i | T_\mu q_i \rangle = \\ &= \sum_{i \in I} \langle q_i | T_\mu P_Q q_i \rangle = \sum_{i \in I} \langle q_i | T_\mu P_Q q_i \rangle + \sum_{j \in J} \langle h_j | T_\mu h_j \rangle = \text{tr}(T_\mu P_Q), \end{aligned}$$

thus $\mu(P) = \text{tr}(AT_\mu)$, for any $P \in \mathfrak{P}(\mathbf{H})$.

In order to give an alternative proof of Gleason theorem [33], we consider a finite-dimensional Hilbert space \mathbf{H} , with $\dim \mathbf{H} \geq 3$, and the unique regular Borel positive measure $\nu_{\mathbf{H}}$ invariant under the action of the unitary operators in \mathbf{H} , with $\nu_{\mathbf{H}}(\mathbb{S}(\mathbf{H})) = 1$, and we prove that for every frame function $f \in \mathcal{L}^2(\mathbb{S}(\mathbf{H}), \nu_{\mathbf{H}})$ there is a unique linear operator $T : \mathbf{H} \rightarrow \mathbf{H}$ such that $f(x) = \langle x|Tx \rangle$ for all $x \in \mathbb{S}(\mathbf{H})$. Sections 2.2 and 2.3 are devoted to the proof of these results. In the next chapter the strong relationship of these results with geometric QM is discussed.

2.2 Generalized complex spherical harmonics

2.2.1 Measure theory on the sphere

To prove that a complex frame function is representable as a quadratic form whenever it is square-integrable w.r.t. the natural measure ν_n , we use the properties of the spaces of *generalized complex spherical harmonics*, in particular some result due to Watanabe [44] and several standard results on Hausdorff compact topological group representations [30].

Let us introduce the unit sphere in \mathbb{C}^n as a $2n - 1$ -dimensional real smooth manifold:

$$\mathbb{S}^{2n-1} := \{x \in \mathbb{C}^n | \langle x|x \rangle = 1\} \quad \text{where} \quad \langle z|w \rangle := \sum_{i=1}^n \bar{z}_i w_i \quad (2.3)$$

ν_n denotes the $U(n)$ -left-invariant (regular and complete) Borel measure on \mathbb{S}^{2n-1} , normalized to $\nu_n(\mathbb{S}^{2n-1}) = 1$, obtained from the two-sided Haar measure on $U(n)$ on the homogeneous space given by the quotient $U(n)/U(n-1) \equiv \mathbb{S}^{2n-1}$ as discussed in Chapter 4 of [11], noticing that both $U(n)$ and $U(n-1)$ are compact and thus unimodular. Let us prove that the measure ν_n is positive.

Lemma 14 *If $A \neq \emptyset$ is an open subset of \mathbb{S}^{2n-1} then $\nu_n(A) > 0$.*

Proof. $\{gA\}_{g \in U(n)}$ is an open covering of \mathbb{S}^{2n-1} . Compactness implies that $\mathbb{S}^{2n-1} = \cup_{k=1}^N g_k A$ for some finite N . If $\nu_n(A) = 0$, sub-additivity and $U(n)$ -left-invariance would imply $\nu_n(\mathbb{S}^{2n-1}) = 0$ that is false. \square

As ν_n is $U(n)$ -left-invariant,

$$U(n) \ni g \rightarrow D_n(g) \quad \text{with } D_n(g)f := f \circ g^{-1} \text{ for } f \in L^2(\mathbb{S}^{2n-1}, d\nu_n) \quad (2.4)$$

defines a faithful unitary representation of $U(n)$ on $L^2(\mathbb{S}^{2n-1}, d\nu_n)$.

Lemma 15 *For every $n = 1, 2, \dots$ the unitary representation (2.4) is strongly continuous.*

Proof. It is enough proving the continuity at $g = I$. If $f \in L^2(\mathbb{S}^{2n-1}, d\nu_n)$ is continuous, $U(n) \times \mathbb{S}^{2n-1} \ni (g, u) \mapsto f(g^{-1}u)$ is jointly continuous and thus bounded by $K < +\infty$ since the domain is compact. Exploiting Lebesgue dominated convergence theorem as $|f \circ g^{-1}(u) - f(u)|^2 \leq K$ and the constant function K being integrable since the measure ν_n is finite:

$$\|D_n(g)f - f\|_2^2 = \int_{\mathbb{S}^{2n-1}} |f \circ g^{-1} - f|^2 d\nu_n \rightarrow 0 \quad \text{as } g \rightarrow I,$$

If f is not continuous, due to Luzin's theorem, there is a sequence of continuous functions f_n converging to f in the norm of $L^2(\mathbb{S}^{2n-1}, d\nu_n)$. Therefore

$$\|f \circ g^{-1} - f\|_2 \leq \|f \circ g^{-1} - f_n g^{-1}\|_2 + \|f_n \circ g^{-1} - f_n\|_2 + \|f_n - f\|_2.$$

If $\epsilon > 0$, there exists k with $\|f \circ g^{-1} - f_k g^{-1}\|_2 = \|f - f_k\|_2 < \epsilon/3$ where we have also used the $U(n)$ -invariance of ν_n . Since f_k is continuous we can apply the previous result getting $\|f_k \circ g^{-1} - f_k\|_2 < \epsilon/3$ if g is sufficiently close to I . \square

We are in a position to define the notion of spherical harmonics we shall use in the rest of the paper. If, $p, q = 0, 1, 2, \dots$, $\mathcal{P}^{p,q}$ denotes the set of polynomials $h : \mathbb{S}^{2n-1} \rightarrow \mathbb{C}$ such that $h(\alpha z_1, \dots, \alpha z_n) = \alpha^p \bar{\alpha}^q h(z_1, \dots, z_n)$ for all $\alpha \in \mathbb{C}$, the standard Laplacian Δ_{2n} on \mathbb{R}^{2n} can be applied to the elements of $\mathcal{P}^{p,q}$ in terms of decomplexified \mathbb{C}^n . Now, we have the following known result (see Theorems 12.2.3, 12.2.7 in [39] and theorem 1.3 in [25]):

Theorem 16 If $\mathbf{H}_{(p,q)}^n := \text{Ker} \Delta_{2n}|_{\mathcal{P}^{p,q}}$, the following facts hold.

(a) The orthogonal decomposition is valid, each $\mathbf{H}_{(p,q)}^n$ being finite-dimensional and closed:

$$L^2(\mathbb{S}^{2n-1}, d\nu_n) = \bigoplus_{p,q=0}^{+\infty} \mathbf{H}_{(p,q)}^n, \quad (2.5)$$

(b) Every $\mathbf{H}_{(p,q)}^n$ is invariant and irreducible under the representation (2.4) of $U(n)$, so that the said representation correspondingly decomposes as

$$D_n(g) = \bigoplus_{p,q=0}^{+\infty} D_n^{p,q}(g) \quad \text{with } D_n^{p,q}(g) := D_n(g)|_{\mathbf{H}_{(p,q)}^n}.$$

(c) If $(p, q) \neq (r, s)$ the irreducible representations $D_n^{p,q}$ and $D_n^{r,s}$ are unitarily inequivalent: there is no unitary operator $U : \mathbf{H}_{(p,q)}^n \rightarrow \mathbf{H}_{(r,s)}^n$ with $UD_n^{p,q}(g) = D_n^{r,s}(g)U$ for every $g \in U(n)$.

Definition 17 For $j \equiv (p, q)$, with $p, q = 0, 1, 2, \dots$, the **generalized complex spherical harmonics** of order j are the elements of $\mathbf{H}_{(p,q)}^n$.

2.2.2 Zonal spherical harmonics

A useful technical lemma is the following.

Lemma 18 For $n \geq 3$, $\mathbf{H}_{(1,1)}^n$ is made of the restrictions to \mathbb{S}^{2n-1} of the polynomials $h^{(1,1)}(z, \bar{z}) = (z|Az) = \bar{z}^t Az$ ($z, \bar{z} \in \mathbb{C}^n$), A being any traceless $n \times n$ matrix.

Proof. $h^{(1,1)}$ is of first-degree in each variables so $h^{(1,1)}(z, \bar{z}) = \bar{z}^t Az$ for some $n \times n$ matrix A . $\Delta_{2n} h^{(1,1)} = 0$ is equivalent to $\text{tr} A = 0$ as one verifies by direct inspection. \square

For $n \geq 3$, there is a special class of spherical harmonics in \mathbf{H}_j^n that are parametrized by vectors $t \in \mathbb{S}^{2n-1}$ [25].

Definition 19 For $n \geq 3$, the **zonal spherical harmonics** are elements of \mathbf{H}_j^n defined as (the scalar product $(\cdot|\cdot)$ being that in (4.22))

$$F_{n,t}^j(u) := R_j^n((u|t)) \quad \forall u \in \mathbb{S}^{2n-1}, \quad (2.6)$$

where the polynomials $R_j^n(z)$ have the generating function

$$(1 - \xi z - \eta \bar{z} + \xi \eta)^{1-n} = \sum_{p,q=0}^{+\infty} R_{p,q}^n(z) \xi^p \eta^q \quad (2.7)$$

with $|z| \leq 1$, $|\eta| < 1$, $|\xi| < 1$.

These zonal spherical harmonics are a generalization of the eigenfunctions of orbital angular momentum with L_z -eigenvalue $m = 0$ as it appears comparing (2.7) with the generating function of Legendre polynomials $P_l(u)$:

$$\frac{1}{\sqrt{1-2tu+t^2}} = \sum_{l=0}^{+\infty} P_l(u)t^l \quad \text{with } |t| < 1, u \in [-1, 1]. \quad (2.8)$$

From (2.7) we get two identities we shall use later:

$$\begin{aligned} p!q!R_{p,q}^n(1) &= (-1)^{p+q}(n-1)n(n+1) \cdots (n+p-2)(n-1)n(n+1) \cdots (n+q-2), \\ p!q!R_{p,q}^n(0) &= (-1)^p \delta_{pq} p!(n-1)n(n+1) \cdots (n+p-2). \end{aligned} \quad (2.9)$$

We intend to show that, in the finite-dimensional, with $\dim(\mathbf{H}) \geq 3$, complex case a frame function $f : \mathbb{S}(\mathbf{H}) \rightarrow \mathbb{C}$, can always be uniquely represented as a quadratic form whenever $f \in \mathcal{L}^2(\mathbb{S}(\mathbf{H}), d\nu)$. We need a preliminary technical result.

Proposition 20 *If $f \in \mathcal{L}^2(\mathbb{S}^{2n-1}, d\nu_n)$, then each projection f_j on \mathbf{H}_j^n verifies, where μ is the Haar measure on $U(n)$ normalized to $\mu(U(n)) = 1$:*

$$f_j(u) = \dim(\mathbf{H}_j^n) \int_{U(n)} \text{tr}(\overline{D^j(g)}) f(g^{-1}u) d\mu(g) \quad \text{a.e. in } u \text{ with respect to } \nu_n, \quad (2.10)$$

where the right-hand side is a continuous function of $u \in \mathbb{S}^{2n-1}$.

If f_j is re-defined on a zero-measure set in order to be continuous and $f \in \mathcal{L}^2(\mathbb{S}^{2n-1}, d\nu_n)$ is a frame function, then f_j is a frame function as well with $W_{f_j} = 0$ when $j \neq (0, 0)$.

Proof. First of all notice that, if $f \in \mathcal{L}^2(\mathbb{S}^{2n-1}, d\nu_n)$, the right-hand side of (2.10) is well defined and continuous. This is because $U(n) \ni g \mapsto \text{tr}(\overline{D^j(g)})$ is continuous – and thus bounded since $U(n)$ is compact – in view of lemma 15 and the fact that $\dim(\mathbf{H}_j^n)$ is finite for theorem 16. Furthermore, for almost all $u \in \mathbb{S}^{2n-1}$ the map $U(n) \ni g \mapsto f(g^{-1}u)$ is $\mathcal{L}^2(U(n), d\mu)$ – and thus $\mathcal{L}^1(U(n), d\mu)$ because the measure is finite – as follows by Fubini-Tonelli theorem and the invariance of ν_n under $U(n)$, it being

$$\int_{U(n)} d\mu(g) \int_{\mathbb{S}^{2n-1}} |f(g^{-1}u)|^2 d\nu_n(u) = \int_{U(n)} d\mu(g) \int_{\mathbb{S}^{2n-1}} |f(u)|^2 d\nu_n(u) = \mu(U(n)) \|f\|_2^2 < +\infty.$$

Actually, in view of the fact that μ is invariant, and $U(n)$ transitively acts on \mathbb{S}^{2n-1} , the

map $U(n) \ni g \mapsto f(g^{-1}u)$ is $\mathcal{L}^2(U(n), d\mu)$ for all $u \in \mathbb{S}^{2n-1}$. Countinuity can be proved by noticing that, as $\mathbb{S}^{2n-1} = U(n)/U(n-1)$, if $u_0 \in \mathbb{S}^{2n-1}$ there is an injective continuous map $\mathbb{S}^{2n-1} \ni u \mapsto g_u$ with $g_u u_0 = u$, that is a continuous left-inverse of the canonical projection $U(n) \rightarrow U(n)/U(n-1)$. Therefore, using the invariance of the Haar measure

$$\int_{U(n)} \text{tr}(\overline{D^j(g)}) f(g^{-1}u) d\mu(g) = \int_{U(n)} \text{tr}(\overline{D^j(g_u g)}) f(g^{-1}u_0) d\mu(g).$$

Since $(u, g) \mapsto \text{tr}(\overline{D^j(g_u g)})$ is continuous due to lemma 15, the measure is finite and $g \mapsto f(g^{-1}u_0)$ is integrable, Lebesgue dominated convergence theorem implies that, as said above, $u \mapsto \int_{U(n)} \text{tr}(\overline{D^j(g_u g)}) f(g^{-1}u_0) d\mu(g)$ is continuous.

Let us pass to prove (2.10) for f containing a finite number of components. So F is finite, $f \in \mathcal{L}^2(\mathbb{S}^{2n-1}, d\nu_n)$ and:

$$f(u) = \sum_{j \in F} f_j(u) = \sum_{j \in F} \sum_{m=1}^{\dim(\mathbf{H}_j^n)} f_m^j Z_m^j(u) \quad f_m^j \in \mathbb{C}$$

where $\{Z_m^j\}_{m=1, \dots, \dim \mathbf{H}_j^n}$ is an orthonormal basis of \mathbf{H}_j^n , with $Z_n^{(0,0)} = 1$, made of continuous functions (it exists in view of the fact that $\mathcal{P}^{p,q}$ is a space of polynomials and exploiting Gramm-Schmidt's procedure), and $f_m^j \in \mathbb{C}$. Then

$$\overline{D_{m_0 m'_0}^{j_0}} f(g^{-1}u) = \sum_{j \in F} \sum_{m, m'} \overline{D_{m_0 m'_0}^{j_0}}(g) D_{mm'}^j(g) f_m^j Z_m^j(u).$$

In view of (c) of theorem 16 and Peter-Weyl theorem, taking the integral over g with respect to the Haar measure on $U(n)$ one has:

$$\int \overline{D_{m_0 m'_0}^{j_0}}(g) f(g^{-1}u) d\mu(g) = \dim(\mathbf{H}_{j_0}^n) f_{m'_0}^{j_0} Z_{m_0}^{j_0}(u),$$

that implies (2.10) when taking the trace, that is summing over $m_0 = m'_0$. To finish with the first part, let us generalize the obtained formula to the case of F infinite. In the following $P_j : L^2(\mathbb{S}^{2n-1}, \nu_n) \rightarrow L^2(\mathbb{S}^{2n-1}, \nu_n)$ is the orthogonal projector onto \mathbf{H}_j^n . The convergence in the norm $\|\cdot\|_2$ implies that in the norm $\|\cdot\|_1$, since $\nu_n(\mathbb{S}^{2n-1}) < +\infty$. So if $h_m \rightarrow f$ in the norm $\|\cdot\|_2$, as P_j is bounded:

$$\lim_{m \rightarrow +\infty}^{\|\cdot\|_1} P_j h_m = \lim_{m \rightarrow +\infty}^{\|\cdot\|_2} P_j h_m = P_j \left(\lim_{m \rightarrow +\infty}^{\|\cdot\|_2} h_m \right) = P_j f.$$

We specialize to the case where each $h_m = \sum_{(p,q)=(0,0)}^{p+q=m} f_{(p,q)}$ so that $h_m \rightarrow f$ as $m \rightarrow +\infty$ in the norm $\|\cdot\|_2$. As every h_m has a finite number of harmonic components the identity above leads to:

$$\dim(\mathbf{H}_j^n) \lim_{m \rightarrow +\infty}^{(\|\cdot\|_1)} \int_{U(n)} \operatorname{tr}(\overline{D^j(g)}) h_m(g^{-1}u) d\mu(g) = P_j f =: f_j.$$

Now notice that, as $U(n) \ni g \mapsto \operatorname{tr}(\overline{D^j(g)})$ is bounded on $U(n)$ by some $K < +\infty$:

$$\begin{aligned} & \left\| \int_{U(n)} \operatorname{tr}(\overline{D^j(g)}) h_m(g^{-1}u) d\mu(g) - \int_{U(n)} \operatorname{tr}(\overline{D^j(g)}) f(g^{-1}u) d\mu(g) \right\|_1 \\ & \leq K \int_{\mathbb{S}^{2n-1}} d\nu(u) \int_{U(n)} d\mu(g) |h_m(g^{-1}u) - f(g^{-1}u)| \\ & = K \int_{U(n)} d\mu(g) \int_{\mathbb{S}^{2n-1}} d\nu(u) |h_m(g^{-1}u) - f(g^{-1}u)| \\ & = K \int_{U(n)} d\mu(g) \int_{\mathbb{S}^{2n-1}} d\nu(u) |h_m(u) - f(u)| = K \mu(U(n)) \|h_m - f\|_1 \rightarrow 0. \end{aligned}$$

We have found that, as wanted:

$$\left\| f_j - \dim(\mathbf{H}_j^n) \int_{U(n)} \operatorname{tr}(\overline{D^j(g)}) f(g^{-1}u) d\mu(g) \right\|_1 = 0.$$

To conclude assume $j \neq (0,0)$ otherwise the thesis is trivial. We notice that, when f_j is taken to be continuous (and it can be done in a unique way in view of lemma 14, referring the Hilbert basis of continuous functions Z_m^j as before), (2.10) must be everywhere true. Therefore, if e_1, e_2, \dots, e_n is a Hilbert basis of \mathbb{C}^n

$$\frac{1}{\dim(\mathbf{H}_j^n)} \sum_k f_j(e_k) = \int_{U(n)} \operatorname{tr}(\overline{D^j(g)}) \sum_k f(g^{-1}e_k) d\mu(g) = \int_{U(n)} \operatorname{tr}(\overline{D^j(g)}) W_f d\mu(g) = 0$$

because W_f is a constant and thus it is proportional to $1 = D^{(0,0)}$ which, in turn, is orthogonal to $D_{mm'}^j$ for $j \neq (0,0)$ in view of Peter-Weyl theorem and (c) of theorem 16. \square

2.3 \mathcal{L}^2 -frame functions as quadratic forms

If \mathbf{H} is a finite-dimensional complex Hilbert space \mathbf{H} , with $\dim \mathbf{H} = n \geq 3$, there is only a regular Borel measure, ν , on $\mathbb{S}(\mathbf{H})$ which is both-sided invariant under the natural action of every unitary operator $U : \mathbf{H} \rightarrow \mathbf{H}$ and $\nu(\mathbb{S}(\mathbf{H})) = 1$. It is the $U(n)$ -invariant measure ν_n induced by any identification of \mathbf{H} with a corresponding \mathbb{C}^n obtained by fixing a orthonormal basis in \mathbf{H} . The uniqueness of ν is due to the fact that different orthonormal basis are connected by means of transformations in $U(n)$.

Theorem 21 *If f is a generally complex frame function on a finite-dimensional complex Hilbert space \mathbf{H} , with $\dim \mathbf{H} \geq 3$ and $f \in \mathcal{L}^2(\mathbb{S}(\mathbf{H}), d\nu)$, there is a unique linear operator $A : \mathbf{H} \rightarrow \mathbf{H}$ such that:*

$$f(z) = \langle z | Az \rangle \quad \forall z \in \mathbb{S}(\mathbf{H}), \quad (2.11)$$

where $\langle | \rangle$ is the inner product in \mathbf{H} . A turns out to be Hermitean if f is real.

