Frame functions in finite-dimensional Quantum Mechanics and its Hamiltonian formulation on complex projective spaces

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V.M. D. Pastorello, *Ann. Henri Poincaré 14 (2013),1435-1443*
V.M. D. Pastorello, arXiv:1311.1720

Summary

Classical (Hamiltonian) Mechanics

Phase space

Classical system with n spatial degrees of freedom: Described in a $2n$-**dimensional symplectic manifold** $(\mathcal{M}, \omega)$.

Sharp state

$(q^1, ..., q^n, p_1, ..., p_n) \equiv s \in \mathcal{M}$

Dynamics

$\mathbb{R} \ni t \mapsto s(t) \in \mathcal{M}$ satisfying Hamilton equations:

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

$H : \mathcal{M} \to \mathbb{R}$ is the Hamiltonian function.
X_H is the **Hamiltonian vector field**: $\omega_s(X_H, \cdot) = dH_s(\cdot)$

Classical states as probability measures

Statistical description (incomplete knowlwdge) $\Longrightarrow$
Statistical state: $\rho : \mathbb{R} \times \mathcal{M} \to [0, +\infty)$ with $\int_{\mathcal{M}} \rho d\mu = 1$

Dynamics

$$\frac{\partial \rho}{\partial t} + \{\rho, H\}_{PB} = 0$$

Expecation values

Physical quantity $f : \mathcal{M} \to \mathbb{R}$, Liouville (symplectic) volume form μ

$$\langle f \rangle_\rho = \int_{\mathcal{M}} f(s)\rho(t,s)d\mu(s)$$

Borel probability measure $\nu_{\rho_t} : \mathcal{B}(\mathcal{M}) \to [0,1], \quad \nu_{\rho_t}(E) := \int_E \rho_t d\mu$

Classical states as probability measures

Propositions in Classical Mechanics

Elementary propositions (at fixed time t) on the system represented by the σ-**boolean lattice** $\mathcal{B}(\mathcal{M})$ of Borel subsets of $\mathcal{M}$.
Logical connectives $\cup, \cap, \subset$. **Tautology** $\mathcal{M}$, **contradiction** $\emptyset$

$A : \mathcal{M} \to \mathbb{R}$ (continuous) physical quantity $\Longrightarrow$
$P_A := A^{-1}([a, b]) \in \mathcal{B}(\mathcal{M})$: «The value of the A, measured at time t, belongs to $[a, b] \subset \mathbb{R}$»

State ρ (at t) probability measure on $\mathcal{B}(\mathcal{M})$: $\nu_{\rho_t}(P) := \int_P \rho_t \, d\mu$

Propositions in Quantum Mechanics?

(elementary) incompatible observables, P, Q cannot be simultaneously measured $\Longrightarrow$ e.g. $P \cap Q$ makes **no** sense $\Longrightarrow$
No Boolean structure admissible

States as measures in Quantum Theories

von Neumann assumptions for QM in Hilbert space

"Quantum system associated with corresponding complex Hilbert space $\mathcal{H}$ s.t. **Quantum propositions** are **orthogonal projectors** on $\mathcal{H}$ and **compatible propositions** are **commuting projectors**
$\Longrightarrow$ **non-Boolean lattice** (standard logic for commuting proj.s)
$\Longrightarrow$ **Observable** = collection of elementary propositions labelled in $\mathcal{B}(\mathbb{R})$ = **self-adjoint operator (spectral theorem)**

Quantum state μ as *generalized probability measures*

$\mu : \mathfrak{P}(\mathcal{H}) \to [0,1]$ ($\mathfrak{P}(\mathcal{H})$ lattice of orthogonal projectors) s.t.
i) $\mu(I) = 1$;
ii) If $\{P_i\}_{i\in\mathbb{N}} \subset \mathfrak{P}(\mathcal{H})$ with $P_iP_j = 0$ for $i \neq j$ then:

$$\mu\left(s\text{-}\sum_i P_i\right) = \sum_i \mu(P_i)$$

States as measures in Quantum Theories

Theorem [Gleason 1957]

If $\dim \mathcal{H} > 2$ separable and $\mu : \mathfrak{P}(\mathcal{H}) \to [0,1]$ is a state,
$\exists! \sigma \in \mathfrak{B}(\mathcal{H})$ s.t.:
i) $\sigma \geq 0$;
ii) $\sigma \in \mathfrak{B}_1(\mathcal{H})$ (σ is trace-class) with $tr(\sigma) = 1$;
iii) $\mu(P) = tr(\sigma P)$ for every $P \in \mathfrak{P}(\mathcal{H})$
($\sigma \in \mathfrak{B}(\mathcal{H})$ satisfying i) and ii) defines a state $\mu(P) = tr(\sigma P)$).