Proof. We start from the uniqueness issue. Let B be another operator satisfying the thesis, so that $\langle z | (A - B)z \rangle = 0 \quad \forall z \in \mathbf{H}$. Choosing $z = x + y$ and then $z = x + iy$ one finds $\langle x | (A - B)y \rangle = 0$ for every $x, y \in \mathbf{H}$, that is $A = B$. We pass to the existence of A identifying \mathbf{H} to \mathbb{C}^n by means of an orthonormal basis $\{e_k\}_{k=1, \dots, n} \subset \mathbf{H}$. $f \in \mathcal{L}^2(\mathbb{S}^{2n-1}, d\nu_n)$ can be decomposed $f = \sum_j f_j$ with $f_j \in \mathbf{H}_j^n$. Lemma 20 implies that, if $g \in U(n)$:

$$\sum_{k=1}^n (D^j(g)f_j)(e_k) = \sum_{k=1}^n f_j(g^{-1}e_k) = 0 \quad \text{if } j \neq (0, 0) \quad (2.12)$$

Assuming $f_j \neq 0$, since the representation D^j is irreducible, the subspace of \mathbf{H}_j^n spanned by all the vectors $D^j(g)f_j \in \mathbf{H}_j^n$ is dense in \mathbf{H}_j^n when g ranges in $U(n)$. As \mathcal{H}_j^n is finite-dimensional, the dense subspace is \mathbf{H}_j^n itself. So it must be $\sum_{k=1}^n Z(e_k) = 0$ for every $Z \in \mathbf{H}_j^n$. In particular it holds for the zonal spherical harmonic F_{n, e_1}^j individuated by e_1 : $\sum_{k=1}^n F_{n, e_1}^j(e_k) = 0$. By definition of zonal spherical harmonics the above expression can be written in these terms: $R_{p, q}^n(1) + (n-1)R_{p, q}^n(0) = 0$, and using relations (2.9):

$$\begin{aligned} & (-1)^{p+q}(n-1)n(n+1) \cdots (n+p-2)(n-1)n(n+1) \cdots (n+q-2) = \\ & = (-1)^p \delta_{pq} p! (n-1)^2 n(n+1) \cdots (n+p-2). \end{aligned} \quad (2.13)$$

(2.13) implies $p = q$. Indeed, if $p \neq q$ the right hand side vanishes, while the left does not. Now, for $n \geq 3$ and $j \neq (0, 0)$ we can write:

$$(n-1)^2 n^2 (n+1)^2 \cdots (n+p-2)^2 = (-1)^p p! (n-1)^2 n(n+1) \cdots (n+p-2). \quad (2.14)$$

The identity (2.14) is verified if and only if $p = 1$. In view of lemma 18, we know that the functions $f_{(1,1)} \in \mathbf{H}_{(1,1)}^n$ have form $f(x) = \langle x | A_0 x \rangle$ with $\text{tr} A_0 = 0$. We conclude that our frame function f can only have the form:

$$f(x) = c + f_{(1,1)}(x) = \langle x | cIx \rangle + \langle x | A_0 x \rangle = \langle x | Ax \rangle \quad x \in \mathbb{S}^{2n-1}.$$

If f is real valued $\langle x | Ax \rangle = \overline{\langle x | Ax \rangle} = \langle x | A^* x \rangle$ and thus $\langle x | (A - A^*)x \rangle = 0$. Exploiting the same argument as that used in the proof of the uniqueness, we conclude that $A = A^*$. \square

The statement of theorem 21 establishes a bijective correspondence between linear operators in a finite-dimensional Hilbert space \mathbf{H} and the frame functions belonging to $\mathcal{L}^2(\mathbb{S}(\mathbf{H}), \nu)$. Thus one can suppose to represent quantum observables and density matrices as function, possibly in a classical-like fashion. Since $f(z) = \langle z|Az\rangle = \text{tr}(A|z\rangle\langle z|) = \text{tr}(AP_z)$, where P_z is the orthogonal projector on the 1-dimensional subspace spanned by $z \in \mathbb{S}(\mathbf{H})$, the frame function f can be viewed as a function defined on the projective space $\mathbf{P}(\mathbf{H})$. In the next chapter we give an equivalent definition of frame function on the projective space which is a good candidate to be a quantum phase space.

Chapter 3

Interplay of Hamiltonian and Quantum formalisms

Content of this chapter is based on the paper [34].

3.1 Complex projective space as a quantum phase space

3.1.1 A classical-like formulation of QM

In his 1979 paper [27], T.W.B. Kibble gave a first suggestion about a geometric formulation of Quantum Mechanics as a Hamiltonian theory in a complex projective space with some remarkable analogies with Classical Mechanics. Examples of other works on this topic are [6, 9]. Geometric Hamiltonian construction is rather effective in finite dimension, if the Hilbert space of a considered quantum theory is infinite-dimensional there are several problems regarding unbounded operators, infinite-dimensional manifolds and measure theory issues that we point out later. The phase space of the Hamiltonian formulation is given by the projective space $\mathbf{P}(\mathbf{H})$ constructed on the Hilbert space \mathbf{H} of the considered quantum theory. $\mathbf{P}(\mathbf{H})$ has a natural almost Kähler structure, i.e. a symplectic form¹ ω is defined on $\mathbf{P}(\mathbf{H})$, beyond a Riemannian metric g and a almost complex structure j which transforms ω into g and viceversa. The presence of a symplectic form allows the definition of a Hamiltonian formalism with the notions of Poisson bracket and Hamiltonian vector fields. Let us recall some fundamental ideas of general Hamiltonian formalism: a diffeomorphism $F : \mathcal{M} \rightarrow \mathcal{M}$ on a symplectic manifold (\mathcal{M}, ω) is said to be *symplectic* if and only if it preserves the symplectic form $F^*\omega = \omega$. For every smooth $f : \mathcal{M} \rightarrow \mathbb{R}$ the associated *Hamiltonian vector field* X_f can be defined as the unique vector field satisfying $\omega_p(X_f, \cdot) = df_p$. When H is the Hamiltonian function of a physical system described in the phase space \mathcal{M} , the integral curves $t \mapsto s(t) \in \mathcal{M}$ of X_H , i.e. the solutions of the *Hamilton equation*:

¹A closed non-degenerate smooth 2-form.

$$\frac{ds}{dt} = X_H(s(t)), \quad (3.1)$$

represent the dynamics of the system. The general evolution along the integral curves of the Hamiltonian vector field X_f defines a one-parameter group of symplectic diffeomorphism called Hamiltonian flow generated by f . The *Poisson bracket* of a pair of functions $f, g : \mathcal{M} \rightarrow \mathbb{R}$ is defined as $\{f, g\} := \omega(X_f, X_g)$ and the commutator of two Hamiltonian vector fields satisfies $[X_f, X_g] = X_{\{f, g\}}$, in fact $f \mapsto X_f$ turn out to be an isomorphism of Lie algebras.

On the *quantum phase space*, an observable should be represented by a real-valued function in a classical-like picture. In this chapter, we define a general prescription $A \mapsto f_A$ to associate a classical-like observable $f_A : \mathbf{P}(\mathbf{H}) \rightarrow \mathbb{R}$ to any quantum observable A (self-adjoint operator in \mathbf{H}) in order to obtain a meaningful Hamiltonian description of quantum dynamics. More precisely, fixing a Hamiltonian operator H and its associated classical-like Hamiltonian function f_H : The equivalence between Schrödinger dynamics given by H and Hamilton dynamics given by the vector field defined by f_H is required. In other words the solutions of Schrödinger equation correspond to the flow lines of Hamiltonian vector field. Furthermore, one can prove that a vector field on $\mathbf{P}(\mathbf{H})$ is Hamiltonian if and only if it is a Killing vector field w.r.t. the Riemannian metric g ; every notion of unitary evolution corresponds to a notion of an evolution along a suitable g -Killing flow.

Another interesting feature of the correspondence between standard QM in \mathbf{H} and the classical-like Hamiltonian QM in $\mathbf{P}(\mathbf{H})$ is the computation of expectation values. Within a classical theory formulated in the phase space \mathcal{M} , the expectation value of a classical observable $f : \mathcal{M} \rightarrow \mathbb{R}$ is computed as the integral of f w.r.t. the measure $\rho d\mu$, where μ is the Liouville volume form induced by the symplectic form on \mathcal{M} and ρ is a probability density satisfying Liouville equation. In QM the expectation value of the observable represented by the self-adjoint operator A is computed as the trace $tr(A\sigma)$, where σ is the density matrix representing the state of the quantum system. We need a correspondence between quantum states and probability densities on $\mathbf{P}(\mathbf{H})$ in such a way quantum expectation values can be computed as classical expectation values.

This chapter is devoted to classify all possible correspondences from quantum and classical-like states (i.e. probability densities on $\mathbf{P}(\mathbf{H})$) on the one hand and quantum and classical-like observables (i.e. real-valued functions on $\mathbf{P}(\mathbf{H})$) on the other hand in order to obtain a quantum theory where evolution is given by a Hamiltonian vector field and expectation values are computed as integrals w.r.t. Liouville measures. In this sense we obtain a classical-like formulation of a *quantum* theory and not a proper *classical* theory, in fact once constructed the observable algebra in terms of classical-like observables we have a non-commutative \star -product given by three contributions: pointwise, Lie and Jordan.

A first intuitive and informal motivation to choose the projective Hilbert space as a phase space for a quantum theory is the following: It represents the pure states of the system so the Schrödinger evolution of a pure state can be seen as a curve in the pro-

jective space which is similar to a classical evolution in a classical phase space. For the same reason, one can choose the Lie group of unitary operators to be the quantum phase space, however projective space has a rich geometric structure to set up a symplectic description. Adopting the point of view of this dissertation we can present the following instance: In every finite-dimensional Hilbert \mathbf{H}_n with $\dim \mathbf{H}_n = n > 2$, there is a bijective correspondence between linear operators and the set of \mathcal{L}^2 -frame functions on $\mathbb{S}(\mathbf{H}_n)$ (theorem 21). Then one suspects of being able to represent self-adjoint operators and density matrices as scalar functions on the unit sphere of the Hilbert space. A frame function on the sphere can be equivalently defined on the projective space, in fact for any frame function $f \in \mathcal{L}^2(\mathbb{S}(\mathbf{H}_n), \nu_n)$ there is a unique linear operator A such that:

$$f(\psi) = \langle \psi | A \psi \rangle = \text{tr}(A |\psi\rangle \langle \psi|),$$

thus we can be understood as a function well-defined on the projective space: $f(p) = \text{tr}(Ap)$ for any $p \in \mathbf{P}(\mathbf{H}_n)$. In this sense the projective space constructed on the Hilbert space of the theory is a good candidate to play the rôle of a phase space. A consistent definition of frame function as a function on $\mathbf{P}(\mathbf{H}_n)$ is introduced further.

3.1.2 Kähler structure of the complex projective space

In this section \mathbf{H}_n denotes a (complex) Hilbert space with finite dimension $n > 1$ and $U(n)$ denotes the group of unitary operators on \mathbf{H}_n . In finite dimensions the sphere $\mathbb{S}(\mathbf{H}_n)$ and the projective space $\mathbf{P}(\mathbf{H}_n)$ have a structure of compact, second countable, topological spaces. Moreover we prove that $\mathbf{P}(\mathbf{H}_n)$ can be equipped with the structure of a real $(2n - 2)$ -dimensional smooth manifold and the projection $\mathbb{S}(\mathbf{H}_n) \rightarrow \mathbf{P}(\mathbf{H}_n) = \mathbb{S}(\mathbf{H}_n)/U(1)$ is a smooth submersion. First of all note that \mathbf{H}_n can be identified with \mathbb{C}^n once choose an orthonormal basis, thus \mathbf{H}_n has the natural structure of a real $2n$ -dimensional smooth manifold which does not depend on the choice of the basis. Such structure can be induced on $\mathbb{S}(\mathbf{H}_n)$ and $\mathbf{P}(\mathbf{H}_n)$. Furthermore, as a consequence of statement 3. of proposition 2, $\mathbf{P}(\mathbf{H}_n)$ can be identified to $\mathbf{S}_p(\mathbf{H}_n)$.

Proposition 22 *The following facts hold in the real smooth manifold \mathbf{H}_n .*

- i) $\mathbb{S}(\mathbf{H}_n)$ is a real $(2n - 1)$ -dimensional embedded submanifold of \mathbf{H}_n .*
- ii) $\mathbf{P}(\mathbf{H}_n)$ can be equipped with a real $(2n - 2)$ -dimensional smooth manifold structure in a way such that both the continuous projection $\pi : \mathbb{S}(\mathbf{H}) \ni \psi \mapsto [\psi] \in \mathbf{P}(\mathbf{H})$ is a smooth submersion and the transitive action of the compact Lie group $U(n)$ on $\mathbf{S}_p(\mathbf{H}_n) \equiv \mathbf{P}(\mathbf{H}_n)$ defined as:*

$$U(n) \times \mathbf{P}(\mathbf{H}_n) \ni (U, p) \mapsto \Phi_U(p) := U p U^{-1} \in \mathbf{S}_p(\mathbf{H}_n), \quad (3.2)$$

is smooth.

Proof. (a) $\mathbb{S}(\mathbf{H}_n)$ is a real $(2n-1)$ -dimensional embedded submanifold of \mathbf{H}_n . Let us sketch how it happens. If $(z_{01}, \dots, z_{0n}) \in \mathbb{S}(\mathbf{H}_n)$, there is an open (in \mathbf{H}_n) neighbourhood O of that point such that for every $(z_1, \dots, z_n) \in O' := \mathbb{S}(\mathbf{H}_n) \cap O$ there is a component, say $z_k = x_k + iy_k$, (the same for all points of O) such that either x_k or y_k can be written as a smooth function of the remaining components z_h , when $(z_1, \dots, z_n) \in O'$. This procedure define a natural local chart on $\mathbb{S}(\mathbf{H}_n)$ with domain O' . Collecting all these charts, that are mutually smoothly compatible, one obtains a smooth differentiable structure on $\mathbb{S}(\mathbf{H}_n)$ making it a real $(2n-1)$ -dimensional embedded submanifold of \mathbf{H}_n .

(b) Similarly $\mathbf{P}(\mathbf{H}_n)$ can be equipped with a real $(2n-2)$ -dimensional smooth manifold structure. Consider $(z_{01}, \dots, z_{0n}) \in [\psi_0] \in \mathbf{P}(\mathbf{H}_n)$. At least one of the components z_{0j} cannot vanish, say z_{0h} . By continuity this fact is valid in an open neighbourhood V of $(z_{01}, \dots, z_{0n}) \in \mathbb{S}(\mathbf{H}_n)$. In that neighbourhood the set of $n-1$ ratios z_j/z_h with $j \neq h$ determine a point on $\mathbf{P}(\mathbf{H}_n)$ biunivocally. These $n-1$ ratios vary in an open neighborhood $V' := \pi(V) \subset \mathbf{P}(\mathbf{H}_n)$ of $[\psi_0]$ when the components (z_1, \dots, z_n) range in V . Decomposing each of these ratios into real and imaginary part, we obtain a real local chart on $V' \subset \mathbf{P}(\mathbf{H}_n)$ with $2n-2$ real coordinates. Collecting all these local charts, that are mutually smoothly compatible, one obtains a smooth differentiable structure on $\mathbf{P}(\mathbf{H}_n)$, making it a $2n-2$ -dimensional real smooth manifold. With the said structures, the canonical projection $\pi : \mathbb{S}(\mathbf{H}_n) \rightarrow \mathbf{P}(\mathbf{H}_n)$ becomes a smooth submersion and the transitive action (3.2) of $U(n)$ on $\mathbf{P}(\mathbf{H}_n)$ turns out to be smooth as one easily proves. \square

It is well-known that the finite-dimensional projective space has a structure of $2n-2$ -dimensional symplectic manifold. Let us summarize the symplectic geometry of $\mathbf{P}(\mathbf{H}_n)$ starting from a useful characterization of the tangent space by means the ransitive action of $U(n)$. Henceforth $iu(n)$ denotes the real vector space of self-adjoint operators on \mathbf{H}_n , $\mathfrak{u}(n)$ is the Lie algebra of $U(n)$.

Proposition 23 *The tangent vectors v at $p \in \mathbf{P}(\mathbf{H}_n) \equiv \mathbf{S}_p(\mathbf{H}_n)$ are all of the elements in $\mathfrak{B}(\mathbf{H}_n)$ of the form: $v = -i[A_v, p]$, for some $A_v \in iu(n)$. Consequently, $A_1, A_2 \in iu(n)$ define the same vector in $T_p\mathbf{P}(\mathbf{H}_n)$ iff $[A_1 - A_2, p] = 0$.*

Proof. The action (3.2) is transitive and smooth so, on the one hand $\mathbf{P}(\mathbf{H}_n)$ is diffeomorphic to the quotient $U(n)/G_p$, where $G_p \subset U(n)$ is the isotropy group of $p \in \mathbf{P}(\mathbf{H}_n)$ and on the other hand the projection $\Pi_p : U(n) \ni U \mapsto UpU^{-1} \in \mathbf{P}(\mathbf{H}_n)$ is a submersion [46, 38] and thus $d\Pi_p|_{U=I} : \mathfrak{u}(n) \rightarrow T_p\mathbf{P}(\mathbf{H}_n)$ is surjective. The thesis is true because $d\Pi_p(B)|_{U=I} = [B, p]$ for every $B \in \mathfrak{u}(n)$ and $\mathfrak{u}(n)$ is the real vector space of anti-self adjoint in $\mathfrak{B}(\mathbf{H})$. \square

Representing tangent vectors in a fixed point of the manifold with operators, one can define the following map for any fixed value of the constant $\kappa > 0$:

$$\omega_p(u, v) := -i\kappa(p[A_u, A_v]) \quad u, v \in T_p\mathbf{P}(\mathbf{H}_n), \quad (3.3)$$

that is a symplectic form being the Kostant-Kirillov form defined on the rank-1 orbit $\mathbf{P}(\mathbf{H}_n) = \frac{U(n)}{U(n-1)U(1)}$ of $U(n)$. It is a well-known fact [6, 9] that a Riemannian metric can be defined on $\mathbf{P}(\mathbf{H}_n)$, the so-called **Fubini-Study metric**:

$$g_p(u, v) := -\kappa \operatorname{tr}(p([A_u, p][A_v, p] + [A_v, p][A_u, p])) \quad u, v \in T_p\mathbf{P}(\mathbf{H}_n), \quad (3.4)$$

adopting the notation $-i[A, p] = p$, Fubini-Study metric assumes the more popular form $ds^2 = g_p(dp, dp) = 2\kappa \operatorname{tr}(p(dp)^2)$, applying the polarization identity. The symplectic form ω and the metric g are compatible in an almost complex structure defined by the class j of linear maps:

$$j_p : T_p\mathbf{P}(\mathbf{H}_n) \ni v \mapsto i[v, p] \in T_p\mathbf{P}(\mathbf{H}_n) \quad p \in \mathbf{P}(\mathbf{H}_n). \quad (3.5)$$

The map $p \mapsto j_p$ is smooth, $j_p j_p = -\mathbb{I}_{T_p\mathbf{P}(\mathbf{H}_n)}$ for every $p \in \mathbf{P}(\mathbf{H}_n)$ and $\omega_p(u, v) = g_p(u, j_p v)$ if $u, v \in T_p\mathbf{P}(\mathbf{H}_n)$. Thus (ω, g, j) is an *almost Kähler structure* on $\mathbf{P}(\mathbf{H}_n)$. Indeed the almost complex form j is also integrable [23], so $\mathbf{P}(\mathbf{H}_n)$ is a *Kähler manifold*. As anticipated the symplectic structure is crucial to state a Hamiltonian formulation of QM in a classical-like fashion while the Fubini-Study metric is useful to characterize Hamiltonian vector fields in such formulation as Killing fields.

From the geometrical point of view, it is well-known [8, 29] that the projective space of an infinite-dimensional Hilbert space can be endowed with a structure of Kähler manifold which is a generalization of the Kähler structure in a finite-dimensional projective space.

3.2 Frame functions on the projective space

3.2.1 From the sphere to the projective space

Definition of frame function and the statement of theorem 21 given in the chapter 2 can be consistently reformulated on $\mathbf{P}(\mathbf{H}_n)$ rather than on the sphere. The unique $U(n)$ -invariant regular positive Borel measure ν_n , determined on $\mathbb{S}(\mathbf{H}_n)$ by its normalization $\nu_n(\mathbb{S}(\mathbf{H}_n)) = 1$, induces a suitable measure μ_n on $\mathbf{P}(\mathbf{H}_n)$ as proved below.

Proposition 24 *Let $\nu_n : \mathbb{S}(\mathbf{H}_n) \rightarrow [0, 1]$ denote the unique $U(n)$ -left-invariant regular Borel measure with $\nu_n(\mathbb{S}(\mathbf{H}_n)) = 1$. There exists a unique positive Borel measure μ_n over $\mathbf{P}(\mathbf{H}_n)$ such that, if $\pi : \mathbb{S}(\mathbf{H}_n) \rightarrow \mathbf{P}(\mathbf{H}_n)$ is the natural projection map, then:*

$$f \circ \pi \in \mathcal{L}^1(\mathbb{S}(\mathbf{H}_n), \nu_n) \quad \text{if} \quad f \in \mathcal{L}^1(\mathbf{P}(\mathbf{H}_n), \mu_n), \quad \text{and} \quad \int_{\mathbf{P}(\mathbf{H}_n)} f d\mu_n = \int_{\mathbb{S}(\mathbf{H}_n)} f \circ \pi d\nu_n.$$

The measure μ_n fulfils the following:

i) Referring to the smooth action (3.2), μ_n is the unique $U(n)$ -left-invariant regular Borel

measure on $\mathbf{P}(\mathbf{H}_n)$ with $\mu_n(\mathbf{P}(\mathbf{H}_n)) = 1$.

ii) It coincides to the Liouville volume form induced by ω up to its normalization.

iii) It coincides to the Riemannian measure induced by g up to its normalization.

Proof. Henceforth $\mathcal{B}(X)$ denotes the Borel σ -algebra on the topological space X . If μ_n exists, the requirement $\int_{\mathbf{P}(\mathbf{H}_n)} f d\mu_n = \int_{\mathbb{S}(\mathbf{H}_n)} f \circ \pi d\nu_n$ entails that, for $f := \chi_E$, it holds:

$$\mu_n(E) = \nu_n(\pi^{-1}(E)) \quad \text{for every } E \in \mathcal{B}(\mathbf{P}(\mathbf{H}_n)). \quad (3.6)$$

That relation proves that, if μ_n exists, it is uniquely determined by ν_n . Let us pass to the existence issue. Since π is continuous, is Borel-measurable and thus $\pi^{-1}(E) \in \mathcal{B}(\mathbb{S}(\mathbf{H}_n))$ if $E \in \mathcal{B}(\mathbf{P}(\mathbf{H}_n))$. Since the other requirements are trivially verified, (3.6) defines, in fact, a positive Borel measure on $\mathbf{P}(\mathbf{H}_n)$. That measure fulfils

$$f \circ \pi \in \mathcal{L}^1(\mathbb{S}(\mathbf{H}_n), \nu_n) \quad \text{if } f \in \mathcal{L}^1(\mathbf{P}(\mathbf{H}_n), \mu_n), \quad \text{and} \quad \int_{\mathbf{P}(\mathbf{H}_n)} f d\mu_n = \int_{\mathbb{S}(\mathbf{H}_n)} f \circ \pi d\nu_n.$$

directly from the definition of integral and $\mu_n(\mathbf{P}(\mathbf{H}_n)) = \nu_n(\pi^{-1}(\mathbf{P}(\mathbf{H}_n))) = \nu_n(\mathbb{S}(\mathbf{H}_n)) = 1$. μ_n is regular because $\mathbf{P}(\mathbf{H}_n)$ is compact it being the image of the compact set $\mathbb{S}(\mathbf{H}_n)$ under the continuous map π with finite measure [39] and this regularity results also applies the the Liouville measure and the Riemannian one. Concerning the invariance under the action of $PU(n)$, it arises from that of μ_n under $U(n)$:

$$\mu_n(E) = \nu_n(\pi^{-1}(E)) = \nu_n(U\pi^{-1}(E)) = \nu_n(\pi^{-1}(UEU^{-1})) = \mu_n(UEU^{-1}) \quad \text{if } U \in U(n).$$

(a) $\mathbf{P}_n(\mathbf{H}_n)$ is homeomorphic to the quotient of compact groups $U(n)/H$ where H is the isotropy group of any point of $\mathbf{P}_n(\mathbf{H}_n)$, since H is closed in the compact group $U(n)$, it is compact as well. Thus there is a non-vanishing $U(n)$ left invariant positive regular Borel measure on $\mathbf{P}_n(\mathbf{H}_n)$, uniquely determined by the volume of $\mathbf{P}_n(\mathbf{H}_n)$ (Chapter 4 of [11]). That measure must thus coincide with μ_n up to a strictly positive multiplicative constant. (b) and (c) the Liouville measure and the Riemannian measure are non-vanishing $U(n)$ left invariant positive regular Borel measure on $\mathbf{P}_n(\mathbf{H}_n)$, because both ω and g are $U(n)$ invariant. Therefore they have to coincide with μ_n up to a strictly positive multiplicative constant. \square

In view of the statement *ii)*, the image of the measure ν_n (which is crucial to state the bijective correspondence between frame functions and linear operators) turns out to be the Liouville form on $\mathbf{P}(\mathbf{H}_n)$, i.e. the measure on the phase space w.r.t. which expectation values are computed. The critical issue to state a definition of of frame function on $\mathbf{P}(\mathbf{H}_n)$ is finding an analogue of orthonormal basis on $\mathbf{P}(\mathbf{H}_n)$. The next result is rather helpful in this sense.

Proposition 25 Let \mathbf{H} be a complex separable Hilbert space and $\pi : \mathbb{S}(\mathbf{H}_n) \rightarrow \mathbf{P}(\mathbf{H}_n)$ the natural projection from the unit sphere to the projective space. A subset N of $\mathbf{P}(\mathbf{H}_n)$ can be written as $\{\pi(\psi)\}_{\psi \in M}$ for some Hilbertian basis M of \mathbf{H} if and only if $d_2(p, p') = \sqrt{2}$ for $p \neq p'$ and N is maximal w.r.t. this property.

Proof. As $d_2(\psi\langle\psi|\cdot\rangle, \phi\langle\phi|\cdot\rangle) = \sqrt{||\psi||^4 + ||\phi||^4 - 2|\langle\psi|\phi\rangle|^2}$ if $\psi, \phi \in \mathbf{H}$, for $\psi, \phi \in \mathbb{S}(\mathbf{H})$, one has $d_2(\psi\langle\psi|\cdot\rangle, \phi\langle\phi|\cdot\rangle) = \sqrt{2}$ if and only if $\psi \perp \phi$. The proof concludes noticing that the maximality property in the thesis is equivalent to that of a Hilbertian basis. \square

For \mathbf{H} n -dimensional Hilbert space \mathbf{H}_n , we have that N is maximal if and only if N contains exactly n elements.

Definition 26 Let \mathbf{H} be separable complex Hilbert space. $N \subset \mathbf{P}(\mathbf{H}_n)$ is called **basis** of $\mathbf{P}(\mathbf{H}_n)$ if $d_2(p, p') = \sqrt{2}$ for $p, p' \in n$ with $p \neq p'$ and N is maximal w.r.t. this property.

The above definition of *disguised basis* allows to introduce an equivalent notion of frame function on the projective space.

Definition 27 A map $f : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{C}$ is called **frame function** if there is $W_f \in \mathbb{C}$ such that:

$$\sum_{i=1}^n f(p_i) = W_f, \quad (3.7)$$

for every basis $\{p_i\}_{i=1, \dots, n}$ of $\mathbf{P}(\mathbf{H}_n)$.

Theorem 21 can be now restated referring to the measure μ_n also completing it by adding some other elementary facts. Statement is (b) is the equivalent result of theorem 21.

Theorem 28 In \mathbf{H}_n the following facts holds.

1. If $A \in \mathfrak{B}(A)$ then

$$F_A(p) := \text{tr}(pA) \quad \text{for } p \in \mathbf{P}(\mathbf{H}_n). \quad (3.8)$$

defines a frame function with $W_{F_A} = \text{tr}A$ which belongs to $\mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), d\mu_n)$.

2. If $F : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{C}$ is a frame function, $n > 2$ and $F \in \mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), d\mu_n)$, then there is a unique $A \in \mathfrak{B}(\mathbf{H}_n)$ such that $F_A = F$.

3. Defining the subspace, closed if $n > 2$:

$$\mathcal{F}^2(\mathbf{H}_n) := \{F : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{C} \mid F \in \mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), d\mu_n) \text{ and } F \text{ is a frame function}\}, \quad (3.9)$$

$M : \mathfrak{B}(\mathbf{H}) \ni A \mapsto F_A \in \mathcal{F}^2(\mathbf{H}_n)$ is a complex vector space injective homomorphism, surjective if $n > 2$, fulfilling the properties:

(i) $A \geq cI$, for some $c \in \mathbb{R}$, if and only if $F_A(x) \geq c$ for all $x \in \mathbf{P}(\mathbf{H}_n)$

(ii) $F_{A^*} = \overline{F_A}$, where the bar denotes the point-wise complex conjugation. In particular $A = A^*$ if and only if F_A is real.

Proof. The proof of the first part of 1. is trivial. F_A is continuous and thus bounded, since $\mathbf{P}(\mathbf{H}_n)$ is compact. Therefore it belongs to $\mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), d\mu_n)$ as $\mu_n(\mathbf{P}(\mathbf{H}_n)) < +\infty$. Concerning 2., we observe that $f(\psi) := F([\psi])$ is a frame function in the sense of definition 13 due to proposition 25. If $F \in \mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), d\mu_n)$, then $f \in \mathcal{L}^2(\mathbb{S}(\mathbf{H}_n), d\nu_n)$ in view of the first statement in proposition 24. Thus, whenever $n \geq 3$, we can take advantage of thm 21, obtaining that there is $A \in \mathfrak{B}(\mathbf{H}_n)$ with $F_A([\psi]) = f_A(\psi) = \langle \psi | A \psi \rangle = \text{tr}(\psi \langle \psi | \cdot \rangle A)$ for all $\psi \in \mathbb{S}(\mathbf{H}_n)$, namely $F = F_A$. A is uniquely determined since, as it is simply proved, in complex Hilbert spaces, if $B : \mathbf{H} \rightarrow \mathbf{H}$ is linear, $\langle \psi | B \psi \rangle = 0$ for all $\psi \in \mathbb{S}(\mathbf{H})$ then $B = 0$. The proof of 3. is evident per direct inspection. Closedness of $\mathcal{F}^2(\mathbf{H}_n)$ for $n \geq 3$ arises from the fact that $\mathcal{F}^2(\mathbf{H}_n)$ is a finite dimensional subspace of a Banach space: The space of quadratic forms on $\mathbf{H}_n \times \mathbf{H}_n$ for 2.. \square

3.2.2 Covariance under unitary transformations

Let us introduce the notion of covariance w.r.t. the group $U(n)$ of a map $\mathcal{G} : \sigma \mapsto f_\sigma$ associating any quantum state σ to a complex-valued function ρ_σ defined on the projective space $\mathbf{P}(\mathbf{H}_n)$. A map \mathcal{G} of this kind is called $U(n)$ -**covariant** if it satisfies the following property:

$$\rho_\sigma(\Phi_U(p)) = \rho_{U^{-1}\sigma U}(p) \quad \forall U \in U(n), \sigma \in \mathbb{S}(\mathbf{H}_n), p \in \mathbf{P}(\mathbf{H}_n), \quad (3.10)$$

where $U \mapsto \Phi_U$ is the smooth representation introduced in (3.2). The importance of the notion of $U(n)$ -covariance is motivated by its interplay with frame functions, shown in the next theorem. Before stating the theorem, we invoke a technical lemma which ensures that for every pair of points on the unit sphere there is a unitary transformation which map a point into the other, up to a phase factor.

Lemma 29 *If \mathbf{H} is a complex Hilbert space and $\phi, \psi \in \mathbb{S}(\mathbf{H})$, then there exists $U \in \mathfrak{B}(\mathbf{H})$ such that $U\phi = \alpha\psi$ for some $\alpha \in \mathbb{C}$, $|\alpha| = 1$, and $U = U^* = U^{-1}$.*

Proof. If ϕ and ψ are linearly dependent, choosing α such that $\phi = \alpha\psi$, we can define $U := I$. In the other case, let \mathbf{K} be the closed subspace spanned by ϕ and ψ . It is enough to find $V : \mathbf{K} \rightarrow \mathbf{K}$ with $V = V^* = V^{-1}$ and $V\phi = \alpha\psi$ for some α with $|\alpha| = 1$. If such a V exists, the wanted U can be defined as $U := V \oplus I$ referring to the orthogonal

decomposition $\mathbf{H} = \mathbf{K} \oplus \mathbf{K}^\perp$. Fixing an orthonormal basis in \mathbf{K} given by ϕ, ϕ_1 , the problem can be tackled in \mathbb{C}^2 . With the Hilbert-space isomorphism from \mathbf{K} to \mathbb{C}^2 , ϕ corresponds to $(1, 0)^t$ and ψ with $(a, b)^t$ where $|a|^2 + |b|^2 = 1$. We can choose α such that $\alpha\psi$ corresponds to (c, d) with $c > 0$, $d \in \mathbb{C}$ and $c^2 + |d|^2 = 1$. To conclude, we only need to find a complex 2×2 matrix M with $M = \overline{M}^t = M^{-1}$ and $M(1, 0)^t = (c, d)^t$. The operator V corresponds to M through the identification of \mathbf{K} and \mathbb{C}^2 we have previously introduced. The wanted M is just the following one:

$$M := \begin{bmatrix} c & \bar{d} \\ d & -c \end{bmatrix}.$$

□

Theorem 30 Assume that $n > 2$ for \mathbf{H}_n .

- i) If $\mathcal{G} : \mathbf{S}(\mathbf{H}_n) \rightarrow \mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$ is a convex-linear and $U(n)$ -covariant map, then $\mathcal{G}(\mathbf{S}(\mathbf{H}_n)) \subset \mathcal{F}^2(\mathbf{H}_n)$.
 ii) If $\mathcal{N} : \mathfrak{B}(\mathbf{H}_n) \rightarrow \mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$ is a \mathbb{C} -linear map satisfying $\mathcal{N}|_{\mathbf{S}(\mathbf{H}_n)} = \mathcal{G}$, with \mathcal{G} as in i), then $\mathcal{N}(\mathbf{S}(\mathbf{H}_n)) \subset \mathcal{F}^2(\mathbf{H}_n)$.

Proof. i) Suppose that $\sigma = \phi\langle\phi|\cdot\rangle$ is a given pure state and suppose that $\{p_i\}_{i=1,2,\dots,n}$ is a basis of $\mathbf{P}(\mathbf{H}_n)$, so that $p_i = \psi_i\langle\psi_i|\cdot\rangle$. With a suitable choice of the arbitrary phase in the definition of the ψ_i , there are n operators U_i such that $U_i\phi = \psi_i$ and $U_i = U_i^* = U_i^{-1}$, (lemma 29). Consequently, taking advantage of the $U(n)$ -covariance: $g_\sigma(p_i) = g_\sigma(U_i\sigma U_i^*) = g_{U_i^*\sigma U_i}(\sigma) = g_{U_i\sigma U_i^*}(\sigma) = g_{p_i}(\sigma)$. Exploiting the convex-linearity:

$$n^{-1} \sum_i g_\sigma(p_i) = \sum_i n^{-1} g_\sigma(p_i) = g_{\sum_i n^{-1} p_i}(\sigma) = g_{n^{-1} \sum_i p_i}(\sigma) = g_{n^{-1} I}(\sigma).$$

$U(n)$ -covariance implies: $g_{n^{-1} I}(\sigma) = g_{U^{-1} n^{-1} I U}(\sigma) = g_{n^{-1} I}(\Phi_U(\sigma))$. Since Φ is transitive on $\mathbf{P}(\mathbf{H}_n)$, we conclude that $n^{-1} \sum_i g_\sigma(p_i) = g_{n^{-1} I}(q) = c$, for every $q \in \mathbf{P}(\mathbf{H}_n)$ and some constant $c \in \mathbb{R}$. Next consider a mixed $\sigma \in \mathbf{S}(\mathbf{H}_n)$. The found result and convex-linearity of \mathcal{G} , representing σ with its spectral decomposition $\sigma = \sum_j q_j \sigma_j$ (σ_j being pure), yield:

$$\sum_i g_\sigma(p_i) = \sum_i g_{\sum_j q_j \sigma_j}(p_i) = \sum_i \sum_j q_j g_{\sigma_j}(p_i) = \sum_j q_j \sum_i g_{\sigma_j}(p_i) = \sum_j q_j n c.$$

As the right most side does not depend on the choice of the basis $\{p_i\}_{i=1,2,\dots,n}$, g_σ must be a frame function, that belongs to \mathcal{L}^2 by hypotheses. (b) of thm 28 implies that $g_\sigma \in \mathcal{F}^2(\mathbf{H}_2)$.
 ii) If $A \in \mathfrak{B}(\mathbf{H}_n)$, decompose it as $A = \frac{1}{2}(A + A^*) + i\frac{1}{2i}(A - A^*)$. Next decompose the self-adjoint operators $\frac{1}{2}(A + A^*)$ and $\frac{1}{2i}(A - A^*)$ into linear combinations of pure states σ_k exploiting the spectral theorem. Each $\mathcal{N}(\sigma_k) = \mathcal{G}(\sigma_k)$ belongs to the linear space \mathcal{F}^2 . Linearity of \mathcal{N} concludes the proof. □

In the next section, a physical meaning of a $U(n)$ -covariance requirement and its crucial rôle are explained.

3.2.3 Trace-integral formulas

To conclude this technical section about frame functions, let us introduce the so-called *trace-integral formulas*. Consider a frame function $F \in \mathcal{L}^2(\mathbb{P}(\mathbb{H}_n), \mu_n)$, we know there exists a unique operator $A \in \mathfrak{B}(\mathbb{H}_n)$ such that $F(p) = \text{tr}(Ap)$ (theorem 21). One can prove that the integral of F with respect the measure μ_n corresponds to the trace of A (the weight W_F of F) and the Hilbert-Schmidt product in $\mathfrak{B}(\mathbb{H}_n)$ is connected with the \mathcal{L}^2 -product in $\mathcal{L}^2(\mathbb{P}(\mathbb{H}_n), \mu_n)$. Similar facts are proved in [20] for self-adjoint operators in terms of integrals w.r.t. the measure induced by Fubini-Study metric. Next theorem extends the results of [20] to non self-adjoint operators without appealing to the Riemannian metric structure.

Theorem 31 *Referring to Theorem 28, if F_A and F_B are frame functions respectively constructed out of A and B in $\mathfrak{B}(\mathbb{H}_n)$, then:*

$$\int_{\mathbb{P}(\mathbb{H}_n)} F_A d\mu_n = \frac{\text{tr}(A)}{n} = \frac{W_F}{n}, \quad (3.11)$$

$$\int_{\mathbb{P}(\mathbb{H}_n)} \overline{F_A} F_B d\mu_n = \frac{1}{n(n+1)} (\text{tr}(A^*B) + \text{tr}(A^*)\text{tr}(B)), \quad (3.12)$$

which inverts as:

$$\text{tr}(A^*B) = n(n+1) \int_{\mathbb{P}(\mathbb{H}_n)} \overline{F_A} F_B d\mu_n - n^2 \int_{\mathbb{P}(\mathbb{H}_n)} \overline{F_A} d\mu_n \int_{\mathbb{P}(\mathbb{H}_n)} F_B d\mu_n. \quad (3.13)$$

Proof. The second identity in (3.11) is immediate. (3.13) arises from (3.12) and (3.11) straightforwardly, so we have to prove (3.11) and (3.12) only. Actually (3.11) follows from (3.12) swapping A and B and taking $B = I$. Therefore we have to establish (3.12) to conclude. To this end, we notice that (3.12) holds true for generic $A, B \in \mathfrak{B}(\mathbb{H}_n)$ if it is valid for A and B self-adjoint. This result arises decomposing A and B in self-adjoint and anti self adjoint part and exploiting linearity in various points. Therefore it is enough proving (3.12) for A and B self-adjoint. Next we observe that, if as before $iu(n)$ is the real vector space of self-adjoint operators: $iu(n) \times iu(n) \ni (A, B) \mapsto (n(n+1))^{-1} (\text{tr}(AB) + \text{tr}(A)\text{tr}(B))$ is a real scalar product. Similarly, the left-hand side of (3.12), restricted to the real vector space of real frame functions is a real scalar product. Taking advantage of the polarization identity, we conclude that (3.12) holds when it does for the corresponding norms on the considered real vector spaces:

$$\int_{\mathbb{P}(\mathbb{H}_n)} F_A^2 d\mu_n = \frac{1}{n(n+1)} (\text{tr}(AA) + \text{tr}(A)^2) \quad \text{for } A \in iu(n). \quad (3.14)$$

Let us establish (3.14) to conclude. We pass from the integration over $\mathbb{P}(\mathbb{H}_n)$ to that over $\mathbb{S}(\mathbb{H}_n)$ just replacing μ_n for ν_n . If $\{e_j\}_{j=1, \dots, n}$ is a Hilbertian basis of \mathbb{H}_n made of

eigenvectors of A such that $Ae_k = \lambda_k e_k$, we can decompose $\psi \in \mathbb{S}(\mathbb{H}_n)$ as follows $\psi = \sum_j \psi_j e_j$ so that:

$$\int_{\mathbb{S}(\mathbb{H}_n)} F_A^2 d\nu_n = \sum_i^n \lambda_i^2 \int_{\mathbb{S}(\mathbb{H}_n)} |\psi_i|^4 d\nu_n + \sum_{i \neq j}^n \lambda_i \lambda_j \int_{\mathbb{S}(\mathbb{H}_n)} |\psi_i|^2 |\psi_j|^2 d\nu_n.$$

In view of the $U(n)$ invariance of ν_n and the transitive action of $U(n)$ on $\mathbb{S}(\mathbb{H}_n)$, we conclude that: $\int_{\mathbb{S}(\mathbb{H}_n)} |\psi_i|^4 d\nu_n(\psi) = a$, where a does not depend on i , on the used Hilbertian basis, and on A . If $\psi, \phi \in \mathbb{S}(\mathbb{H}_n)$ are a pair of vectors satisfying $\psi \perp \phi$, for every choice of $i, j = 1, \dots, n$ with $i \neq j$, there exist $U_{i,j} \in U(n)$ such that, both verifies $U_{i,j} e_i = \psi$ and $U_{i,j} e_j = \phi$. The invariance of ν_n under $U(n)$ thus proves that, for $i \neq j$: $\int_{\mathbb{S}(\mathbb{H}_n)} |\psi_i|^2 |\psi_j|^2 d\nu_n(\psi) = b$ where b does not depend on A , on the used Hilbertian basis and on the couple $i, j = 1, \dots, n$ provided $i \neq j$. Summing up:

$$\int_{\mathbb{S}(\mathbb{H}_n)} F_A^2 d\nu_n = a \operatorname{tr}(A^2) + b \sum_{i \neq j}^n \lambda_i \lambda_j = \int_{\mathbb{S}(\mathbb{H}_n)} F_A^2 d\nu_n = a \operatorname{tr}(A^2) + b \sum_{i,j}^n \lambda_i \lambda_j - b \operatorname{tr}(A^2).$$

That is, redefining $d := a - b$:

$$\int_{\mathbb{P}(\mathbb{H}_n)} F_A^2 d\mu_n = d \operatorname{tr}(A^2) + b (\operatorname{tr}(A))^2. \quad (3.15)$$

To determine the constants d and b we first choose $A = I$ obtaining: $1 = dn + bn^2$. To grasp another condition, consider the real vector space of self-adjoint operators $iu(n)$ and complete $\frac{I}{\sqrt{n}}$ to a Hilbert-Schmidt-orthonormal basis of $iu(n)$ by adding self-adjoint operators $T_1, T_2, \dots, T_{n^2-1}$. Notice that $(I|T_k)_2 = 0$ means $\operatorname{tr}(T_k) = 0$. Thus, if $p \in \mathbb{P}(\mathbb{H}_n)$: $p = \frac{I}{n} + \sum_k p_k T_k$ with $p_k = \operatorname{tr}(p T_k) \in \mathbb{R}$. The condition $\operatorname{Tr}(p^2) = 1$ ((2) in proposition 2) is equivalent to $\sum_k p_k^2 = 1 - \frac{1}{n}$, so that

$$\sum_{k=1}^{n^2-1} \int_{\mathbb{P}(\mathbb{H}_n)} F_{T_k}(p)^2 d\mu_n(p) = \int_{\mathbb{P}(\mathbb{H}_n)} \sum_{i=1}^{n^2-1} p_k^2 d\mu_n(p) = \left(1 - \frac{1}{n}\right) \int_{\mathbb{P}(\mathbb{H}_n)} d\mu_n(p) = \left(1 - \frac{1}{n}\right).$$

Inserting this result in the left-hand side of (3.15):

$$\left(1 - \frac{1}{n}\right) = \sum_{i=1}^{n^2-1} d \operatorname{tr}(T_i T_i) + b \sum_{i=1}^{n^2-1} (\operatorname{tr}(T_i))^2, \quad \text{i.e.} \quad \left(1 - \frac{1}{n}\right) = \sum_{i=1}^{n^2-1} d + b \sum_{i=1}^{n^2-1} (0)^2.$$

Summing up, we have the pair of equations for b and d : $1 - 1/n = d(n^2 - 1)$ and $1 = dn + bn^2$ with solution $d = b = (n(n+1))^{-1}$ that, inserted in (3.15), yields (3.14). \square

3.3 Hamiltonian formalism for Quantum Mechanics

3.3.1 Quantum dynamics as a Hamiltonian flow

As anticipated in the initial part of the chapter, there is a nice interplay of Hamiltonian and Quantum formalism [6, 9]. The key-idea behind this interplay is the association of a quantum observable $A \in \mathfrak{iu}(n)$ to a real function f_A defined on $\mathbf{P}(\mathbf{H}_n)$, i.e. a *classical-like observable*. A natural definition for a classical-like observable is a slightly generalized expectation value function:

$$f_A : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{R} \quad f_A(p) := \kappa \operatorname{tr}(Ap) + \operatorname{ctr}(A), \quad (3.16)$$

where $\kappa > 0$ is the free parameter appearing in the symplectic form and $c \in \mathbb{R}$ is an arbitrary constant. Definition (3.16) works well as an observable in a Hamiltonian picture as shown by the following theorem.