Density matrices

$$\mathfrak{D}(\mathcal{H}) = \{\sigma \in \mathfrak{B}_1(\mathcal{H}) | \sigma \geq 0, tr(\sigma) = 1\}$$

* $\mathfrak{D}(\mathcal{H})$ is closed and convex in $\mathfrak{B}_1(\mathcal{H})$.
* extremal points said **pure states**: $|\psi\rangle\langle\psi|$ with $\psi \in \mathcal{H}$, $\| \psi \| = 1$.
* convex combinations of pure states exhaust $\mathfrak{D}(\mathcal{H})$ (strong top.)

Frame functions

$\mathbb{S}(\mathcal{H}) = \{\psi \in \mathcal{H} : \| \psi \| = 1\}$, $\mathcal{H}$ separable

$f : \mathbb{S}(\mathcal{H}) \to \mathbb{C}$ is a **frame funtion** if $\exists W_f \in \mathbb{C}$ s.t.

$$\sum_{\psi \in N} f(\psi) = W_f \qquad \forall N \text{ orthonormal basis of } \mathcal{H}.$$

Quantum states $\mu : \mathfrak{P}(\mathcal{H}) \to [0,1]$ define **real bounded** frame functions: $f_\mu(\psi) := \mu(p_\psi) \in [0,1] \qquad p_\psi = |\psi\rangle\langle\psi|$

$$W_{f_\mu} = \sum_{\psi \in N} f_\mu(\psi) = \sum_{\psi \in N} \mu(p_\psi) = \mu\left(\sum_{\psi \in N} p_\psi\right) = \mu(I) = 1$$

Core of Gleason theorem: $\forall$ *real bounded* frame function f $\exists$ a self-adjoint trace class operator A s.t. $f(\psi) = \langle\psi|A\psi\rangle$

Frame functions

$$2 < \dim \mathcal{H}_n = n < +\infty \, , \, \mathbb{S}(\mathcal{H}) = \mathbb{S}^{2n-1}$$

$$\mathcal{L}^2(\mathbb{S}^{2n-1}, \nu'_n) = \left\{ f : \mathbb{S}^{2n-1} \to \mathbb{C} \,|\, \int_{\mathbb{S}^{2n-1}} \overline{f(x)} f(x) d\nu'_n(x) < +\infty \right\}$$

$\nu'_n : \mathcal{B}(\mathbb{S}^{2n-1}) \to [0,1]$ is the unique regular Borel measure s.t.:
i) $\nu'_n(\mathbb{S}^{2n-1}) = 1$;
ii) $\nu'_n(UE) = \nu_n(E) \quad \forall U \in U(n), \forall E \in \mathcal{B}(\mathbb{S}^{2n-1})$.
ν_n is obtained from the Haar measure on $U(n)$.

Theorem [V.M., D.Pastorello Ann.Henri Poincaré 2013]

Let $\mathcal{H}$ be a Hilbert space with $2 < \dim \mathcal{H}_n < +\infty$. For every frame function $f \in \mathcal{L}^2(\mathbb{S}^{2n-1}, \nu'_n)$, $\exists!\ A \in \mathfrak{B}(\mathcal{H})$ s.t.:
$f(\psi) = \langle \psi | A\psi \rangle \quad \forall \psi \in \mathbb{S}^{2n-1}$

$\Longrightarrow$ extension to $n = +\infty$ alternative form. of Gleason theorem

Proof essentially based on Peter-Weyl theorem and Harmonic analysis on $U(n)$.

$$\mathcal{L}^2(\mathbb{S}^{2n-1}, d\nu_n) = \bigoplus_{p,q=0}^{\infty} \mathcal{H}^n_{(p,q)}$$

Decomposition into orthogonal $U(n)$-invariant and irreducible subspaces. The elements of $\mathcal{H}^n_{(p,q)}$, called **generalized spherical harmonics of order** $j = (p, q)$, are restrictions of **homogeneous complex polynomials** $h(z_1, ..., z_n)$ s.t.:
i) $h(\alpha z_1, ..., \alpha z_n) = \alpha^p \overline{\alpha}^q h(z_1, ..., z_n)$ for any $\alpha \in \mathbb{C}$
ii) $\Delta h(z_1, ..., z_n) = 0$ in $\mathbb{R}^{2n}$
If $f \in \mathcal{L}^2(\mathbb{S}^{2n-1}, \nu_n)$ is a frame function, then (via theory of **zonal spherical harmonics**) $f \in \mathcal{H}^n_{(0,0)} \oplus \mathcal{H}^n_{(1,1)} \Longrightarrow f(\cdot) = \langle \cdot | A \cdot \rangle$.