Theorem 32 *Consider a quantum system described on \mathbf{H}_n . Equip $\mathbf{P}(\mathbf{H}_n)$ with the triple (ω, g, j) as before. For every $A \in \mathfrak{iu}(n)$, define the function $f_A : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{R}$ as in (3.16). Then the Hamiltonian field associated with f_A reads:*

$$X_{f_A}(p) = -i[A, p] \quad \text{for all } p \in \mathbf{P}(\mathbf{H}_n), \quad (3.17)$$

and the following facts hold:

1. $\mathbb{R} \ni t \mapsto p(t) \in \mathbf{S}_p(\mathbf{H}_n)$ is the evolution of a pure quantum state fulfilling Schrödinger equation

$$\frac{dp(t)}{dt} = -i[H, p(t)], \quad (3.18)$$

with Hamiltonian $H \in \mathfrak{iu}(n)$ if and only if $\mathbb{R} \ni t \mapsto p(t) \in \mathbf{P}(\mathbf{H}_n)$ satisfies Hamilton equations

$$\frac{dp(t)}{dt} = X_{f_H}(p(t)), \quad (3.19)$$

with Hamiltonian function $\mathbf{H} := f_H$.

Similarly, Hamiltonian evolution of classical observables is equivalent to the Heisenberg evolution of corresponding quantum observables: $f_A(p(t)) = f_{e^{itH} A e^{-itH}}(p)$.

2. If $A, H \in \mathfrak{iu}(n)$, then:

$$\{f_A, f_H\} = f_{-i[A, H]}. \quad (3.20)$$

So in particular A is a quantum constant of motion if and only if f_A is a classical constant of motion when $\mathbf{H} = f_H$ is the Hamiltonian function.

3. If $U \in U(n)$ the map $\Phi_U : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbf{P}(\mathbf{H}_n)$ as in (3.2), describing the action of the quantum symmetry U on states, is both a symplectic diffeomorphism and an isometry of $\mathbf{P}(\mathbf{H}_n)$ and thus X_{f_A} is a g -Killing fields for every $A \in \mathfrak{iu}(n)$. Finally the covariance relation holds:

$$f_A(\Phi_U(p)) = f_{U^{-1}AU}(p) \quad \text{for all } A \in \mathfrak{iu}(n), p \in \mathbf{P}(\mathbf{H}_n), \text{ and } U \in U(n).$$

Proof. Regarding (3.17), consider a smooth curve $\mathbb{R} \ni t \mapsto p(t) \in \mathbf{P}(\mathbf{H}_n)$ such that $\dot{p}(0) = v = -i[B_v, p]$, (3.16) implies:

$$\langle df_A(p), v \rangle = \kappa \frac{d}{dt} \Big|_{t=0} \text{tr}(p(t)A) = -i\kappa \text{tr}([B_v, p], A) = -i\kappa \text{tr}(p[A, B]) = \omega_p(-i[A, p], v).$$

Since it must also hold $\omega_p(X_{f_A}(p), v) = \langle df_A(p), v \rangle$ we conclude that $\omega_p(X_{f_A}(p) + i[A, p], v) = 0$ for every $v \in T_p\mathbf{P}(\mathbf{H}_n)$. As ω_p is non-degenerate, (3.17) follows.

1. In view of (3.17), Hamilton equation $\frac{dp}{dt} = X_{f_H}(p(t))$ is the same as Schrödinger equation $\frac{dp}{dt} = -i[H, p(t)]$. Now the final statement is obvious form (3.16) and the cyclic property of the trace:

$$\begin{aligned} f_A(p(t)) &= f_A(e^{-itH} p e^{itH}) = \kappa \text{tr}(e^{-itH} p e^{itH} A) + \text{ctr}(A) = \kappa \text{tr}(p e^{itH} A e^{-itH}) + \text{ctr}(e^{-itH} e^{itH} A) \\ &= \kappa \text{tr}(p e^{itH} A e^{-itH}) + \text{ctr}(p e^{itH} A e^{-itH}) = f_{e^{itH} A e^{-itH}}(p). \end{aligned}$$

2. The first statement immediately arises using $\{f_A, f_B\} := \omega(X_{f_A}, X_{f_B})$ and (3.17) noticing that $\text{tr}(-i[A, B]) = 0$. Next observe that, since \mathbf{H}_n has finite dimension and so no problems with domains arise, A is a constant of motion with respect to the Hamiltonian $B = H$ iff $[A, H] = 0$. This is equivalent to say $\langle \psi | [A, H] \psi \rangle = 0$ for all $\psi \in \mathbb{S}(\mathbf{H}_n)$, that is $\text{tr}(p[A, H]) = 0$ for all $p \in \mathbf{P}(\mathbf{H}_n)$, that is $f_{-i[A, B]} - \text{tr}(-i[A, B]) = 0$. In view of the very identity (3.20), that is equivalent to say (where $\mathbf{H} = f_H$) $\{f_A, \mathbf{H}\} = 0$, that is eventually equivalent to say that f_A is a constant of motion in Hamiltonian formulation.

3. The first part of (c) is an evident consequence of the fact that referring to (3.2): $\Phi_U^* \omega = \omega$ and $\Phi_U^* g = g$ for all $U \in U(n)$. In other words $\omega_p(u, v)$ and $g_p(u, v)$ are invariant if replacing p, A_v, A_u for $UpU^{-1}, UA_vU^{-1}, UA_uU^{-1}$ simultaneously as one checks immediately. The last statement is immediately proved by direct inspection. \square

The statement 1. of the above theorem establishes the equivalence between Schrödinger and Hamilton dynamics which is the most important feature of a Hamiltonian description of a quantum system. In other words the solutions of Schrödinger equation with Hamiltonian operator H are given by the flow lines of the Hamiltonian vector field associated to f_H .

3.3.2 Quantum expectation values as classical-like averages

In view of theorem 32, definition (3.16) gives rise to a meaningful classical-like observable. However there are two open questions at least: i) Is there a more general correspondence than (3.16)? ii) Is there any criterion to fix the constants κ and c ? In particular, a fixed value of κ would imply the existence of a preferred symplectic form (3.3) on $\mathbf{P}(\mathbf{H}_n)$ (and a Kähler structure at all). In order to answer these questions giving a more complete characterization of classical-like observables we have to investigate how the expectation values of quantum and classical-like observables are related.

In the Hamiltonian formulation of a classical theory, the state (at time t) of a system with $2n$ degrees of freedom is represented by a Liouville density ρ that is a probability density on the phase space \mathcal{M} . Any physical quantity is represented by a real function f on \mathcal{M} , a classical observable, the expectation value of f is the integral of the pointwise product of ρ and f with respect to the positive Borel measure $m := \omega \wedge \cdots \wedge (n \text{ times}) \wedge \cdots \wedge \omega$, called *Liouville measure*:

$$\mathbb{E}_\rho(f) := \int_{\mathcal{M}} \rho(p) f(p) \, dm(p). \quad (3.21)$$

In any local chart of the symplectic atlas of \mathcal{M} , the measure m corresponds to Lebesgue measure. If there is no a kind of classical uncertainty on the initial condition of the system then its time evolution is completely deterministic and the state at time t is represented by a single point in \mathcal{M} for every t . Suppose $s_0 \in \mathcal{M}$ is the state of the system at time t_0 , in this case ρ is given by the Dirac measure $\delta_{s_0} : \mathfrak{B}(\mathcal{M}) \rightarrow [0, 1]$ with $\delta_{s_0}(E) = 1$ if $s_0 \in E$ and $\delta_{s_0}(E) = 0$ otherwise. The expectation value of f on a sharp state represented by s_0 is the value of f in that point:

$$\mathbb{E}_{s_0}(f) := \int_{\mathcal{M}} f(p) \, d\delta_{s_0}(p) = f(s_0). \quad (3.22)$$

In Quantum Mechanics, the expectation value of the observable $A \in i\mathfrak{u}(n)$ on the state $\sigma \in \mathcal{S}(\mathbf{H}_n)$ is:

$$\langle A \rangle_\sigma := \text{tr}(\sigma A). \quad (3.23)$$

One can conjecture the existence of a correspondence $\mathcal{S}(\mathbf{H}_n) \ni \sigma \mapsto \rho_\sigma : \mathbf{P}(\mathbf{H}_n) \rightarrow [0, 1]$ such that ρ_σ is a Liouville density on $\mathbf{P}(\mathbf{H}_n)$ describing the quantum state σ with:

$$\text{tr}(A\sigma) = \int_{\mathbf{P}(\mathbf{H}_n)} f_A(p) \rho_\sigma(p) d\mu_n(p) \quad \text{for every } A \in i\mathfrak{u}(n) \text{ and } \sigma \in \mathcal{S}(\mathbf{H}_n), \quad (3.24)$$

where μ_n is the measure introduced in proposition 24. Such a correspondence is presented

in [20]: Classical-like observable is of the simplest form $f_A(p) = \text{tr}(Ap)$ and the Liouville density is given by:

$$\rho_\sigma(p) := \text{tr}(\sigma p) - \frac{1}{n+1}, \quad (3.25)$$

the quantum expectation value $\text{tr}(A\sigma)$ is then calculated as the product $f_A\rho_\sigma$ w.r.t. the measure $n(n+1)\mu_n$. Despite the nice correspondence of expectation values, one notes that (3.25) is not a positive definite function, so ρ_σ cannot be interpreted as a probability density. The next chapter is devoted to the study of all possible correspondences $A \mapsto f_A$ and $\sigma \mapsto \rho_\sigma$ satisfying natural requirements and giving rise to all possible prescriptions to set up a classical-like Hamiltonian formulation of a quantum theory.

Chapter 4

Geometric Hamiltonian Quantum Mechanics

Content of this chapter is based on the paper [34].

4.1 Prescription for the *inverse quantization*

Assuming the correspondence of quantum and classical-like observables given by (3.16), theorem 32 is true independently from the values of constant $\kappa > 0$ and $c \in \mathbb{R}$. Validity of theorem 32 is crucial for a well-formulated Hamiltonian theory, so we investigate how is the most general way to construct classical-like observable (and Liouville densities) preserving the validity of the theorem. We want to state a prescription for an *inverse quantization* by definition of a map associating quantum observables with functions on $P(H_n)$:

$$\mathcal{O} : \mathfrak{iu}(n) \ni A \mapsto f_A : P(H_n) \rightarrow \mathbb{R}, \quad (4.1)$$

and a map associating density matrices with functions $P(H_n)$:

$$\mathcal{S} : S(H_n) \ni \sigma \mapsto \rho_\sigma : P(H_n) \rightarrow \mathbb{R}. \quad (4.2)$$

Let us clarify the meaning of the expression *inverse quantization*: It is not a procedure to obtain a *classical theory* but a *classical-like formulation* of a *quantum theory*, where there are several analogies with a classical Hamiltonian theory like dynamics encoded in the flow of a vector field on a symplectic manifold. In section 4.3 the *quantumness* of the obtained Hamiltonian theory will be clear in the structure of C^* -algebra of classical-like observables.

In (4.2) we do not require that ρ_σ is valued in $[0, 1]$, like a proper Liouville density, because even if ρ_σ is not a normalized positive function the construction of a theory

without non-physical results is possible, e.g. [20] discussed in the last chapter. However we can isolate the cases where ρ_σ can be really interpreted as a probability density on the quantum phase space.

4.1.1 Quantum observables as real scalar function on quantum phase space

In order to find the most general form of the map \mathcal{O} , an axiomatic approach can be adopted making a list of physically meaningful requirements. Below there is such a list and a following discussion.

Requirements on observables correspondence $\mathcal{O} : i\mathfrak{u}(n) \ni A \mapsto f_A$ with $f_A : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{R}$

(O1) \mathcal{O} is injective.

(O2) \mathcal{O} is \mathbb{R} -linear.

(O3) If $H \in i\mathfrak{u}(n)$, then f_H is C^1 so that X_{f_H} can be defined. A curve $p = p(t) \in \mathbf{P}(\mathbf{H}_n)$, $t \in (a, b)$, satisfies Hamilton's equation if and only if it satisfies Schrödinger's one:

$$\frac{dp}{dt} = X_{f_H}(p(t)) \quad \text{for } t \in (a, b) \quad \text{is equivalent to} \quad \frac{dp}{dt} = -i[H, p(t)] \quad \text{for } t \in (a, b).$$

(O4) \mathcal{O} is $U(n)$ -covariant.

(O5) If $A \in i\mathfrak{u}(n)$ then: $\min \text{sp}(A) \leq f_A(p) \leq \max \text{sp}(A)$ for $p \in \mathbf{P}(\mathbf{H}_n)$.

Requirement (O1) simply says that the map \mathcal{O} produces a faithful image of the set of quantum observables in terms of the classical-like ones. (O2) establishes that the structure of real vector space enjoyed by the set of quantum observables is preserved. (O3) is the crucial requirement about the equivalence between Schrödinger dynamics and Hamilton dynamics already introduced and discussed. (O4) is a natural covariance requirement to avoid the existence of a preferred point on the quantum phase space. (O5) is the most elementary possible relation between the values of A , i.e. the elements of the spectrum $\text{sp}(A)$, and the values of f_A , i.e. the points of the range. However there is no unique way to compare a continuous set of values (the range) with a discrete one (the spectrum).

Applying theorem 30, we can immediately observe that requirements (O2) and (O4) imply that f_A is a frame function, then there exists an operator $A' \in \mathfrak{B}(\mathbf{H}_n)$ such that $f_A = \text{tr}(A'p)$; establishing the relationship between A and A' is not obvious, but it is a way to construct a general \mathcal{O} satisfying above list of requirements.

The next is one of the main results presented in this dissertation. It is a theorem establishing that the classical-like observables must have the form already introduced in (3.16) for $n > 2$.

Theorem 33 *Consider a quantum system described on \mathbf{H}_n with $n > 1$. Assume the almost Kähler structure (ω, g, j) on $\mathbf{P}(\mathbf{H}_n)$, with the constant $\kappa > 0$ fixed arbitrarily. The*

following facts hold concerning the map $\mathcal{O} : i\mathfrak{u}(n) \ni A \mapsto f_A$.

- i) The requirements (O1)-(O4) are valid if and only if \mathcal{O} has the form (3.16) for some constant $c \in \mathbb{R}$ (so that, in particular, theorem 32 holds) and $\kappa + nc \neq 0$.
- ii) If the requirements (O1)-(O4) are valid, then \mathcal{O} extends to the whole $\mathfrak{B}(\mathbf{H})$ by complex-linearity giving rise to an injective map that, if $n > 2$, satisfies $\mathcal{O}(\mathfrak{B}(\mathbf{H}_n)) = \mathcal{F}^2(\mathbf{H}_n)$.

Proof. i) If \mathcal{O} has the form (3.16) then (O2)-(O4) are valid. Let us prove the converse. Assuming (O3), from the definition of Hamiltonian field, it must be $\omega_p(X_{f_H}, u_A) = \langle df_H, u_A \rangle$, for every $H \in i\mathfrak{u}(n)$, $p \in \mathbf{P}(\mathbf{H}_n)$ and $u_B = -i[p, B] \in T_p\mathbf{P}(\mathbf{H}_n)$. The definition of ω and some elementary computations permit to re-write the identity above as $\langle df_H, -i[p, B] \rangle = \kappa \text{tr}(H(-i[p, B]))$. Consider a smooth curve $q = q(s)$ in $\mathbf{P}(\mathbf{H}_n)$ such that $q(s_0) = p$ and $\dot{q}(s_0) = -i[p, B]$. The identity above, taking advantage of the linearity of the trace, entails:

$$\frac{d}{ds} f_H(q(s))|_{s=s_0} = \frac{d}{ds} \kappa \text{tr}(Hq(s))|_{s=s_0} = \kappa \text{tr} \left(H \frac{dq}{ds} \Big|_{s=s_0} \right).$$

Since s_0 is arbitray, we have found that:

$$\frac{d}{ds} f_H(q(s)) = \kappa \text{tr} \left(H \frac{dq}{ds} \right).$$

Integrating in s and swapping the integral with the symbol of trace by linearity, we finally obtain $f_H(p) = \kappa \text{tr}(Hp) + C_H$, where $p \in \mathbf{P}(\mathbf{H}_n)$ is arbitrary. The map $H \mapsto C_H = f_H(p) - \kappa \text{tr}(Hp)$ must be linear for (O2). By Riesz' theorem, referring to the Hilbert-Schmidt (real) scalar product we have that there exists $B \in i\mathfrak{u}(n)$ such that $C_H = \text{tr}(BH)$ for all $H \in i\mathfrak{u}(n)$. (O4) easily implies that $\text{tr}(BUHU^{-1}) = \text{tr}(BH)$ for al $U \in U(n)$ and $H \in i\mathfrak{u}(n)$. Choosing $H = \psi \langle \psi | \cdot \rangle$ with $\psi \in \mathbb{S}(\mathbf{H}_n)$ and noticing that $U(n)$ acts transitively on $\mathbb{S}(\mathbf{H}_n)$ we conclude that $\langle \psi | B \psi \rangle = c$ for some constant $c \in \mathbb{R}$ and all $\psi \in \mathbb{S}(\mathbf{H}_n)$. From polarization identity it easily implies that $B = cI$, so that $f_A = \kappa \text{tr}(pA) + c \text{tr}(A)$ for all $A \in i\mathfrak{u}(n)$ as requested. Let us prove that \mathcal{O} is injective if and only if (O1) holds. Exploiting $\kappa \neq 0$, and dealing with as done above, one easily sees that $f_A = 0$ is equivalent to $A = -c\kappa^{-1} \text{tr}(A)I$. Computing the trace of both sides one immediately sees that this equation has $A = 0$ as the unique solution if $1 + nc/\kappa \neq 0$, namely $\kappa + nc \neq 0$. Conversely, if $A + c\kappa^{-1} \text{tr}(A)I = 0$ has $A = 0$ as unique solution, $I + c\kappa^{-1} \text{tr}(I)I \neq 0$, namely $\kappa + nc \neq 0$. ii) Assuming (O1)-(O4) and extending \mathcal{O} by complex linearity, exactly as before, \mathcal{O} turns out to be injective. If $n > 2$, the elements of $\mathcal{F}^2(\mathbf{H}_n)$ are of the form F_B for every $B \in \mathfrak{B}(\mathbf{H}_n)$ (statement 2. of theorem 28). For a fixed B , $\mathcal{O}(A) = F_B$, if $A := \kappa^{-1}B - c[\kappa(\kappa + nc)]^{-1} \text{tr}(B)I$, so that \mathcal{O} is onto $\mathcal{F}^2(\mathbf{H}_n)$. \square

4.1.2 Quantum states as Liouville densities on quantum phase space

A similar axiomatic approach can be adopted also to find a general form of the map \mathcal{S} , constructing Liouville denisties (possibly positive and normalized) associated to quantum states.

Requirements on states correspondence $\mathcal{S} : \mathcal{S}(\mathbf{H}_n) \ni \sigma \mapsto \rho_\sigma$ with $\rho_\sigma : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{R}$

(S1) If $\sigma \in \mathcal{S}(\mathbf{H}_n)$, then $\rho_\sigma(p) \geq 0$ for $p \in \mathbf{P}(\mathbf{H}_n)$.

(S2) \mathcal{S} is convex linear.

(S3) With μ_n as in theorem 24, if $\sigma \in \mathcal{S}(\mathbf{H}_n)$, then $\rho_\sigma \in \mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$ (so that $\rho_\sigma \in \mathcal{L}^1(\mathbf{P}(\mathbf{H}_n), \mu_n)$) and

$$\int_{\mathbf{P}(\mathbf{H}_n)} \rho_\sigma d\mu_n = 1 .$$

(S4) \mathcal{S} is $U(n)$ -covariant.

(S5) If $\sigma \in \mathcal{S}(\mathbf{H}_n)$ and $A \in iu(n)$ then, assuming $f_A \in \mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$:

$$tr(\sigma A) = \int_{\mathbf{P}(\mathbf{H}_n)} \rho_\sigma f_A d\mu_n .$$

(S1) is the requirement of positivity according to the interpretation of density probability. (S2) establishes that the natural convex structure of the set of quantum states is preserved. (S3) is the normalization to 1 of ρ_σ , taking in to account that if ρ_σ is \mathcal{L}^2 then it is \mathcal{L}^1 . The covariance requirement (S4), similar to (O4), implies that Hamiltonian evolution of ρ_σ is equivalent to Schrödinger evolution of σ . (S5) requires the equivalence between the quantum expectation value $\langle A \rangle_\sigma$ computed in the standard formalism as $tr(A\sigma)$ and the classical-like expectation value computed in the Hamiltonian formalism as an integral. If $f_A = \mathcal{O}(A)$, with \mathcal{O} satisfying (O3), then $f_A \in \mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$ since $|f_A|^2$ is continuous and thus bounded on the compact space $\mathbf{P}(\mathbf{H}_n)$ and the measure μ_n is finite. In the following there is the proof that for $n > 2$ the densities ρ_σ representing quantum states must be frame functions.

Theorem 34 Consider a quantum system described on \mathbf{H}_n with $n > 2$. Assume the almost Kähler structure (ω, g, j) on $\mathbf{P}(\mathbf{H}_n)$, with the constant $\kappa > 0$ fixed arbitrarily and the map $\mathcal{O} : iu(n) \ni A \mapsto f_A$ of the form (3.16) for some constant $c \in \mathbb{R}$. The following fact hold.

i) The requirements (S2)-(S5) are valid if and only if both in the definition (3.16) of \mathcal{O} :

$$\kappa = \kappa , \quad c = c_\kappa \tag{4.3}$$

and \mathcal{S} associates states σ with frame functions of the form:

$$\rho_\sigma(p) := \kappa'_\kappa tr(\sigma p) + c'_\kappa \tag{4.4}$$

where

$$c_\kappa := \frac{1 - \kappa}{n} , \quad \kappa'_\kappa := \frac{n(n+1)}{\kappa} , \quad c'_\kappa := \frac{\kappa - (n+1)}{\kappa} . \tag{4.5}$$

\mathcal{O} is injective because of the former of the following consequent identities:

$$\kappa + nc_\kappa = 1 \quad \text{and} \quad \kappa'_\kappa + nc'_\kappa = n . \tag{4.6}$$

ii) If (S2)-(S5) are true, also \mathcal{S} is injective.

Proof. i) If (4.3), (4.4), (4.5) are valid, one sees that (S2)-(S5) hold true. In particular, \mathcal{O} is injective because $\kappa + nc_\kappa = 1 \neq 0$ and ii) of thm 33 holds. It remains to prove that (S2)-(S5) are valid, then (4.3), (4.4), (4.5) hold. We start (for $n > 2$) by assuming that a map \mathcal{S} verifying (S2)-(S5) and \mathcal{O} of the form (3.16) with $\kappa > 0$ and $c \in \mathbb{R}$. As the first step we prove that ρ_σ is a frame function, next we shall establish its form. (S2) and (S4), together with (i) in thm 30 imply that: $\rho_\sigma(p) = tr(\sigma'p)$ for all $p \in \mathbf{P}(\mathbf{H}_n)$, where (i) of (3) of thm 28 entail that σ' is some self-adjoint operator associated with the given σ . Using the fact that the total integral of ρ_σ has value 1 from (S3), taking (3.11) into account, we find $tr\sigma' = n$. Finally (S5) together the form of \mathcal{O} require that the following identity holds true for all self-adjoint $A \in \mathfrak{B}(\mathbf{H}_n)$ and $\sigma \in \mathbf{S}(\mathbf{H}_n)$:

$$tr(\sigma A) = \int_{\mathbf{P}(\mathbf{H}_n)} tr(\sigma'p) (\kappa tr(Ap) + ctrA) d\mu_n(p). \quad (4.7)$$

The right-hand side can be expanded taking (3.12), (3.11) and $tr\sigma' = n$ into account:

$$tr(\sigma A) = \frac{\kappa}{n(n+1)} tr(\sigma' A) + tr(A) \left(\frac{\kappa}{n+1} + c \right).$$

Consequently, for every $A = A^*$:

$$tr \left(\left(\sigma - \frac{\kappa}{n(n+1)} \sigma' \right) A \right) = tr(A) \left(\frac{\kappa}{n+1} + c \right).$$

Choosing $A = p \in \mathbf{S}_p(\mathbf{H}_n)$, arbitrariness of p easily entails that, for some $\beta_\sigma \in \mathbb{R}$:

$$\sigma - \frac{\kappa}{n(n+1)} \sigma' = \beta_\sigma I,$$

namely, for some constants $\kappa' > 0$ and $c' \in \mathbb{R}$:

$$f_\sigma(p) = \kappa' tr(\sigma p) + c'.$$

Inserting again this expression in (4.7) he have:

$$tr(\sigma A) = \int (\kappa' tr(\sigma p) + c') (\kappa tr(Ap) + ctrA) d\mu_n(p).$$

Finally, using again (3.11), (3.12) and $\mu_n(\mathbf{P}(\mathbf{H}_n)) = 1$ we obtain:

$$\left(1 - \frac{\kappa\kappa'}{n(n+1)} \right) tr(\sigma A) + tr(A) \left(\frac{\kappa\kappa'}{n(n+1)} + cc' + \frac{ck'}{n} + \frac{c'k}{n} \right) = 0$$

that has to hold for all $A \in iu(n)$ and $\sigma \in \mathbf{S}(\mathbf{H}_n)$ and for some $\kappa, \kappa' > 0$ and $c, c' \in \mathbb{R}$. Arbitrariness of A and σ easily lead to the first two requirements of the following triple:

$$1 - \frac{\kappa\kappa'}{n(n+1)} = 0, \quad \frac{\kappa\kappa'}{n(n+1)} + cc' + \frac{ck'}{n} + \frac{c'k}{n} = 0, \quad 1 = \frac{\kappa'}{n} + c',$$

the third requirement immediately arises from (S3) using (3.11). This system can completely be solved parametrizing κ, κ', c in terms of c' with $c' < 1$ in order to verify the requirement $\kappa > 0$ in the definition of f_A . Finally, parametrizing the solutions in terms of κ : $\kappa, c_\kappa, \kappa'_\kappa, c'_\kappa$ we have (4.5).

ii) If $\rho_\sigma = \rho_{\sigma'}$, exploiting $\kappa'_\kappa \neq 0$, one has $tr((\sigma - \sigma')p) = 0$ for every $p \in \mathbf{P}(\mathbf{H}_n)$. Namely $\langle \psi | (\sigma - \sigma') \psi \rangle = 0$ for every $\psi \in \mathbf{H}_n$. Polarization leads to $\sigma - \sigma' = 0$. \square

The fact ρ_σ can be represented by a frame function for expectation values of observables $f_A \in \mathcal{F}^2(\mathbf{H}_n)$ is an immediate consequence of Riesz' theorem, noticing that $\mathcal{F}^2(\mathbf{P}(\mathbf{H}))$ is a closed subspace of $L^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$.

The pair of identities (4.6) respectively imply that: A quantum observable $A = aI$, with $a \in \mathbb{R}$ constant, corresponds to f_A constantly attaining the value a ; and (2) that the completely unpolarized state $\sigma = n^{-1}I$ gives rise to the classical trivial Liouville density $\rho_\sigma = 1$ constantly.

4.2 Self-consistency of the geometric Hamiltonian formulation

4.2.1 Complete characterization of classical-like observables

One of the most remarkable contributions of the presented results is the classification of all possible prescriptions to set up a Hamiltonian formulation of a finite-dimensional quantum theory. From *quantum observables* to *classical-like observables* the inverse quantization map is:

$$\mathcal{O} : A \mapsto f_A \quad \text{with} \quad f_A(p) = \kappa tr(Ap) - \frac{1 - \kappa}{n} tr(A), \quad (4.8)$$

and from *density matrices* to *Liouville densities* the inverse quantization map is:

$$\mathcal{S} : \sigma \mapsto \rho_\sigma \quad \text{with} \quad \rho_\sigma(p) = \frac{n(n+1)}{\kappa} tr(\sigma p) + \frac{\kappa - (n+1)}{\kappa}, \quad (4.9)$$

so the only degree of freedom of the whole construction is $\kappa > 0$, which is the "geometric degree of freedom" imposed by the Kähler structure of $\mathbf{P}(\mathbf{H}_n)$. κ labels the infinite prescriptions: For $\kappa = 1$ one has $c_\kappa = 0$ and thus: $f_A(p) = F_A(p) = tr(pA)$, defining the simplest relation between quantum and classical observables. While the choice $\kappa = n + 1$ implies $\kappa'_\kappa = n$, $c'_\kappa = 0$, so that: $\rho_\sigma(p) = nF_\sigma(p) = ntr(p\sigma)$ are positive Liouville densities with the most elementary form allowed by our hypotheses. This form may further be simplified changing the normalization of the measure. Leaving \mathcal{O} unchanged, one may indeed redefine $\mu_n \rightarrow \mu'_n := n\mu_n$ and $\rho_\sigma \rightarrow \rho'_\sigma := n^{-1}\rho_\sigma$ to obtain $\rho'_\sigma = F_\sigma$ exactly, preserving (S1)-(S5) with ρ'_σ in place of ρ_σ , but $\mu'_n(\mathbf{P}(\mathbf{H}_n)) = n$.

A significative development with respect to the celebrated results in [27, 20, 6, 9] is the complete characterization of classical-like observable made possible by the machinery of

frame functions. We know that the set of real frame functions belonging to $\mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$, for $n > 2$ provides the set of quantum observables in terms of classical-like objects. While a well-known characterization of these observables is presented in [9], they are the functions on the projective space whose Hamiltonian fields are g -Killing fields. Another characterization is the following.

Proposition 35 For $n > 2$, let \mathcal{O} and \mathcal{S} be as in (a) of theorem 34.

A map $f : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{R}$ in $\mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$ verifies $f = \mathcal{O}(A)$ for some $A \in iu(n)$ if and only if there are constants $a, b \in \mathbb{R}$ with $a \neq 0$ and

$$\int_{\mathbf{P}(\mathbf{H}_n)} \rho_{p_0}(p) f(p) d\mu_n(p) = a f(p_0) + b \quad \text{for every } p_0 \in \mathbf{S}_p(\mathbf{H}_n). \quad (4.10)$$

Proof. If $f = f_A$ one has immediately:

$$\int_{\mathbf{P}(\mathbf{H}_n)} \rho_{p_0}(p) f(p) d\mu_n(p) = \text{tr}(p_0 A) = \kappa^{-1} f(p_0) - \kappa^{-1} c_\kappa \text{tr}(A) \quad \text{for every } p_0 \in \mathbf{S}_p(\mathbf{H}_n).$$

Conversely, assume that (4.10) holds for a map $f : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{R}$ in $\mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$. If $\{p_i\}_{i=1, \dots, n}$ is a basis of $\mathbf{P}(\mathbf{H}_n)$ one has:

$$\begin{aligned} n^{-1} a \left(\sum_i f(p_i) \right) + b &= \int_{\mathbf{P}(\mathbf{H}_n)} \sum_i n^{-1} \rho_{p_i}(p) f(p) d\mu_n(p) = \int_{\mathbf{P}(\mathbf{H}_n)} \rho_{\sum_i n^{-1} p_i}(p) f(p) d\mu_n(p) \\ &= \int_{\mathbf{P}(\mathbf{H}_n)} \rho_{n^{-1} I}(p) f(p) d\mu_n(p) = \int_{\mathbf{P}(\mathbf{H}_n)} f(p) d\mu_n(p). \end{aligned}$$

So that

$$\sum_i f(p_i) = \frac{n}{a} \int_{\mathbf{P}(\mathbf{H}_n)} f(p) d\mu_n(p) - \frac{nb}{a}$$

that does not depend on the choice of the basis $\{p_i\}_{i=1, \dots, n}$. In view of (b) in thm 28, f is a real frame function. Due to (d) of thm 34, $f = \mathcal{O}(A)$ per some $A \in iu(n)$. \square

With the choice, $\kappa = 1$, the proposition above specializes to $a = 1$ and $b = 0$. This gives rise to a suggestive interpretation of the Liouville densities of pure states:

$$\int_{\mathbf{P}(\mathbf{H}_n)} \rho_{p_0}(p) f_A(p) d\mu_n(p) = f_A(p_0).$$

If $\kappa = 1$, a map $f : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{R}$ in $\mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$ can be written as $f = f_A$ for some $A \in iu(n)$ if and only if f “sees” the density ρ_{p_0} of any pure state p_0 as a Dirac delta localized at p_0 itself. Despite this strong analogy with classical expectation values on sharp states, for $\kappa = 1$ ρ_σ cannot be interpreted as a proper probability density because it is not positive definite.

In the hypothesis of theorem 33 and theorem 34, requirements (O5) and (S1) are not involved. The following theorem implies that they are incompatible.

Theorem 36 For $n > 1$, with \mathcal{O} and \mathcal{S} defined in agreement with (4.3), (4.4), (4.5), (4.5) for some $\kappa > 0$, the following facts are valid.

(a) (S1) holds if and only if $\kappa \in [n + 1, +\infty)$.

(b) (O5) holds if and only if $\kappa \in (0, 1]$ whereas, in the general case $\kappa > 0$ one has:

$$\min f_A = \min sp(A) + c_\kappa(tr(A) - n \min sp(A)), \quad (4.11)$$

$$\max f_A = \max sp(A) + c_\kappa(tr(A) - n \max sp(A)), \quad (4.12)$$

and furthermore, for $A = iu(n)$:

$$\|f_A\|_\infty \leq (1 + 2n|c_\kappa|)\|A\| \quad \text{if } \kappa \in [n + 1, +\infty), \quad (4.13)$$

$$\|f_A\|_\infty \leq \|A\| \quad \text{if } \kappa \in (0, 1], \quad (4.14)$$

where \leq can be replaced by $=$ if $\kappa = 1$.

Proof. (a) if (4.3), (4.4), (4.5), (4.5) are valid, (S1) holds if and only if $\kappa'_\kappa > 0$ and $c'_\kappa \geq 0$ (notice that $\sigma \geq 0$ for a state by hypotheses and there are states with $tr(p\sigma) = 0$ for some $p \in \mathcal{P}(\mathbf{H}_n)$). From (4.5), $\kappa'_\kappa > 0$ and $c'_\kappa \geq 0$ are equivalent to $\kappa \in [n + 1, +\infty)$.

(b) We know that, since A is self-adjoint and \mathbf{H}_n is finite dimensional, $\min sp(A) = \min_{\|\psi\|=1} \langle \psi | A \psi \rangle = \min_{p \in \mathcal{P}(\mathbf{H}_n)} tr(pA)$. Therefore $\min f_A = \kappa \min sp(A) + c_\kappa tr(A)$. Using $\kappa + nc_\kappa = 1$ we immediately have (4.11). The proof of (4.12) is analogous. Next notice that $tr(A) - n \min sp(A) \geq 0$ and $tr(A) - n \max sp(A) \leq 0$ so that (4.11)-(4.12) imply (O1) if and only if $c_\kappa \geq 0$, namely $\kappa \in (0, 1]$. The proof of the remaining estimates easily follows using an analogous procedure, noticing that $\kappa > 0$ and exploiting the inequalities $|tr(A)| \leq tr|A| \leq n\|A\|$ which arises from $\|A\| = \max\{|\lambda| \mid \lambda \in sp(A)\}$ and $\max_{p \in \mathcal{P}(\mathbf{H}_n)} |tr(pA)| = \|A\|$. The latter implies the validity of the last statement in (b) out of the fact that $c_\kappa = 0$ if $\kappa = 1$. \square

What is the preferable assumption? The positivity of the classical-like states or the fact that the range of a classical-like observable is bounded by the bounds of the spectrum of associated self-adjoint operator? Indeed the failure of (O5) is not so strong as it could seem at first glance, since there is no unique way to compare a continuous set of reals (the range of f_A) with a discrete set of real numbers (the spectrum of A) and the only physically sensible comparison relies upon the identity (3.24) that is satisfied. In particular, this identity assures that all elements of $sp(A)$ are always obtained as expectation values of f_A with respect to suitable classical-like states: If $a \in sp(A)$, picking out $p_a \in \mathcal{S}_p(\mathbf{H}_n)$ such that $p_a = |\psi_a\rangle\langle\psi_a|$, where ψ_a is a normalized eigenvector of A with eigenvalue a , one has $\mathbb{E}_{\rho_{\sigma_a}}(f_A) = \langle A \rangle_{\sigma_a} = a$.

If $\kappa = 1$, the elements $sp(A)$ coincides to the singular values of f_A (i.e. $df_A(p) = 0$ iff $f_A(p) \in sp(A)$) as one easily proves. Moreover the choice $\kappa = 1$ seems to be mandatory in a infinite-dimensional extension of the Hamiltonian formulation.

4.2.2 Re-quantization of the classical-like picture

The aim of this section is finding a way to calculate explicitly an operator from the associated function on the projective space (re-quantization). In other words we construct the inverse \mathcal{O}^{-1} of the map \mathcal{O} . Indeed the term *re-quantization* is used with the following meaning: It is a prescription to associate a self-adjoint operator to each classical-like observable and a density matrix to each Liouville density, thus it is the translation from the Hamiltonian formalism to the standard formalism of QM.

Theorem 37 *Let \mathbf{H}_n a finite-dimensional Hilbert space with dimension n larger than 2. Let $\mathcal{F}^2(\mathbf{H}_n)$ be the space of square-integrable frame functions on \mathbf{H}_n . If $\rho \in \mathcal{F}^2(\mathbf{H}_n)$, then the operator $\sigma \in \mathfrak{B}(\mathbf{H}_n)$ such that $\rho(p) = \text{tr}(\sigma p)$ is given by:*

$$\sigma = (n + 1) \int_{\mathbf{P}(\mathbf{H}_n)} \rho(p) \left(p - \frac{1}{n + 1} \mathbb{I} \right) d\mu_n(p) \quad (4.15)$$

where \mathbb{I} is the identity operator.

Proof. Let φ be a vector of the unit sphere $\mathbb{S}^{2n-1} = \{\psi \in \mathbf{H}_n \mid \|\psi\| = 1\}$. Since a point $p \in \mathbf{P}(\mathbf{H}_n)$ can be represented by a rank-1 orthogonal projector then we can take the standard expectation value $\langle \varphi | p \varphi \rangle = \text{tr}(p |\varphi\rangle\langle\varphi|)$ on the normalized pure state $|\varphi\rangle\langle\varphi|$. $f_\varphi(p) := \text{tr}(p |\varphi\rangle\langle\varphi|)$ is the frame function associated to the operator $|\varphi\rangle\langle\varphi|$. Applying (3.12) we can write the following relation:

$$\int_{\mathbf{P}(\mathbf{H}_n)} f_\varphi(p) \rho(p) d\mu_n(p) = \frac{1}{n + 1} (\text{tr}(|\varphi\rangle\langle\varphi| \sigma) + \text{tr}(\sigma)),$$

Thus:

$$\text{tr}(|\varphi\rangle\langle\varphi| \sigma) = \langle \varphi | \sigma \varphi \rangle = (n + 1) \int_{\mathbf{P}(\mathbf{H}_n)} \rho(p) \langle \varphi | p \varphi \rangle d\mu_n(p) - \text{tr}(\sigma),$$

the second equality is true for every $\varphi \in \mathbb{S}^{2n-1}$ i.e. for every $\varphi \in \mathbf{H}_n$ by sesquilinearity. Thus:

$$\sigma = (n + 1) \int_{\mathbf{P}(\mathbf{H}_n)} \rho(p) p d\mu_n(p) - \text{tr}(\sigma) \mathbb{I},$$

using (3.11):

$$\sigma = (n + 1) \int_{\mathbf{P}(\mathbf{H}_n)} \rho(p) p d\mu_n(p) - \int_{\mathbf{P}(\mathbf{H}_n)} \rho(p) d\mu_n(p) \mathbb{I},$$

that is the statement of the proposition:

$$\sigma = (n + 1) \int_{\mathbf{P}(\mathbf{H}_n)} \rho(p) \left(p - \frac{1}{n + 1} \mathbb{I} \right) d\mu_n(p).$$

□

So, starting from a function $\rho \in \mathcal{F}^2(\mathbf{H})$ one can obtain the associated operator ($\sigma \in \mathfrak{B}(\mathbf{H}_n)$) s.t. $\rho(p) = \text{tr}(\sigma p)$ by the smearing of ρ with the operator:

$$\mathfrak{B}(\mathbf{H}_n) \ni \mathfrak{S}(p) := (n+1)p - \mathbb{I} \quad p \in \mathbf{P}(\mathbf{H}_n), \quad (4.16)$$

$$\sigma = \int_{\mathbf{P}(\mathbf{H}_n)} \rho(p) \mathfrak{S}(p) d\mu_n(p). \quad (4.17)$$

For this reason let us call the operator-valued function $\mathfrak{S} : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathfrak{B}(\mathbf{H}_n)$ *re-quantization distribution* since its smearing action on each Liouville density gives the correspondent density matrix. The statement of theorem 37 can be used to construct a re-quantization prescription to obtain a quantum observable (a self-adjoint operator) smearing a classical-like observable with a re-quantization distribution. We calculate the inverse map of $\mathcal{O} : i\mathfrak{u}(n) \ni A \mapsto f_A$ defined in (3) in the general form. Let $A \in i\mathfrak{u}(n)$, by direct computation:

$$\int_{\mathbf{P}(\mathbf{H}_n)} f_A(p) \mathfrak{S}(p) d\mu_n(p) = \kappa \int_{\mathbf{P}(\mathbf{H}_n)} \text{tr}(Ap) \mathfrak{S}(p) d\mu_n(p) + \frac{1-\kappa}{n} \text{tr}(A) \int_{\mathbf{P}(\mathbf{H}_n)} \mathfrak{S}(p) d\mu_n(p),$$

exploiting the statement of theorem 37 and noting that $\int \mathfrak{S}(p) d\nu(p) = \mathbb{I}$, we can write:

$$\int_{\mathbf{P}(\mathbf{H}_n)} f_A(p) \mathfrak{S}(p) d\mu_n(p) = \kappa A + \frac{1-\kappa}{n} \text{tr}(A) \mathbb{I},$$

an easy computation shows $\int f_A(p) d\nu(p) = \text{tr}(A)$ for every $\kappa > 0$, thus:

$$A = \frac{1}{\kappa} \int_{\mathbf{P}(\mathbf{H}_n)} f_A(p) \left[\mathfrak{S}(p) - \frac{1-\kappa}{n} \mathbb{I} \right] d\mu_n(p). \quad (4.18)$$

The general re-quantization distribution for observables, i.e. the operator-valued function $\mathfrak{D} : \mathbf{P}(\mathbf{H}_n) \rightarrow \mathfrak{B}(\mathbf{H}_n)$ such that for any $A \in i\mathfrak{u}(n)$:

$$A = \int_{\mathbf{P}(\mathbf{H}_n)} f_A(p) \mathfrak{D}(p) d\mu_n(p)$$

is given by:

$$\mathfrak{D}(p) = \frac{(n+1)}{\kappa} p - \left(\frac{n+1-\kappa}{\kappa n} \right) \mathbb{I}. \quad (4.19)$$

In the choice $\kappa = n+1$, where the action of \mathcal{O} is given by $\mathcal{O}(A) = f_A$ with $f_A(p) = \text{tr}(Ap) - \text{tr}(A)$ and the action of \mathcal{S} is simply $\mathcal{S}(\sigma) = \rho_\sigma$ with $\rho_\sigma(p) = \text{tr}(\sigma p)$, re-quantization distribution is simply $\mathfrak{D}(p) = p$ for observables and (4.16) for states. Then re-quantization procedure is given by the following formulas:

$$A = \int_{\mathbf{P}(\mathbf{H}_n)} f_A(p) p d\mu_n(p), \quad (4.20)$$

$$\sigma = \int_{\mathbf{P}(\mathbf{H}_n)} \rho_\sigma(p) \mathfrak{S}(p) d\mu_n(p), \quad (4.21)$$

for every classical-like observable (real functions in $\mathcal{F}^2(\mathbf{H}_n)$) and Liouville density on $\mathbf{P}(\mathbf{H}_n)$. (4.20) turns out to be a sort of continuous spectral decomposition of the operator A .