Projective space as phase space

$\mathcal{P}(\mathcal{H}_n) = \frac{U(n)}{U(n-1)U(1)}$ **projective space** of $\mathcal{H}_n$. ν_n unique normalized $U(n)$ invariant regular Borel mesure on $\mathcal{P}(\mathcal{H}_n)$.
A frame function $f : \mathbb{S}(\mathcal{H}_n) \to \mathbb{C}$ is well-defined as functin on $\mathcal{P}(\mathcal{H}_n)$

$$f(\psi) = \langle\psi|A\psi\rangle = tr(Ap_\psi) =: f(p_\psi) \quad p_\psi \in \mathcal{P}(\mathcal{H}_n)$$

Moreover

$$f \in \mathcal{L}^2(\mathcal{P}(\mathcal{H}_n), \nu_n) \text{ iff } f \in \mathcal{L}^2(\mathbb{S}(\mathcal{H}_n), \nu'_n)$$

Geometry of $\mathcal{P}(\mathcal{H}_n)$

$\mathcal{P}(\mathcal{H}_n)$ real smooth $(2n-2)$-dimensional manifold.
Tangent vectors at $p \in \mathcal{P}(\mathcal{H}_n)$:

$$v = -i[A_v, p] \in T_p\mathcal{P}(\mathcal{H}_n) \text{ for some } A_v \in i\mathfrak{u}(n),$$

$\mathfrak{u}(n)$ is the Lie algebra of $U(n)$.

Projective space as phase space

Well known Kähler structure on $\mathcal{P}(\mathcal{H}_n)$

-) **Symplectic form** : $\omega_p(u,v) := -ik\, tr\,(p[A_u, A_v]) \qquad k > 0$

-) **Fubini-Study metric**:

$$g_p(u,v) = -ktr\,(p\,([A_u,p][A_v,p] + [A_v,p][A_u,p]))$$

-) **Almost complex form**:

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

$p \mapsto j_p$ smooth, $j_p j_p = -id$ and $\omega_p(u,v) = g_p(u, j_p v)$.

$(\mathcal{P}(\mathcal{H}_n), \omega, g, j)$ is a Kähler manifold

Geometric Hamiltonian QM

Essentially known with various approaches

Correspondence *quantum observables* – *classical-like observables*:

$$\mathcal{O}(\mathcal{H}_n) : i\mathfrak{u}(n) \ni A \quad \longmapsto \quad f_A : \mathcal{P}(\mathcal{H}_n) \to \mathbb{R}, \quad \text{s.t.}$$

Schrödinger dynamics due to H equivalent to the **flow of** X_{f_H}.

Kibble ('79), Ashtekar Schilling ('95), Brody-Hughston (2001)

Open issues

Correspondence *quantum states* – *Liouville densities on* $\mathcal{P}(\mathcal{H}_n)$

$$\mathcal{S} : \mathfrak{D}(\mathcal{H}_n) \ni \sigma \quad \longmapsto \quad \rho_\sigma : \mathcal{P}(\mathcal{H}_n) \to [0, +\infty) \quad s.t.$$

$$\int_{\mathcal{P}(\mathcal{H})} \rho_\sigma d\nu_n = 1 \quad \text{and} \quad \langle A \rangle_\sigma = tr(A\sigma) = \int_{\mathcal{P}(\mathcal{H})} f_A \rho_\sigma d\nu_n$$

Gibbons ('92) (partially negative result)

Geometric Hamiltonian QM

Physical requirements on $\mathcal{O} : i\mathfrak{u}(n) \ni A \mapsto f_A$

O1) $\mathcal{O}$ is injective;
O2) $\mathcal{O}$ is $\mathbb{R}$-linear;
O3) If $H \in i\mathfrak{u}(n)$ then $\mathcal{O}(H) = f_H \in C^1(\mathcal{P}(\mathcal{H}_n))$ and X_{f_H} can be defined with

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

O4) $U(n)$-covariance: $f_A(UpU^{-1}) = f_{U^{-1}AU}(p)$ for any $U \in U(n)$;

Theorem [V.M., D.Pastorello 2014]

$\mathcal{O} : A \mapsto f_A$ satisfies O1) - O4) $\Longleftrightarrow$ f_A is a frame function
$f_A(p) = k\, tr(Ap) + c\, tr(A)$

with $c \in \mathbb{R}$ and $k + nc \neq 0$.

Geometric Hamiltonian QM

$\mathcal{O} : A \mapsto f_A$ satisfies O1) - O4) $\Rightarrow f_A(p) = k\, tr(Ap) + c\, tr(A)$

Sketch of proof:

O3) If $A \in i\mathfrak{u}(n)$ then X_{f_A} is well-defined: $\omega_p(X_{f_A}, u_B) = df_{A_p}(u_B)$ for $p \in \mathcal{P}(\mathcal{H}_n)$ and $u_B = -i[B,p] \in T_p\mathcal{P}(\mathcal{H}_n)$.

$$ktr(A(-i[B,p])) = df_{A_p}(-i[B,p])$$

Let $q = q(s) \in \mathcal{P}(\mathcal{H}_n)$ be a curve s.t. $q(s_0) = p$, $\dot{q}(s_0) = -i[B,p]$:

$$\frac{d}{ds} f_A(q(s)) = ktr\left(A\frac{dq}{ds}\right) \Rightarrow f_A(p) = ktr(Ap) + c_A$$

O2) $\mathcal{O}$ is linear $\Rightarrow$ $A \mapsto c_A$ is linear, thus $\exists C \in i\mathfrak{u}(n)$ s.t. $tr(CA) = c_A$.

O4) $U(n)$-covariance of $\mathcal{O} \Rightarrow$ $C = c\mathbb{I}$ $c \in \mathbb{R}$

Geometric Hamiltonian QM

Physical requirements on $\mathcal{S} : \mathfrak{D}(\mathcal{H}_n) \ni \sigma \mapsto \rho_\sigma$

S1) $\rho_\sigma \geq 0$ for every $\sigma \in \mathfrak{D}(\mathcal{H}_n)$;
S2) $\mathcal{S}$ is convex-linear;
S3) $\rho_\sigma \in \mathcal{L}^2(\mathcal{P}(\mathcal{H}), \nu_n)$ (and thus $\rho_\sigma \in \mathcal{L}^1$) and

$$\int_{\mathcal{P}(\mathcal{H})} \rho_\sigma d\nu_n = 1;$$

S4) $\rho_\sigma(UpU^{-1}) = \rho_{U^{-1}\sigma U}(p)$
S5) If $A \in i\mathfrak{u}(n)$ and $f_A = \mathcal{O}(A)$ then:

$$tr(A\sigma) = \int_{\mathcal{P}(\mathcal{H}_n)} f_A \rho_\sigma d\nu_n$$

Geometric Hamiltonian QM

Theorem [V.M., D.Pastorello 2014]

$\mathcal{S} : \sigma \mapsto \rho_\sigma$ satisfies S2) - S5) $\iff$ $\rho_\sigma(p) = k' tr(Ap) + c'$

$$\text{with} \quad k' = \frac{n(n+1)}{k}, \quad c' = \frac{k-(n+1)}{k}, \quad c = \frac{1-k}{n}.$$

S1) holds iff $k \in [n+1, +\infty)$.
k is the only degree of freedom of the construction.

The proof relies on this key result [V.M., D.Pastorello 2014]

Consider $\mathfrak{G} : \mathfrak{D}(\mathcal{H}_n) \ni \sigma \mapsto f_\sigma$ where $f_\sigma : \mathcal{P}(\mathcal{H}_n) \to \mathbb{C}$.
Proposition: If $\mathfrak{G}$ is $U(n)$-covariant [i.e. $f_\sigma(UpU^{-1}) = f_{U\sigma U^{-1}}(p)$] and convex-linear then:

$$\mathfrak{G}(\mathfrak{D}(\mathcal{H}_n)) \subset \mathcal{F}^2(\mathcal{H}_n),$$

where $\mathcal{F}^2(\mathcal{H}) = \{f \in \mathcal{L}^2(\mathcal{P}(\mathcal{H}), \nu_n) | f \text{ is a frame function}\}$.

Geometric Hamiltonian QM

Physical requirements on $\mathcal{S} : \mathfrak{D}(\mathcal{H}_n) \ni \sigma \mapsto \rho_\sigma$

S2) $\mathcal{S}$ is convex-linear and S4) $\rho_\sigma(UpU^{-1}) = \rho_{U^{-1}\sigma U}(p)$

imply ρ_σ is a $\mathcal{L}^2$-frame function!
$\Rightarrow \exists T \in i\mathfrak{u}^*(n)$ s.t. $\rho_\sigma(p) = tr(Tp)$ and $\int \rho_\sigma d\nu_n = n^{-1}tr(T)$.