4.3 Observable C^* -algebra in geometric Hamiltonian formulation

Since the machinery of frame functions allows a complete characterization of classical-like observable associated to quantum observables, as explained in the last section, we can investigate the structure of the C^* -algebra enjoyed by the set of \mathcal{L}^2 -frame functions. In this section we assume to work with \mathcal{O} of the form (3.16), holding (4.3), (4.4), (4.5), (4.5). The observables of the systems we are considering are the self-adjoint elements of $\mathfrak{B}(\mathbf{H}_n)$. Considering also complex combinations of observables we recover the whole C^* -algebra $\mathfrak{B}(\mathbf{H}_n)$. The map \mathcal{O} , defined with respect to a choice of $\kappa > 0$, can be extended by linearity to a map indicated with the same symbol:

$$\mathcal{O} : \mathfrak{B}(\mathbf{H}_n) \ni A \mapsto f_A := \kappa F_A + c_\kappa \text{tr}(A) \in \mathcal{F}^2(\mathbf{H}_n).$$

From (d) in theorem 34, this map turns out to be an isomorphism of complex vector spaces with the further property that

$$\mathcal{O}^{-1}(\bar{f}) = (\mathcal{O}^{-1}(f))^* \quad \text{for all } f \in \mathcal{F}^2(\mathbf{H}_n).$$

Obviously \mathcal{O} can be used to induce on $\mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$ a structure of $*$ -algebra, defining a (distributive and associative) $*$ -algebra product:

$$f \star g := \mathcal{O}(\mathcal{O}^{-1}(f)\mathcal{O}^{-1}(g)) \quad \text{for all } f, g \in \mathcal{F}^2(\mathbf{H}_n). \quad (4.22)$$

With this product $\mathcal{F}^2(\mathbf{H}_n)$ becomes a C^* -algebra with unit, given by the constantly function 1, with involution given by the standard complex conjugation and norm:

$$\|f\| := \|\mathcal{O}^{-1}(f)\| \quad \text{for all } f \in \mathcal{F}^2(\mathbf{H}_n), \quad (4.23)$$

where the norm in the right-hand side is the C^* -norm of $\mathfrak{B}(\mathbf{H}_n)$. With these definitions, \mathcal{O} turns out to be a C^* -algebra isomorphism. The proofs are straightforward.

An intriguing issue is whether the C^* -algebra norm and products can be recast using the geometric structure already present on $\mathbf{P}(\mathbf{H}_n)$. Concerning the norm, we observe that it is enough to know the explicit expression for the case of f real, the general case then arises

form that and the C^* -algebra property $\|a^*a\| = \|a\|^2$, once one has an explicit expression for the product \star , that we will obtain shortly. As a matter of fact $\|f\| = \sqrt{\|\bar{f} \star f\|}$. Focus on $f \in \mathcal{F}^2(\mathbf{P}(\mathbf{H}_n))$ real, so that we can write $f = \kappa F_A + c_\kappa \text{tr}(A)$ for some $A \in iu(n)$. Since A is self-adjoint:

$$\|F_A\|_\infty = \sup_{p \in \mathbf{P}(\mathbf{H}_n)} |\text{tr}(pA)| = \sup_{\psi \in \mathbb{S}(\mathbf{H}_n)} |\langle \psi | A \psi \rangle| = \|A\| = \|f\|.$$

As a consequence, taking advantage from (3.11), from the explicit expression of f_A (50), and exploiting $\kappa + nc_\kappa = 1$, we immediately have a geometric expression for $\|f\|$.

Proposition 38 *If $n > 2$ and $f \in \mathcal{F}^2(\mathbf{H}_n)$ is real, referring to the C^* -algebra norm in (50) (everything defined for a choice of $\kappa > 0$) we have:*

$$\|f\| = \frac{1}{\kappa} \left\| f - (1 - \kappa) \int_{\mathbf{P}(\mathbf{H}_n)} f d\mu_n \right\|_\infty. \quad (4.24)$$

Even dropping the requirement $f \in \mathcal{F}^2(\mathbf{H}_n)$ and assuming, more generally, $f \in C^0(\mathbf{P}(\mathbf{H}_n))$, the right-hand side of (4.24) defines a norm. The same holds true if working in $L^\infty(C^0(\mathbf{P}(\mathbf{H}_n)), \mu_n)$ and interpreting $\|\cdot\|_\infty$ as the natural norm referred to the essential supremum computed with respect to μ_n . The proofs are straightforward.

We write down two cases explicitly. The case $\kappa = n + 1$, with $\mu'_n := n\mu_n$:

$$\|f\| = \frac{1}{n+1} \left\| f + \int_{\mathbf{P}(\mathbf{H}_n)} f d\mu'_n \right\|_\infty, \quad \text{for every real } f \in \mathcal{F}^2(\mathbf{H}_n),$$

and the case considered by Gibbons, $\kappa = 1$:

$$\|f\| = \|f\|_\infty, \quad \text{for every real } f \in \mathcal{F}^2(\mathbf{H}_n).$$

Let us finally pass to the product \star , stating a corresponding theorem.

Theorem 39 *Let $n > 2$ and $f, g \in \mathcal{F}^2(\mathbf{H}_n)$. If $G_p : T_p^*\mathbf{P}(\mathbf{H}_n) \times T_p^*\mathbf{P}(\mathbf{H}_n) \rightarrow \mathbb{R}$ denotes the scalar product on 1-forms canonically induced by the metric g on $\mathbf{P}(\mathbf{H}_n)$, referring to the C^* -algebra product in (4.22), we have:*

$$\begin{aligned} f \star g &= \frac{i}{2} \{f, g\} + \frac{1}{2} G(df, dg) + \frac{fg}{\kappa} + \frac{1-\kappa}{\kappa} \left(\frac{n+1}{\kappa} \int_{\mathbf{P}(\mathbf{H}_n)} f g d\mu_n - f \int_{\mathbf{P}(\mathbf{H}_n)} g d\mu_n - g \int_{\mathbf{P}(\mathbf{H}_n)} f d\mu_n \right) \\ &\quad + \frac{1-\kappa}{\kappa^2} (\kappa - (n+1)) \int_{\mathbf{P}(\mathbf{H}_n)} f d\mu_n \int_{\mathbf{P}(\mathbf{H}_n)} g d\mu_n \end{aligned} \quad (4.25)$$

with, as usual, $\kappa > 0$. In particular, for $\kappa = n + 1$ and defining $\mu'_n := n\mu_n$:

$$f \star g = \frac{i}{2}\{f, g\} + \frac{1}{2}G(df, dg) + \frac{1}{n+1} \left(fg - \int_{\mathbb{P}(\mathbb{H}_n)} fg d\mu'_n + f \int_{\mathbb{P}(\mathbb{H}_n)} g d\mu'_n + g \int_{\mathbb{P}(\mathbb{H}_n)} f d\mu'_n \right)$$

and, for $\kappa = 1$:

$$f \star g = \frac{i}{2}\{f, g\} + \frac{1}{2}G(df, dg) + fg. \quad (4.26)$$

Proof. First of all we notice that, the following identity holds, $g(X_f, X_g) = G(df, dg)$, that immediately follows from $g(X_f, j \cdot) = \omega(X_h, \cdot) = df$, $jj = -I$ and $g(ju, jv) = g(u, v)$. So we replace $G(df, dg)$ for $g(X_f, X_g)$ in the following. Define $f := f_A$ and $g := f_B$. With this choice $f \star g = f_{AB} = \kappa F_{AB} + c_\kappa tr(AB)$. Therefore:

$$f_{AB}(p) = \kappa tr(pAB) + c_\kappa tr(AB) = \frac{\kappa}{2} \kappa tr(p[A, B]) + \frac{\kappa}{2} tr(p(AB + BA)) + c_\kappa tr(AB).$$

A straightforward computation proves that

$$tr(p(AB + BA)) = -tr(p[p, A][p, B]) - tr(p[p, B][p, A]) + 2tr(pA)tr(pB).$$

Reminding the definition of ω , $\{\cdot, \cdot\}$, X_h and g presented in section 3.1, and putting all together we find:

$$(f \star g)(p) = f_{AB}(p) = \frac{i}{2}\{f, g\} + \frac{1}{2}g(X_f, X_g) + \kappa tr(pA)tr(pB) + c_\kappa tr(AB).$$

From $\kappa + nc_\kappa = 1$ and using (3.11), one easily finds

$$\int_{\mathbb{P}(\mathbb{H}_n)} f_A d\mu = \kappa \int_{\mathbb{P}(\mathbb{H}_n)} F_A d\mu + c_\kappa tr(A) = \frac{1}{n} tr(A) = \int_{\mathbb{P}(\mathbb{H}_n)} F_A d\mu,$$

and a similar result for B in place of A . Using (3.13) and the definition of f_A (f_B) in terms of F_A (F_B):

$$\begin{aligned} f \star g &= \frac{i}{2}\{f, g\} + \frac{1}{2}g(X_f, X_g) + \frac{1}{\kappa} \left(f - nc_\kappa \int_{\mathbb{P}(\mathbb{H}_n)} f d\mu_n \right) \left(g - nc_\kappa \int_{\mathbb{P}(\mathbb{H}_n)} g d\mu_n \right) \\ &- c_\kappa n^2 \int_{\mathbb{P}(\mathbb{H}_n)} f d\mu_n \int_{\mathbb{P}(\mathbb{H}_n)} g d\mu_n + \frac{c_\kappa n(n+1)}{\kappa^2} \int_{\mathbb{P}(\mathbb{H}_n)} \left(f - nc_\kappa \int_{\mathbb{P}(\mathbb{H}_n)} f d\mu_n \right) \left(g - nc_\kappa \int_{\mathbb{P}(\mathbb{H}_n)} g d\mu_n \right) d\mu_n. \end{aligned}$$

Using again $\kappa + nc_\kappa = 1$ we obtain (4.25). \square

The formula 4.25 explicitly shows the structure of Lie-Jordan-Banach algebra of $\mathcal{F}^2(\mathbf{H}_n)$. For $\kappa = 1$ the standard deviation $(\Delta A)_\psi$ coincides to $\frac{1}{2}G_p(df_A, df_A)$, this allows to write down a geometrical formulation of Heisenberg inequality. For other choices of κ it is still possible, but the expression is more complicated. A formula similar to (4.22) for $n = 2$ (stated on the 2-dimensional Bloch sphere) and for the case $\kappa = 1$ is mentioned in [12].

Chapter 5

Geometric Hamiltonian approach to composite quantum systems

Content of this chapter is based on [36].

One of the reasons why finite-dimensional QM is interesting regards the *quantum information theory*. The aim of this chapter is investigating if the self-consistent geometric Hamiltonian formulation of finite-dimensional QM admits any application to this topic. First of all we have to study how describe a composite quantum system with the Hamiltonian formalism. Considering a bipartite system described in a Hilbert space given by the tensor product $H_1 \otimes H_2$, the quantum phase space for the Hamiltonian description should be $P(H_1 \otimes H_2)$ and not $P(H_1) \times P(H_2)$ as suggested by the analogy with Classical Mechanics. In the first section we tackle this issue, studying how Liouville densities of a composite system can be characterized.

5.1 Liouville densities for composite systems

In Classical Mechanics the phase space of a composite system is given by the cartesian product of phase spaces of each subsystem. While if one consider a quantum composite system then the phase space must be the projective space of the tensor product of the Hilbert spaces of the subsystems, according to standard Quantum Mechanics. We can consider a bipartite quantum system which consists in two subsystems described in the finite-dimensional Hilbert spaces H and K : The phase space (in the geometric Hamiltonian sense) of the system is given by $P(H \otimes K)$ and not by $P(H) \times P(K)$, however the second one is embedded in the first one by *Segre embedding*. Let us recall few fundamental ideas: Considering two finite dimensional Hilbert spaces H and K , let us recall how the tensor product of Hilbert spaces $H \otimes K$ is defined: the *tensor product* of two vectros $\psi \in H$ and $\phi \in K$, denoted by $\psi \otimes \phi$, is defined as the following bilinear form:

$$\psi \otimes \phi : H \times K \rightarrow \mathbb{C} \quad \psi \otimes \phi(\eta, \zeta) := \langle \psi | \eta \rangle_H \langle \phi | \zeta \rangle_K, \quad (5.1)$$

where $\langle | \rangle_{\mathbf{H}}$ and $\langle | \rangle_{\mathbf{K}}$ are the inner products on \mathbf{H} and \mathbf{K} respectively. We denote with $\mathbf{H} \otimes \mathbf{K}$ the vector space spanned by all $\psi \otimes \phi$. For $\psi \otimes \phi, \psi' \otimes \phi' \in \mathbf{H} \otimes \mathbf{K}$, we can define an inner product:

$$\langle \psi \otimes \phi | \psi' \otimes \phi' \rangle := \langle \psi | \psi' \rangle_{\mathbf{H}} \langle \phi | \phi' \rangle_{\mathbf{K}}. \quad (5.2)$$

Above definition extends to $\mathbf{H} \otimes \mathbf{K}$ which turns out to be a Hilbert space called *tensor product of Hilbert spaces* \mathbf{H} and \mathbf{K} . In the same way we can define the tensor product of a countable quantity of Hilbert spaces. Consider $A \in \mathfrak{B}(\mathbf{H})$ and $B \in \mathfrak{B}(\mathbf{K})$, the *tensor product of two operators*, $A \otimes B$, can be defined in the following way on the product vectors $\psi \otimes \phi$:

$$A \otimes B(\psi \otimes \phi) := A\psi \otimes B\phi, \quad (5.3)$$

and the action extends to whole Hilbert space $\mathbf{H} \otimes \mathbf{K}$ by linearity. The span of all $A \otimes B$ can be denoted by $\mathfrak{B}(\mathbf{H}) \otimes \mathfrak{B}(\mathbf{K})$ and it coincides with $\mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$ as a general result on Von Neumann algebras. Of course, not all the operators in $\mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$ are in the product form $A \otimes B$, but considering a general operator in $\mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$ we can define a notion of *restriction* of such operator to \mathbf{H} or \mathbf{K} , via the so-called *partial trace*.

Definition 40 Let be $A \in \mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$. The **partial trace** of A w.r.t. \mathbf{K} (similarly \mathbf{H}) is the unique operator $tr_{\mathbf{K}}(A) \in \mathfrak{B}(\mathbf{H})$ such that:

$$tr [tr_{\mathbf{K}}(A)B] = tr[A(B \otimes \mathbb{I}_{\mathbf{K}})] \quad \forall B \in \mathfrak{B}(\mathbf{H}). \quad (5.4)$$

where $\mathbb{I}_{\mathbf{K}}$ denotes the identity operator on \mathbf{K} .

Consider a quantum system made up by two quantum subsystems which are described by the observable algebras $\mathfrak{B}(\mathbf{H})$ and $\mathfrak{B}(\mathbf{K})$. According to standard quantum theory the observable algebra of the composite system is given by the tensor product $\mathfrak{B}(\mathbf{H}) \otimes \mathfrak{B}(\mathbf{K}) = \mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$.

Definition 41 A state $\sigma \in \mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$ is called **separable** if it can be written as:

$$\sigma = \sum_i \lambda_i \sigma_i^{(1)} \otimes \sigma_i^{(2)},$$

whit weights $\lambda_i > 0$ and states $\sigma_i^{(1)} \in \mathfrak{B}(\mathbf{H})$, $\sigma_i^{(2)} \in \mathfrak{B}(\mathbf{K})$; otherwise it is called **entangled**.

According to the above definition, a pure state $\sigma \in \mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$ is separable if and only if it is of product form $\sigma = \sigma_1 \otimes \sigma_2$. In this regard let us introduce the well-known *Segre embedding*. The tensor product map $\otimes : \mathbf{H} \times \mathbf{K} \rightarrow \mathbf{H} \otimes \mathbf{K}$ induces a canonical embedding of the cartesian product of complex projective spaces in the complex projective space of the tensor product, called **Segre embedding**:

$$\begin{aligned} \text{Seg} &: \mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K}) \rightarrow \mathbf{P}(\mathbf{H} \otimes \mathbf{K}), \\ \text{Seg} &: (|\psi\rangle\langle\psi|, |\phi\rangle\langle\phi|) \mapsto |\psi \otimes \phi\rangle\langle\psi \otimes \phi|, \quad \|\psi\| = \|\phi\| = 1. \end{aligned} \quad (5.5)$$

The action of Segre embedding can be written as $\text{Seg}(p_1, p_2) = p_1 \otimes p_2$ for $p_1 \in \mathbf{P}(\mathbf{H})$ and $p_2 \in \mathbf{P}(\mathbf{K})$, representing pure states as points of projective space. In the standard formulation, the image $\text{Seg}(\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K}))$ gives the separable pure states of the composite system. Here we use the Segre embedding to explicitly construct the isomorphism between $\mathcal{F}^2(\mathbf{H}) \otimes \mathcal{F}^2(\mathbf{K})$ and $\mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$.

Proposition 42 *Let \mathbf{H} and \mathbf{K} be finite-dimensional Hilbert spaces with $\dim \mathbf{H}, \dim \mathbf{K} > 2$. The map $\mathcal{I} : \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K}) \rightarrow \mathcal{F}^2(\mathbf{H}) \otimes \mathcal{F}^2(\mathbf{K})$ defined as the pull-back by Segre embedding:*

$$\mathcal{I}(f) = \text{Seg}^* f \quad (5.6)$$

is an isomorphism.

Proof. For any $f \in \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$, its image function $\mathcal{I}(f) : (p_1, p_2) \mapsto f \circ \text{Seg}(p_1, p_2)$ belongs to $\mathcal{F}^2(\mathbf{H}) \otimes \mathcal{F}^2(\mathbf{K})$. We have to show that \mathcal{I} is bijective.

The generic element g of $\mathcal{F}^2(\mathbf{H}) \otimes \mathcal{F}^2(\mathbf{K})$ is the function given by the finite sum:

$$g : (p_1, p_2) \mapsto \sum_{i \in I} g_1^{(i)}(p_1) g_2^{(i)}(p_2),$$

with $g_1^{(i)} \in \mathcal{F}^2(\mathbf{H})$ and $g_2^{(i)} \in \mathcal{F}^2(\mathbf{K})$ for every $i \in I$. The function g can be written as:

$$g : (p_1, p_2) \mapsto \sum_{i \in I} \text{tr}(A_1^{(i)} p_1) \text{tr}(A_2^{(i)} p_2),$$

with $A_1^{(i)} \in \mathfrak{B}(\mathbf{H})$ and $A_2^{(i)} \in \mathfrak{B}(\mathbf{K})$ for every $i \in I$. We define the action of the map $\mathcal{J} : \mathcal{F}^2(\mathbf{H}) \otimes \mathcal{F}^2(\mathbf{K}) \rightarrow \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ as:

$$\mathcal{J}(g) : \mathbf{P}(\mathbf{H} \otimes \mathbf{K}) \rightarrow \mathbb{C}$$

$$\mathcal{J}(g) : p \mapsto \sum_{i \in I} \text{tr} \left(A_1^{(i)} \otimes A_2^{(i)} p \right) = \text{tr} \left(\sum_{i \in I} A_1^{(i)} \otimes A_2^{(i)} p \right).$$

The direct calculation shows that $\mathcal{J} = \mathcal{I}^{-1}$, so \mathcal{I} is a bijection. \square

One can prove the above result establishes a C^* -algebraic isomorphism, however only the isomorphism of vector spaces is useful for us, considering the convex set $\mathbf{S}(\mathbf{H} \otimes \mathbf{K}) \subset \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ of Liouville densities. The hypothesis $\dim \mathbf{H}, \dim \mathbf{K} > 2$ is mandatory because we exploit the isomorphisms $\mathcal{F}^2(\mathbf{H}) \simeq \mathfrak{B}(\mathbf{H})$ and $\mathcal{F}^2(\mathbf{K}) \simeq \mathfrak{B}(\mathbf{K})$.

5.2 Quantum entanglement in geometric Hamiltonian picture

5.2.1 A notion of separability

In this section we introduce the machinery to describe quantum entanglement of a bipartite system in terms of Liouville densities defined on the phase space given by the projective Hilbert space. As *inverse-quantization scheme* for states (to obtain Liouville densities from density matrices) we consider the isomorphism of vector spaces $\mathcal{S} : \mathfrak{B}(\mathbf{H} \otimes \mathbf{K}) \rightarrow \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ given by $\mathcal{S}(\sigma)(p) = \text{tr}(\sigma p)$ for every $\sigma \in \mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$, we also consider the isomorphisms $\mathcal{S}_{\mathbf{H}} : \mathfrak{B}(\mathbf{H}) \rightarrow \mathcal{F}^2(\mathbf{H})$ and $\mathcal{S}_{\mathbf{K}} : \mathfrak{B}(\mathbf{K}) \rightarrow \mathcal{F}^2(\mathbf{K})$ defined for the subsystems.

Since a pure state of a bipartite system is separable if and only if it is represented by a pure tensor in $\mathbf{H} \otimes \mathbf{K}$, we want to investigate how product form is encoded in frame functions formalism. Henceforth we assume $\dim \mathbf{H}, \dim \mathbf{K} > 2$ without further specifications.

The following result shows a necessary and sufficient condition on $\rho \in \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ so that $\rho = \mathcal{S}(\sigma_1 \otimes \sigma_2)$ with $\sigma_1 \in \mathfrak{B}(\mathbf{H})$ and $\sigma_2 \in \mathfrak{B}(\mathbf{K})$. In other words there is a criterion to check if a function in $\mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ is associated to an operator in the product form.

Proposition 43 *Let be $\rho \in \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$, the operator $\sigma = \mathcal{S}^{-1}(\rho) \in \mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$ is given by a product $\sigma = \sigma_1 \otimes \sigma_2$ with $\sigma_1 \in \mathfrak{B}(\mathbf{H})$ and $\sigma_2 \in \mathfrak{B}(\mathbf{K})$ if and only if there are $\rho_1 \in \mathcal{F}^2(\mathbf{H})$, $\rho_2 \in \mathcal{F}^2(\mathbf{K})$ such that:*

$$(\rho \circ \text{Seg})(p_1, p_2) = \rho_1(p_1)\rho_2(p_2) \quad \forall (p_1, p_2) \in \mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K}), \quad (5.7)$$

where $\text{Seg} : \mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K}) \rightarrow \mathbf{P}(\mathbf{H} \otimes \mathbf{K})$ is the Segre embedding $\text{Seg} : (p_1, p_2) \mapsto p_1 \otimes p_2$. Moreover the functions ρ_1 and ρ_2 satisfy $\rho_1 = \mathcal{S}_{\mathbf{H}}(\sigma_1)$ and $\rho_2 = \mathcal{S}_{\mathbf{K}}(\sigma_2)$.

In this case we say that the function ρ is of the **product form** writing $\rho = \rho_1 \diamond \rho_2$.

Proof. Let us suppose that $\rho = \mathcal{S}(\sigma)$, i.e. $\rho(p) = \text{tr}(\sigma p)$, where $\sigma = \sigma_1 \otimes \sigma_2$ with $\sigma_1 \in \mathfrak{B}(\mathbf{H})$ and $\sigma_2 \in \mathfrak{B}(\mathbf{K})$. Just calculate, for any $p_1 \in \mathbf{P}(\mathbf{H})$ and $p_2 \in \mathbf{P}(\mathbf{K})$:

$$(\rho \circ \text{Seg})(p_1, p_2) = \rho(p_1 \otimes p_2) = \text{tr}(\sigma p_1 \otimes p_2) = \text{tr}(\sigma_1 p_1 \otimes \sigma_2 p_2) = \text{tr}(\sigma_1 p_1)\text{tr}(\sigma_2 p_2)$$

put: $\rho_1(p_1) = \text{tr}(\sigma_1 p_1)$ and $\rho_2(p_2) = \text{tr}(\sigma_2 p_2)$. Thus we proved that (5.7) holds if:

$$\rho(p) = \text{tr}(\sigma_1 \otimes \sigma_2 p) \quad p \in \mathbf{P}(\mathbf{H} \otimes \mathbf{K}), \quad (5.8)$$

now let us prove that (5.7) *only if* (5.8). The function $\hat{\rho} : (p_1, p_2) \mapsto \rho_1(p_1)\rho_2(p_2)$ is an element of $\mathcal{F}^2(\mathbf{H}) \otimes \mathcal{F}^2(\mathbf{K})$. Since $\mathcal{F}^2(\mathbf{H}) \otimes \mathcal{F}^2(\mathbf{K})$ and $\mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ are isomorphic (Proposition 42) then for any function $\hat{\rho} \in \mathcal{F}^2(\mathbf{H}) \otimes \mathcal{F}^2(\mathbf{K})$ there is a unique function

$\rho \in \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ such that $\hat{\rho} = \mathcal{I}(\rho) = \rho \circ \text{Seg}$. Thus the function $\rho \in \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ satisfying (5.7) is unique and given by (5.8). \square

In proposition 43, we have introduced the product \diamond corresponding to tensor product between operators, i.e. $\mathcal{S}(A \otimes B) = \mathcal{S}_{\mathbf{H}}(A) \diamond \mathcal{S}_{\mathbf{K}}(B)$ for every $A \in \mathfrak{B}(\mathbf{H})$ and $B \in \mathfrak{B}(\mathbf{K})$. Since \mathcal{S} is linear, the vector space $\mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ is the span of all $\rho_1 \diamond \rho_2$. Applying the result of Proposition 37 we can give an explicit definition of the \diamond -product. The natural idea is representing $\sigma_1 \otimes \sigma_2$ in terms of the integral introduced in Proposition 37. Consider the re-quantization distributions $\mathfrak{S}_{\mathbf{H}} : \mathbf{P}(\mathbf{H}) \rightarrow \mathfrak{B}(\mathbf{H})$ and $\mathfrak{S}_{\mathbf{K}} : \mathbf{P}(\mathbf{K}) \rightarrow \mathfrak{B}(\mathbf{K})$ according to definition (4.16):

Proposition 44 *Let be $\rho_1 \in \mathcal{F}^2(\mathbf{H})$ and $\rho_2 \in \mathcal{F}^2(\mathbf{K})$. The function $\rho \in \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ such that $\mathcal{S}^{-1}(\rho) = \mathcal{S}_{\mathbf{H}}^{-1}(\rho_1) \otimes \mathcal{S}_{\mathbf{K}}^{-1}(\rho_2)$ is given by:*

$$\rho(p) = \int_{\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K})} \rho_1(p_1) \rho_2(p_2) \text{tr} [p \mathfrak{S}_{\mathbf{H}}(p_1) \otimes \mathfrak{S}_{\mathbf{K}}(p_2)] d\mu_{\mathbf{H}}(p_1) d\mu_{\mathbf{K}}(p_2) =: (\rho_1 \diamond \rho_2)(p), \quad (5.9)$$

where $\mu_{\mathbf{H}}$ and $\mu_{\mathbf{K}}$ are the Liouville measures respectively defined on the manifolds $\mathbf{P}(\mathbf{H})$ and $\mathbf{P}(\mathbf{K})$.

Proof. The thesis is a direct result of these two steps: representation of the operator $\mathcal{S}_{\mathbf{H}}^{-1}(\rho_1) \otimes \mathcal{S}_{\mathbf{K}}^{-1}(\rho_2)$ with the integral formula (4.17) and the calculation of $\rho = \mathcal{S}(\mathcal{S}_{\mathbf{H}}^{-1}(\rho_1) \otimes \mathcal{S}_{\mathbf{K}}^{-1}(\rho_2))$. \square

The product function $\rho_1 \diamond \rho_2$ is given by a smearing on the cartesian product $\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K})$ with a kernel $\mathfrak{T} : \mathbf{P}(\mathbf{H} \otimes \mathbf{K}) \times \mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K}) \rightarrow \mathbb{C}$ which does not depend on ρ_1 and ρ_2 but only on the quantization distributions on $\mathbf{P}(\mathbf{H})$ and $\mathbf{P}(\mathbf{K})$ given by $\mathfrak{T}(p, p_1, p_2) = \text{tr}[p \mathfrak{S}_{\mathbf{H}}(p_1) \otimes \mathfrak{S}_{\mathbf{K}}(p_2)]$, thus:

$$(\rho_1 \diamond \rho_2)(p) = \int_{\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K})} \rho_1(p_1) \rho_2(p_2) \mathfrak{T}(p, p_1, p_2) d\mu_{\mathbf{H}}(p_1) d\mu_{\mathbf{K}}(p_2). \quad (5.10)$$

With a very compact notation, we can write: $\rho_1 \diamond \rho_2 = \int \rho_1 \otimes \rho_2 \mathfrak{T} d\nu_{\mathbf{H}} d\nu_{\mathbf{K}}$.

We can define an analogous notion of partial trace for functions in $\mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ that are not of product form $\rho_1 \diamond \rho_2$. In Definition 40, partial trace of $\sigma \in \mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$, denoted as $\text{tr}_{\mathbf{K}}(\sigma)$, is defined as the unique operator such that

$$\text{tr}(\text{tr}_{\mathbf{K}}(\sigma)A) = \text{tr}(\sigma A \otimes \mathbb{I}_{\mathbf{K}}) \quad \forall A \in \mathfrak{B}(\mathbf{H}).$$

A slightly alternative definition is the following: the **partial trace** with respect to \mathbf{K} is the injective map $tr_{\mathbf{K}} : \mathfrak{B}(\mathbf{H} \otimes \mathbf{K}) \rightarrow \mathfrak{B}(\mathbf{H})$ given by:

$$tr_{\mathbf{K}}(\sigma \otimes \sigma') := \sigma tr(\sigma') \quad \forall \sigma \in \mathfrak{B}(\mathbf{H}), \forall \sigma' \in \mathfrak{B}(\mathbf{K}), \quad (5.11)$$

and extended to whole $\mathfrak{B}(\mathbf{H} \otimes \mathbf{K})$ by linearity. In order to apply the tool of partial trace in the approach of this paper, we define a map, we can say *partial integral*, using the trace-integral formula already introduced in (3.11).

Definition 45 Let $\mathcal{F}^2(\mathbf{H} \otimes \mathbf{K}) \ni \rho \mapsto \rho_{\mathbf{K}} \in \mathcal{F}^2(\mathbf{H})$ be a map defined on product elements by:

$$(\rho_1 \diamond \rho_2)_{\mathbf{K}}(p_1) := \rho_1(p_1) \int_{\mathbf{P}(\mathbf{K})} \rho_2(p_2) d\mu_{\mathbf{K}}(p_2), \quad (5.12)$$

for any pair $\rho_1 \in \mathcal{F}^2(\mathbf{H})$ and $\rho_2 \in \mathcal{F}^2(\mathbf{K})$ and extended by linearity to whole $\mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$. We call the map $\rho \mapsto \rho_{\mathbf{K}}$ the **partial integral** w.r.t. $\mathbf{P}(\mathbf{K})$.

In case of quantum states, the partial integral can be interpreted as the integration of a Liouville density describing a state of a composite system w.r.t. to a marginal measure obtaining a *marginal* probability density.

Proposition 46 If $\rho \mapsto \rho_{\mathbf{K}}$ is the partial integral on $\mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ w.r.t. $\mathbf{P}(\mathbf{K})$, then:
i) $\rho_{\mathbf{K}}$ has this form:

$$\rho_{\mathbf{K}}(p_1) = \int_{\mathbf{P}(\mathbf{K})} (\rho \circ Seg)(p_1, p_2) d\mu_{\mathbf{K}}(p_2) \quad \forall \rho \in \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K}). \quad (5.13)$$

ii) The following relation holds:

$$tr_{\mathbf{K}} [\mathcal{S}^{-1}(\rho)] = \mathcal{S}_{\mathbf{H}}^{-1}(\rho_{\mathbf{K}}) \quad \forall \rho \in \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K}). \quad (5.14)$$

Analogous statements for $\rho \mapsto \rho_{\mathbf{H}}$.

Proof. The generic element $\rho \in \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ can be written as a finite sum:

$$\rho = \sum_{i \in I} \rho_1^{(i)} \diamond \rho_2^{(i)},$$

with $\rho_1^{(i)} \in \mathcal{F}^2(\mathbf{H})$ and $\rho_2^{(i)} \in \mathcal{F}^2(\mathbf{K})$ for every $i \in I$. Calculating the partial integral as in (5.12):

$$\rho_{\mathbf{K}} = \sum_{i \in I} \rho_1^{(i)} \int_{\mathbf{P}(\mathbf{K})} \rho_2^{(i)} d\mu_{\mathbf{K}}.$$

Let us show that above expression is equivalent to (5.13): By definition of Segre embedding, we have $(\rho \circ \text{Seg})(p_1, p_2) = \rho(p_1 \otimes p_2)$, $\forall (p_1, p_2) \in \mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K})$, in particular:

$$(\rho \circ \text{Seg})(p_1, p_2) = \sum_{i \in I} \rho_1^{(i)}(p_1) \rho_2^{(i)}(p_2).$$

Integrating w.r.t. $\nu_{\mathbf{K}}$:

$$\int_{\mathbf{P}(\mathbf{K})} \rho \circ \text{Seg} \, d\mu_{\mathbf{K}} = \sum_{i \in I} \rho_1^{(i)} \int_{\mathbf{P}(\mathbf{K})} \rho_2^{(i)} \, d\mu_{\mathbf{K}} = \rho_{\mathbf{K}}.$$

Let us prove the statement ii). By linearity and Proposition 43:

$$\mathcal{S}^{-1}(\rho) = \sum_{i \in I} \mathcal{S}_{\mathbf{H}}^{-1}(\rho_1^{(i)}) \otimes \mathcal{S}_{\mathbf{K}}^{-1}(\rho_2^{(i)}),$$

applying the partial trace $\text{tr}_{\mathbf{K}}$:

$$\text{tr}_{\mathbf{K}} [\mathcal{S}^{-1}(\rho)] = \sum_{i \in I} \mathcal{S}_{\mathbf{H}}^{-1}(\rho_1^{(i)}) \int_{\mathbf{P}(\mathbf{K})} \rho_2^{(i)} \, d\mu_{\mathbf{K}} = \mathcal{S}_{\mathbf{H}}^{-1} \left(\sum_{i \in I} \rho_1^{(i)} \int_{\mathbf{P}(\mathbf{K})} \rho_2^{(i)} \, d\mu_{\mathbf{K}} \right) = \mathcal{S}_{\mathbf{H}}^{-1}(\rho_{\mathbf{K}}).$$

□

The statement of this proposition can be used to prove the next result showing how integrals of frame functions over $\mathbf{P}(\mathbf{H} \otimes \mathbf{K})$ can be computed.

Theorem 47 *Let \mathbf{H} and \mathbf{K} be finite-dimensional Hilbert spaces with $\dim \mathbf{H}, \dim \mathbf{K} > 2$. Consider projective spaces $\mathbf{P}(\mathbf{H})$, $\mathbf{P}(\mathbf{K})$, $\mathbf{P}(\mathbf{H} \otimes \mathbf{K})$, each equipped with the discussed almost complex Kähler structure. $\mu_{\mathbf{H}}$, $\mu_{\mathbf{K}}$ and μ denotes the respective Liouville measures. $\mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ denotes the vector space of frame functions in $\mathcal{L}^2(\mathfrak{B}(\mathbf{H} \otimes \mathbf{K}), \nu)$.*

The following fact holds for any $\rho \in \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$:

$$\int_{\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K})} \rho \circ \text{Seg} \, d\mu_{\mathbf{H}} d\mu_{\mathbf{K}} = \int_{\mathbf{P}(\mathbf{H} \otimes \mathbf{K})} \rho \, d\mu, \quad (5.15)$$

where $d\mu_{\mathbf{H}} d\mu_{\mathbf{K}}$ is the standard product measure on $\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K})$.

Proof. Let $\mathcal{S} : \mathfrak{B}(\mathbf{H} \otimes \mathbf{K}) \rightarrow \mathcal{F}^2(\mathbf{H} \otimes \mathbf{K})$ be the isomorphism defined as $\mathcal{S}(\sigma) = \rho$ such that $\rho(p) = \text{tr}(\sigma p)$ for every $p \in \mathbf{P}(\mathbf{H} \otimes \mathbf{K})$. Trace integral formula (3.11) holds:

$$\int_{\mathbf{P}(\mathbf{H} \otimes \mathbf{K})} \rho \, d\mu = \text{tr} [\mathcal{S}^{-1}(\rho)].$$

Using statement (b) of Proposition 46:

$$\text{tr} (\text{tr}_{\mathbb{K}} [\mathcal{S}^{-1}(\rho)]) = \int_{\mathbb{P}(\mathbb{H})} \rho_{\mathbb{K}} d\mu_{\mathbb{H}} \quad (5.16)$$

Since $\text{tr} (\text{tr}_{\mathbb{K}} [\mathcal{S}^{-1}(\rho)]) = \text{tr} [\mathcal{S}^{-1}(\rho)]$ by definition of partial trace, the theorem is proved by statement (a) of Proposition 46. \square

5.2.2 A measure of entanglement

Let us recall the set of Liouville densities is denoted by $\mathbb{S}(\mathbb{H})$ and the subset of densities representing pure states is denoted as $\mathbb{S}_p(\mathbb{H})$. In the following there is the definition of separable and entangled states in terms of Liouville densities.

Definition 48 Let $\rho \in \mathbb{S}_p(\mathbb{H} \otimes \mathbb{K})$ be a Liouville density representing a pure state of the composite system described on $\mathbb{P}(\mathbb{H} \otimes \mathbb{K})$. ρ is said to be a **separable pure state** if there are $\rho_1 \in \mathbb{S}_p(\mathbb{H})$ and $\rho_2 \in \mathbb{S}_p(\mathbb{K})$ such that $\rho = \rho_1 \diamond \rho_2$. In other words, ρ is said to be a **separable pure state** if:

$$(\rho \circ \text{Seg})(p_1, p_2) = \rho_{\mathbb{K}}(p_1)\rho_{\mathbb{H}}(p_2) \quad \forall (p_1, p_2) \in \mathbb{P}(\mathbb{H}) \times \mathbb{P}(\mathbb{K}) \quad (5.17)$$

where $\rho_{\mathbb{H}}$ and $\rho_{\mathbb{K}}$ are the partials integrals of ρ w.r.t. $\mathbb{P}(\mathbb{H})$ and $\mathbb{P}(\mathbb{K})$ respectively. We denote the set of separable pure states as $\mathbb{S}_p^{\text{sep}}(\mathbb{H} \otimes \mathbb{K})$.

The elements of the convex hull $\mathbb{S}^{\text{sep}}(\mathbb{H} \otimes \mathbb{K}) := \text{conv}[\mathbb{S}_p^{\text{sep}}(\mathbb{H} \otimes \mathbb{K})]$ are called **separable mixed states**. Finally, the states belonging to $\mathcal{E}(\mathbb{H} \otimes \mathbb{K}) := \mathbb{S}(\mathbb{H} \otimes \mathbb{K}) \setminus \mathbb{S}^{\text{sep}}(\mathbb{H} \otimes \mathbb{K})$ are called **entangled states**.

Definition 48 suggests that the measure of the subset in $\mathbb{P}(\mathbb{H}) \times \mathbb{P}(\mathbb{K})$ where the equation $\rho \circ \text{Seg} = \rho_{\mathbb{K}}\rho_{\mathbb{H}}$ fails can be considered an entanglement measure of the state ρ .

From the physical point of view this idea of entanglement measure does not take into account the distinguishability of entangled states. Below the proposal of an entanglement measure based on a L^2 -distance.

Let us introduce a real map $E : \mathbb{S}(\mathbb{H} \otimes \mathbb{K}) \rightarrow \mathbb{R}$ defined by:

$$E(\rho) := \left(\int_{\mathbb{P}(\mathbb{H}) \times \mathbb{P}(\mathbb{K})} |F_{\rho}|^2 d\mu_{\mathbb{H}} d\mu_{\mathbb{K}} \right)^{\frac{1}{2}} \quad \forall \rho \in \mathbb{S}_p(\mathbb{H} \otimes \mathbb{K}), \quad (5.18)$$

where

$$F_{\rho}(p_1, p_2) := (\rho \circ \text{Seg})(p_1, p_2) - \rho_{\mathbb{K}}(p_1)\rho_{\mathbb{H}}(p_2), \quad (5.19)$$

and the extension of E to $\mathbb{S}(\mathbb{H} \otimes \mathbb{K})$ is given by the convex roof:

$$E(\rho) := \inf_{\rho = \sum \lambda_i \rho_i} \sum_i \lambda_i E(\rho_i) \quad \forall \rho \in \mathbf{S}(\mathbf{H} \otimes \mathbf{K}), \quad (5.20)$$

where the infimum is taken on all the possible convex combinations of ρ in terms of pure states $\rho_i \in \mathbf{S}_p(\mathbf{H} \otimes \mathbf{K})$ and the coefficients λ_i are the statistical weights of the mixture. Since $F_\rho \in \mathcal{L}^2(\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K}), d\nu_{\mathbf{H}} d\nu_{\mathbf{K}})$ for any $\rho \in \mathbf{S}_p(\mathbf{H} \otimes \mathbf{K})$ by definition (5.19), $E(\rho)$ is its L^2 -norm.

Another natural idea to define an entanglement measure seems to be given by the calculation of the integral of F_ρ itself on $\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K})$, however it is always zero. In fact, by definition of F_ρ and theorem 47, we have:

$$\int_{\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K})} F_\rho d\mu_{\mathbf{H}} d\mu_{\mathbf{K}} = \int_{\mathbf{P}(\mathbf{H} \otimes \mathbf{K})} \rho \circ \text{Seg} d\mu - \int_{\mathbf{P}(\mathbf{H})} \rho_{\mathbf{K}} d\mu_{\mathbf{H}} \int_{\mathbf{P}(\mathbf{K})} \rho_{\mathbf{H}} d\mu_{\mathbf{K}} = 0,$$

since $\rho, \rho_{\mathbf{K}}, \rho_{\mathbf{H}}$ are each normalized to 1 w.r.t. appropriate measures.

Let us recall the following technical lemma [19] about the extension of functions from the extremal points to the convex hull, its statement is a convenient tool to check if the map E is a good entanglement measure.

Lemma 49 *Let X be the set of extremal points of a convex set K in a finite dimensional vector space. Let X_0 be a compact subset of X and $K_0 = \text{conv}(X_0)$ its convex hull.*

For any non-negative continuous function $E : X \rightarrow \mathbb{R}^+$ which vanishes exactly on X_0 , its convex extension, defined as in (5.20), is convex on K and vanishes exactly on K_0 . Moreover, if E is invariant under unitary transformations then its convex extension is so.

In quantum information theory an axiomatic approach can be adopted to find good candidates of entanglement measures (e.g. [26], [43]), for instance requiring that the candidate function assigns to each quantum state of a bipartite system a positive real number and it vanishes on separable states. Another requirement is the invariance of the entanglement measure w.r.t. local unitary transformations. The entanglement measure should be a convex function because entanglement cannot be generated by mixing two states, moreover it should be a continuous function for this physical reason: A small perturbation of a state must correspond to a small change of entanglement. The following proposition shows that E satisfies a list of properties of a good entanglement measure.

Proposition 50 *The map $E : \mathbf{S}(\mathbf{H} \otimes \mathbf{K}) \ni \rho \mapsto E(\rho)$ satisfies the following properties:*

- i) $E(\rho) \in \mathbb{R}^+$ for every $\rho \in \mathbf{S}(\mathbf{H} \otimes \mathbf{K})$;
- ii) $E(\rho) = 0$ if and only if ρ is separable;
- iii) E is invariant under the action of the unitary group;
- iv) E is a convex function;
- v) E is continuous w.r.t. the uniform norm topology.