S3) $\int \rho_\sigma d\nu_n = 1 \;\Rightarrow\; tr(T) = n$

S5) $tr(\sigma A) = \int tr(Tp) f_A d\nu_n$ with $f_A(p) = ktr(Ap) + ctr(A)$.
$\Rightarrow \;\; T = k'\sigma + c'I$

$$\rho_\sigma(p) = tr(Tp) = k'tr(\sigma p) + c'.$$

Translation of a Quantum theory into a Classical-like theory

* From *quantum observables* to *classical-like observables*:

$$f_A(p) = k\, tr(Ap) - \frac{1-k}{n} tr(A)$$

* From *denisty matrices* to *Liouville densities (positive iff* $k \in [n+1, \infty)$:

$$\rho_\sigma(p) = \frac{n(n+1)}{k} tr(\sigma p) + \frac{k-(n+1)}{k}$$

Characterization of classical-like observables

$f : \mathcal{P}(\mathcal{H}_n) \to \mathbb{R}$ in $\mathcal{L}^2(\mathcal{P}(\mathcal{H}_n), \nu_n))$ satisfies $f = \mathcal{O}(A)$ for some $A \in i\mathfrak{u}(n))$ iff

$$\int_{\mathcal{P}(\mathcal{H}_n)} \rho_{p_0} f d\nu_n = \alpha f(p_0) + \beta \qquad \forall \text{pure states } p_0.$$

C*-algebra of classical-like observables

$\mathcal{O} : i\mathfrak{u}(n) \ni A \mapsto f_A$ linear extension $\mathcal{O} : \mathfrak{B}(\mathcal{H}) \to \mathcal{F}^2(\mathcal{H})$

$$\mathcal{F}^2(\mathcal{H}) = \left\{ f \in \mathcal{L}^2(\mathcal{P}(\mathcal{H}), \nu_n) | f \text{ is a frame function} \right\}$$

$\mathcal{F}^2(\mathcal{H})$ as C*-algebra of observables

-) Involution: $A = \mathcal{O}(f)$, $A^* = \mathcal{O}(\overline{f})$;
-) $\star$ - product: $f \star g = \mathcal{O}\left(\mathcal{O}^{-1}(f)\mathcal{O}^{-1}(g)\right)$:

$$f \star g = \frac{i}{2}\{f, g\}_{PB} + \frac{1}{2}G(df, dg) + fg \qquad k = 1$$

(more complicated form for $k \neq 1$)
-) Norm: $|||f||| = \| \mathcal{O}^{-1}(f) \|$

$$|||f||| = \frac{1}{k}\left\| f - \frac{1-k}{n}\int_{\mathcal{P}(\mathcal{H})} f \; d\nu_n \right\|_{\infty} \qquad k > 0$$

Re-quantization of classical-like picture

Observable algebra: $\mathcal{F}^2(\mathcal{H})$.

Inverse of the map $\mathcal{O} : i\mathfrak{u}(n) \ni A \mapsto f_A \in \mathcal{F}^2(\mathcal{H})$

Define $\mathfrak{O} : \mathcal{P}(\mathcal{H}) \to \mathfrak{B}(\mathcal{H})$ s.t.

$$\mathfrak{O}(p) := \frac{n+1}{k} p - \left(\frac{n+1-k}{kn}\right) \mathbb{I}.$$

If $f : \mathcal{P}(\mathcal{H}) \to \mathbb{R}$ belongs to the image of $\mathcal{O}$, the associated operator is

$$A = \int_{\mathcal{P}(\mathcal{H})} f(p) \mathfrak{O}(p) d\nu(p).$$

The integral is computed in weak sense. For $k = n+1$:
$A = \int f(p) p d\nu$.

Some conclusions and open issues

- Square-integrable frame functions on projective (finite dimensonal) Hilbert space are an interesting tool to characterize quantum objects (both states and observables) as scalar functions.
- Finite-dimensional QM can be formulated as a proper Hamiltonian in the complex projective space with its Kähler structure. The formulation concerns both observables and states. Maps associating quantum objects to classical like objects finxed. Positivity issue completely clarified.
- **Open issue 1**. Description of composite fineite -dimensional quantum systems within this geometric Hamiltonian framework (cartesian product vs tensor product, D.Pastorello, arXiv:1408.1839, in print.)
- **Open issue 2**. Infnite dimensional case, *there is no unitarily invariant measure* on the projective space (work in progress with S. Mazzucchi and D. Pastorello).

Thank you for your attention!