Proof. i) $E(\rho)$ is the integral of a non-negative function for any pure state ρ . Convex combinations preserve non-negativity.

ii) The non-negative function $|F_\rho|^2$ vanishes everywhere on $\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K})$ if and only if ρ is a separable pure state and then $F_\rho = 0$ everywhere. Furthermore, since F_ρ is a continuous function, if $F_\rho = 0$ a.e. then $F_\rho = 0$ everywhere. The proof for mixed state is in iv) below.

iii) The action of the unitary group on $\mathcal{F}^2(\mathbf{H}_n)$ is given by $[U(f)](p) = f(U_p U^{-1})$, where $U \in U(n)$ and we used the same symbol for the representative operator. We need to prove that:

$$E(U \otimes V \rho) = E(\rho),$$

for every $U \in U(n)$, $V \in U(m)$ where $\dim \mathbf{H} = n$ and $\dim \mathbf{K} = m$.

$$\begin{aligned} E(U \otimes V \rho) &= \left(\int |F_{U \otimes V \rho}(p_1, p_2)|^2 d\mu_{\mathbf{H}}(p_1) d\mu_{\mathbf{K}}(p_2) \right)^{\frac{1}{2}} \\ &= \left(\int |F_\rho(U p_1 U^{-1}, V p_2 V^{-1})|^2 d\mu_{\mathbf{H}}(p_1) d\mu_{\mathbf{K}}(p_2) \right)^{\frac{1}{2}} \\ &= \left(\int |F_\rho(p_1, p_2)|^2 d\mu_{\mathbf{H}}(U p_1 U^{-1}) d\mu_{\mathbf{K}}(V p_2 V^{-1}) \right)^{\frac{1}{2}} \\ &= \left(\int |F_\rho(p_1, p_2)|^2 d\mu_{\mathbf{H}}(p_1) d\mu_{\mathbf{K}}(p_2) \right)^{\frac{1}{2}} = E(\rho), \end{aligned}$$

where we used the unitary invariance of the measures $\mu_{\mathbf{H}}$ and $\mu_{\mathbf{K}}$. The identity $F_{U \otimes V \rho}(p_1, p_2) = F_\rho(U p_1 U^{-1}, V p_2 V^{-1})$, that is valid for any pair (p_1, p_2) , can be checked directly from definition (5.19). The result holds even for mixed states, see lemma 49.

v) Consider a sequence of pure states $\{\rho_n\}$ that is uniformly convergent to $\rho \in \mathbf{S}_p(\mathbf{H} \otimes \mathbf{K})$, thus we have the pointwise convergence $\rho_n \rightarrow \rho$ as $n \rightarrow \infty$. Then $\rho_n \circ \text{Seg} \rightarrow \rho \circ \text{Seg}$ pointwise.

$\{\rho_n \circ \text{Seg}\}$ is a sequence of positive bounded functions thus it is dominated by an integrable function and we can apply the dominated convergence theorem, obtaining:

$$\lim_{n \rightarrow \infty} \rho_{n\mathbf{K}} = \lim_{n \rightarrow \infty} \int (\rho_n \circ \text{Seg}) d\mu_{\mathbf{K}} = \int (\rho \circ \text{Seg}) d\mu_{\mathbf{K}} = \rho_{\mathbf{K}}.$$

There is pointwise convergence of the sequences of partial integrals: $\rho_{n\mathbf{K}} \rightarrow \rho_{\mathbf{K}}$, $\rho_{n\mathbf{H}} \rightarrow \rho_{\mathbf{H}}$. Thus we have the following pointwise limit:

$$\lim_{n \rightarrow \infty} F_{\rho_n}(p_1, p_2) = F_\rho(p_1, p_2) \quad \forall (p_1, p_2) \in \mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K}).$$

Applying the dominated convergence theorem once again:

$$\lim_{n \rightarrow \infty} E(\rho_n) = \lim_{n \rightarrow \infty} \sqrt{\int |F_{\rho_n}|^2 d\mu_{\mathbf{H}} d\mu_{\mathbf{K}}} = \sqrt{\int |F_\rho|^2 d\mu_{\mathbf{H}} d\mu_{\mathbf{K}}} = E(\rho).$$

iv) We apply lemma 49. $E : \mathbf{S}(\mathbf{H} \otimes \mathbf{K}) \rightarrow \mathbb{R}^+$ is the convex extension of a non-negative continuous function defined on the extremal elements of $\mathbf{S}(\mathbf{H} \otimes \mathbf{K})$ that vanishes on the separable pure states, then it is a convex function vanishing exactly on the set of separable states. □

In standard QM, state distinguishability is quantified by the *trace-distance* between density matrices: $d(\sigma, \sigma') = \frac{1}{2} \|\sigma - \sigma'\|_1 = \frac{1}{2} \text{tr}(|\sigma - \sigma'|)$. Thus a good entanglement measure on the set of density matrices should be continuous w.r.t. the topology induced by $\|\cdot\|_1$. If \mathbf{H} is a finite-dimensional Hilbert space then the topology induced by $\|\cdot\|_1$ on $\mathfrak{B}(\mathbf{H})$ coincides with the topology induced by the norm $\|T\| := \sup_{\|\psi\|=1} |\langle \psi | T \psi \rangle| = \sup_{p \in \mathbf{P}(\mathbf{H})} |\text{tr}(Tp)| = \|\mathcal{S}(T)\|_\infty$. For this reason the continuity w.r.t. the uniform norm topology is remarkable in order to use E as an entanglement measure.

Definition 51 *Let $\mathbf{S}(\mathbf{H} \otimes \mathbf{K})$ be the set of Liouville densities on $\mathbf{P}(\mathbf{H} \otimes \mathbf{K})$ describing physical states of a bipartite quantum system. The map $E : \mathbf{S}(\mathbf{H} \otimes \mathbf{K}) \rightarrow \mathbb{R}$ defined on the extremal points by (5.18) and extended by (5.20) to the convex hull is called **standard Hamiltonian entanglement measure**.*

In the introductory section, we stress that the Hilbert-Schmidt distance between density matrices coincides up to a multiplicative constant with the \mathcal{L}^2 -distance between associate Liouville densities. Thus we can express in terms of Liouville densities a well-known entanglement measure defined as the Hilbert-Schmidt distance of an entangled state from the set of separable states. Consider a density matrix $\sigma_* \in \mathfrak{B}(\mathbf{H})$ of a bipartite system, an entanglement measure proposed in [47] is:

$$D(\sigma_*) = \min_{\sigma \in \mathbf{S}^{sep}} \|\sigma - \sigma_*\|_{HS}, \quad (5.21)$$

where \mathbf{S}^{sep} is the convex set of separable density matrices. Thus we can introduce another measure of entanglement carried by a Liouville density $\rho \in \mathbf{S}(\mathbf{H} \otimes \mathbf{K})$ in thi way:

$$D(\rho) = \min_{\eta \in \mathbf{S}^{sep}(\mathbf{H} \otimes \mathbf{K})} \sqrt{\int_{\mathbf{P}(\mathbf{H} \otimes \mathbf{K})} |\rho - \eta|^2 d\mu}. \quad (5.22)$$

Even this definition is based on a \mathcal{L}^2 -distance but in the space $\mathcal{L}^2(\mathbf{P}(\mathbf{H} \otimes \mathbf{K}), d\nu)$ instead in $\mathcal{L}^2(\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K}), d\mu_{\mathbf{H}} d\nu_{\mathbf{K}})$ like in our proposal. The letter has no a direct analogous in the standard formalism of density matrices, because \mathcal{L}^2 -distance is computed for functions that are not defined on the projective space $\mathbf{P}(\mathbf{H} \otimes \mathbf{K})$ but on the cartesian product $\mathbf{P}(\mathbf{H}) \times \mathbf{P}(\mathbf{K})$ which is the *classical-like* phase space of the bipartite system.

The entanglement measure based on Hilbert-Schmidt distance is connected with the violation degree of a generalized Bell inequality as shown by Bertlmann-Narnhofer-Thirring

theorem [5]. To study this connection from the point of view of Hamiltonian formalism we introduce the *witness inequality* in the next section.

5.3 Separability criteria for Liouville densities

Using the developed machinery we can translate two celebrated separability criteria in the language of Hamiltonian formulation.

Proposition 52 *For any Liouville density $\rho \in \mathcal{S}(\mathbf{H} \otimes \mathbf{K})$ representing an entangled state there is an observable $f : \mathcal{P}(\mathbf{H} \otimes \mathbf{K}) \rightarrow \mathbb{R}$ (called **entanglement witness**) such that:*

$$\int_{\mathcal{P}(\mathbf{H} \otimes \mathbf{K})} f \rho d\mu < 0 \quad \text{and} \quad \int_{\mathcal{P}(\mathbf{H} \otimes \mathbf{K})} f \eta d\mu \geq 0, \quad (5.23)$$

for every separable Liouville density η .

Proof. For any entangled density matrix σ in $\mathbf{H} \otimes \mathbf{K}$ there is a Hermitian operator A (i.e. a quantum observable) such that $\text{tr}(A\sigma) < 0$ and $\text{tr}(A\theta) \geq 0$ for every separable density matrix θ (see e.g. Lemma 1 [24]). Applying trace-integral formulas:

$$\text{tr}(A\sigma) = \int_{\mathcal{P}(\mathbf{H} \otimes \mathbf{K})} f \rho d\mu \quad , \quad \text{tr}(A\theta) = \int_{\mathcal{P}(\mathbf{H} \otimes \mathbf{K})} f \eta d\mu$$

where $\rho = \mathcal{S}(\sigma)$, $\eta = \mathcal{S}(\theta)$ and $f = \mathcal{O}(A)$, i.e. f represents a quantum observable. □

To make above result useful, we recall when a real function $f \in \mathcal{L}^2(\mathcal{P}(\mathbf{H} \otimes \mathbf{K}), d\mu)$ represents a quantum observable (i.e. when it verifies $f = \mathcal{O}(A)$ for some $A \in \text{iu}(n)$). A necessary and sufficient condition, obtained applying proposition 25 in [34], is:

$$\int_{\mathcal{P}(\mathbf{H} \otimes \mathbf{K})} f \mathcal{S}(p_0) d\mu = d^2 f(p_0), \quad (5.24)$$

for every pure state p_0 , where $d = \dim \mathbf{H} \times \dim \mathbf{K}$.

An *entanglement witness* can be defined as a non-positive observable such that its expectation value on every separable state is a positive number. The second inequality in (5.23) is violated by an entangled state, first equation in (5.23). The violation of the inequality:

$$\int_{\mathcal{P}(\mathbf{H} \otimes \mathbf{K})} f \rho d\mu \geq 0 \quad \text{with } f \text{ entanglement witness} \quad (5.25)$$

is a good criterion to test if a state is entangled, it can be called *generalized Bell inequality* in the Hamiltonian formalism. The maximal violation of operatorial generalized Bell inequality is connected with Hilbert-Schmidt entanglement measure (5.21) by the Bertlmann-Narnhofer-Thirring theorem [5]. Thus (5.25) and (5.22) can be used to obtain a Hamiltonian version of BNT theorem.

Proposition 53 *A Liouville density $\rho \in \mathbf{S}(\mathbf{H} \otimes \mathbf{K})$ describes a separable state if and only if:*

$$\int_{\mathbf{P}(\mathbf{H} \otimes \mathbf{K})} \rho f d\mu \geq 0, \quad (5.26)$$

for any quantum observables f satisfying:

$$\int_{\mathbf{P}(\mathbf{H} \otimes \mathbf{K})} \eta_1 \diamond \eta_2 f d\mu \geq 0 \quad (5.27)$$

for all $\eta_1 \in \mathcal{F}^2(\mathbf{H})$ and $\eta_2 \in \mathcal{F}^2(\mathbf{K})$ such that:

$$G(d\eta_1, d\eta_1) = 2(\eta_1 - \eta_1^2) \quad (5.28)$$

$$R(d\eta_2, d\eta_2) = 2(\eta_2 - \eta_2^2) \quad (5.29)$$

where G and R are the scalar products of one-forms respectively induced by the Fubini-Study metrics on $\mathbf{P}(\mathbf{H})$ and $\mathbf{P}(\mathbf{K})$.

Proof. A density matrix σ on $\mathbf{H} \otimes \mathbf{K}$ is separable if and only if $\text{tr}(\sigma A) \geq 0$ for any Hermitian operator A satisfying $\text{tr}((P \otimes Q)A) \geq 0$ for all orthogonal projectors P and Q on \mathbf{H} and \mathbf{K} respectively (e.g. theorem 1 in [24]). The statement of the proposition is the translation of this fact in the classical-like functions formalism. Consider the real functions $g = \mathcal{S}(\tau) \in \mathcal{F}^2(\mathbf{H})$ and $g' = \mathcal{S}(\tau') \in \mathcal{F}^2(\mathbf{H})$ for $\tau, \tau' \in \mathfrak{B}(\mathbf{H})$, then a direct computation [34] produces:

$$\mathcal{S}(\tau\tau') = \mathcal{S}(\mathcal{S}^{-1}(g)\mathcal{S}^{-1}(g')) = \frac{i}{2}\{g, g'\}_{PB} + \frac{1}{2}G(dg, dg') + gg'.$$

If $\tau' = \tau$ then the Poisson bracket is zero, moreover if τ is an orthogonal projector:

$$g = \mathcal{S}(\tau) = \frac{1}{2}G(dg, dg) + g^2, \quad (5.30)$$

i.e. $G(dg, dg) = 2(g - g^2)$. The converse is true because \mathcal{S} is bijective: If $g = \mathcal{S}(\tau)$ satisfies (5.30) then τ is an orthogonal projector.

If $\eta_1 \in \mathcal{F}^2(\mathbf{H})$ satisfies (4.3) and $\eta_2 \in \mathcal{F}^2(\mathbf{K})$ satisfies (4.4) then the operators $P = \mathcal{S}_{\mathbf{H}}^{-1}(\eta_1)$ and $Q = \mathcal{S}_{\mathbf{K}}^{-1}(\eta_2)$ are orthogonal projectors. And using (5.9) as the definition

of \diamond we have $\mathcal{S}(P \otimes Q) = \eta_1 \diamond \eta_2$. We can use trace-integral formulas as in the proof of proposition 52 to obtain (5.26) and (5.27). \square

Conclusions

The main results about the geometric Hamiltonian formulation of finite-dimensional Quantum Mechanics and its interplay with the standard formalism presented in this dissertation has been developed applying the machinery of frame functions and their properties. More precisely, we have considered frame functions belonging to $\mathcal{L}^2(\mathbf{P}(\mathbf{H}_n), \mu_n)$ where μ_n is the natural Liouville measure defined on the Kähler manifold $\mathbf{P}(\mathbf{H}_n)$ and coincides with a unique measure induced by the Haar measure on the unitary group $U(n)$. The complete characterization of classical-like observables (and classical-like states) allows to construct a one-parameter class of prescriptions to obtain a self-consistent geometric Hamiltonian formulation of a finite-dimensional quantum theory. The parameter is $\kappa > 0$ which labels the all possible Kählerian structures on the projective space. For any $\kappa > 0$, an inverse prescription to obtain a "standard" quantum observable (a self-adjoint operator) from the associated classical-like observable has been discussed in terms of an integration on the Hilbert projective space. Since frame functions allow to completely characterize quantum observables in terms of classical-like observables, the algebra of observables has been concretely constructed as a C^* -algebra of functions with a non-commutative product.

Description of finite-dimensional quantum systems is crucial in quantum information, so the geometric formalism has been applied to define and characterize the notion of quantum entanglement within the description of a bipartite quantum system. An analogous of the partial trace is defined and its interpretation as an integration w.r.t. to a marginal probability measure has been pointed out and used to propose a new entanglement measure, providing a map which satisfies several good properties of an entanglement measure. At the end of the last chapter there are some comments about the translation of known separability criteria in terms of geometric Hamiltonian formulation.

For obvious physical reasons, a cogent direction of investigation is the infinite-dimensional extension of the presented results. The projective space on a infinite-dimensional Hilbert space is endowed with a Kähler structure as well in the finite-dimensional case, thus one would have a good geometric framework. However the very difficult issue is the definition of a Liouville measure on such infinite-dimensional quantum phase space. In this way, one should use a machinery beyond standard measure theory like the ideas that have been developed to study mathematical foundations of Feynman path integrals.

Bibliography

- [1] R. Abraham, J.E. Marsden. *Foundations of Mechanics*. AMS Chelsea Publishing (1978).
- [2] P. Aniello, J. Clemente-Gallardo, G. Marmo, G.F. Volkert. *Classical tensors and quantum entanglement I: Pure states*. Int.J.Geom.Meth.Mod.Phys. 7(3) (2010) pp. 485-503.
- [3] P. Aniello, J. Clemente-Gallardo, G. Marmo, G.F. Volkert. *Classical tensors and quantum entanglement II: Mixed states*. Int. J. Geom. Meth. Mod. Phys. 08:853-883 (2011).
- [4] P. Aniello, J. Clemente-Gallardo, G. Marmo, G.F. Volkert. *From Geometric Quantum Mechanics to Quantum Information* arXiv:1101.0625.
- [5] R.A. Bertlmann, H. Narnhofer, W. Thirring. *Geometric picture of entanglement and Bell inequalities*. Phys. Rev. A **66** (2002) 032319.
- [6] A. Ashtekar and T. A. Schilling, *Geometry of quantum mechanics*, AIP Conference Proceedings, **342**, 471-478 (1995).
- [7] G.Birkhoff and J. von Neumann, *The logic of quantum mechanics*, Annals of Mathematics 37, 415 (1936).
- [8] A. Bloch, *An infinite-dimensional Hamiltonian system on projective Hilbert space*, Transactions of the American Mathematical Society 302, n.2 (1987).
- [9] D. C. Brody, L. P. Hughston. *Geometric quantum mechanics*, Journal of Geometry and Physics **38** 19-53 (2001).
- [10] A.Benvegnù, N.Sansonetto and M.Spera *Remarks on geometric quantum mechanics*, Journal of Geometry and Physics **51** 229-243 (2004).
- [11] A.O. Barut and R. Raczka. *Theory of Group Representations and Applications*. World Scientific, Singapore, (2000).

- [12] J. F. Carinena, A. Ibort, G. Marmo, G. Morandi. *Geometrical description of algebraic structures: Applications to Quantum Mechanics*, AIP Conf.Proc. **1130** 47-59 (2009).
- [13] R. Cirelli, P. Lanzavecchia, and A. Mania, *Normal pure states of the von neumann algebra of bounded operators as kahler manifold* J. Phys. A: Mathematical and General, **16**, . 3829 (1983).
- [14] P.A.M. Dirac *The principles of Quantum Mechanics* Oxford Clarendon Press (1958).
- [15] A. Dvurečenskij. *Gleason's theorem and its applications* Kluwer academic publishers (1992).
- [16] F. Falchetto, L. Ferro, A. Ibort and G. Marmo. *Reduction of Lie-Jordan Banach algebras and quantum states* J. Phys. A: Math. Theor. **46** 015201 (2013).
- [17] P. Facchi, L. Ferro, G. Marmo and S. Pascazio, *Defining quantumness via the Jordan product*, Preprint arXiv:1309.4635v1.
- [18] J. Grabowski, M. Kuś and G. Marmo. *Geometry of quantum systems: density states and entanglement*, J. Phys. A: Math. Gen. **38** 10217-10244 (2005).
- [19] J. Grabowski, M. Kuś and G. Marmo. *Segre maps and entanglement for multipartite systems of indistinguishable particles*, J. Phys. A: **38** 105301 (2011).
- [20] G.W. Gibbons. *Typical states and density matrices* Journal of Geometry and Physics **8** 147-162 (1992)
- [21] A. M. Gleason. *Measures on the closed subspaces of a Hilbert space*, Journal of Mathematics and Mechanics, Vol.6, No.6, 885-893 (1957).
- [22] B.C. Hall *Quantum Theory for Mathematicians* Springer, Graduate Texts in Mathematics (2013).
- [23] R. Hartshorne, *Algebraic Geometry*, Springer Science+Business Media, Inc. (1977).
- [24] M. Horodecki, P. Horodecki, R. Horodecki *Separability of mixed states: Necessary and sufficient conditions* , Phys. Lett. **A 223**, no. 1-2,1-8 (1996).
- [25] K. D. Johnson and N. R. Wallach. *Composition series and intertwining operators for spherical principal series I.*, Trans. Am. Math. Soc. **229**, 137-173 (1977) Volume 229, 1977.

-
- [26] M. Keyl *Fundamentals of Quantum Information Theory*, Phys. Rep. **369**, no. 5 431-548 (2002).
- [27] T. W. B. Kibble *Geometrization of Quantum Mechanics*, Commun. Math. Phys. **65**, 189-201 (1979).
- [28] A.A. Kirillov *Representation Theory and Noncommutative Harmonic Analysis I* Springer-Verlag (1994).
- [29] S. Kobayashi *Geometry of bounded domains*, Trans. Amer. Math. Soc. 92, pp 267-290 (1959).
- [30] G. W. Mackey. *Induced representations of locally compact groups I*, The Annals of Mathematics, Second Series, Vol.55, No.1, 101-139 (1951).
- [31] S. Mazzucchi *Mathematical Feynman Path Integrals and their Applications*, World Scientific Publishing Co.Pte.Ltd. (2009).
- [32] V. Moretti *Spectral Theory and Quantum Mechanics*, Springer (2013).
- [33] V. Moretti and D. Pastorello. *Generalized Complex Spherical Harmonics, Frame Functions, and Gleason Theorem* Ann. Henri Poincaré **14**,1435-1443 (2013).
- [34] V. Moretti and D. Pastorello. *Frame functions in finite-dimensional Quantum Mechanics and its Hamiltonian formulation on complex projective spaces*, Submitted to CMP arXiv:1311.1720.
- [35] V. Ovsienko and S. Tabachnikov. *Projective Differential Geometry: Old and New*. Cambridge University Press (2005).
- [36] D. Pastorello. *A geometric Hamiltonian description of composite quantum systems and quantum entanglement*. arXiv: 1408.1839.
- [37] E. Prugovečki. *Quantum Mechanics in Hilbert Space*. Academic Press (1971).
- [38] B. O'Neill , *Semi-Riemannian geometry*, Academic Press, San Diego (1983).
- [39] W. Rudin *Real and complex analysis* McGraw-Hill Book Co. (1986).
- [40] W. Rudin *Functional Analysis* McGraw-Hill Book Co. (1986).
- [41] F. Strocchi *An introduction to the mathematical structure of Quantum Mechanics (2nd edition)* World Scientific Publishing Co. Pte. Ltd. (2008).
- [42] B. Simon *Representations of Finite and Compact Groups* Graduate Studies in Mathematics Vol. 10 American Physical Society (1996).

- [43] V. Vedral, M.B. Plenio, M.A. Rippin, P.L. Knight. *Quantifying entanglement*, Phys.Rev.Lett. 78.12 (1997), p. 4.
- [44] S. Watanabe. *Spherical Harmonics on $U(n)/U(n-1)$ and Associated Hilbert Spaces of Analytic Functions*, Tokyo J. Math **23**, 352-360 (2000).
- [45] S. Watanabe. *Generating functions and integral representations for the spherical functions on some classical Gelfand pairs*, Kyoto J. Math **33** 1125-1142 (1993).
- [46] F.W. Warner. *Foundations of Differentiable Manifolds and Lie Groups*, Springer, Berlin, (1983).
- [47] C.Witte, M.Trucks. *A new entanglement measure induced by the Hilbert-Schmidt norm*. Phys.Lett.A 257 (1998) p.12.

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