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On basic stratified structures in quantum information geometry

Martin Bureš*, Arsen Khvedelidze, Dimitar Mladenov, Stanislav Velkov

*IEAP, CTU Prague, Czechia & JINR Dubna, Russia

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Introduction

Modern applications of quantum mechanics renewed interest in the properties of the set of density matrices of finite size.
The state space $\mathfrak{P}_N$ of an N-level quantum system consists of $N \times N$ Hermitean, normalized semi-positive matrices,

$$\mathfrak{P}_N = \{\, X \in M_N(\mathbb{C}) \,|\, X = X^\dagger\,,\ X \geq 0\,,\ \mathrm{Tr}\, X = 1 \,\}\,.$$

The studies of the state space $\mathfrak{P}_N$ include various points of view, among them

- study of $\mathfrak{P}_N$ within convex geometry;
- study of topological properties of $\mathfrak{P}_N$;
- study of differential-geometrical structures on $\mathfrak{P}_N$.

We present the underlying stratified structure of $\mathfrak{P}_N$ (cf. [1]). The goal of research - to calculate the general metric on the whole stratified space.

[1] F. D'Andrea and D. Franco, On the pseudo-manifold of quantum states, Differential Geometry and its Applications 78, 101800 (2021).

Stratified structure of the state space

- Classical mechanics can be formulated in terms of time evolution of physical systems living in a manifold and of functions defined on such a manifold
- An algebraic formulation that works both in classical and quantum mechanics consists in studying the time evolution of states of a C*-algebra (whose self-adjoint elements we may interpret as the observables of our system) space of classical mechanics
- An interesting question is to investigate whether the state space S(A) of a C*-algebra A admits a differentiable structure, in some generalized sense.

Stratified structure of the state space

- The aim of paper[2] is to show that the state space of an arbitrary finite-dimensional C*-algebra is indeed a "good" singular space: it is a stratified space in the sense of Whitney whose structure can be described rather explicitly
- Whitney stratified spaces are a class of singular spaces that are as close as possible to smooth manifolds.
- When working with such spaces, many issues can be addressed by working them out separately on each stratum, reducing many problems to questions about smooth manifolds
- The notion of stratified space is supposed to be a notion of topological space that is not necessarily a manifold, but which is filtered into "strata" that are.

[2] F. D'Andrea and D. Franco, On the pseudo-manifold of quantum states, Differential Geometry and its Applications 78, 101800 (2021).

Stratified spaces - decomposition of a topological space

Definition

Let I be a set. An *I-decomposition* of a topological space X is a locally finite collection of disjoint locally closed subsets $S_i \subset X$, one for each $i \in I$, such that

(1) $X = \bigcup_{i \in I} S_i$,

(2) $S_i \cap \overline{S_j} \neq \emptyset$ implies $S_i \subset \overline{S_j}$.

The sets $\{S_i\}$ are called *pieces* of the decomposition, and a topological space X equipped with an I-decomposition will be called an *I-decomposed space*.

Stratified spaces - decomposition of a topological space

- "locally finite" - every point has a neighborhood which intersects only finitely many pieces
- a set $S \subset X$ is "locally closed" if it is the intersection of an open and a closed subset of X.
- Condition (2) is the so-called frontier condition, saying that if a piece S_i intersects the closure of S_j, it must lie in the frontier $\overline{S_j} \setminus S_j$.
- An example is the decomposition of $M_n(C)$ into subsets of matrices of fixed rank. It follows that any subset of $M_n(C)$ is a decomposed space, in particular the set of density matrices of a finite-dimensional C^*-algebra is a decomposed space. In this example, I is totally ordered and the least element, the unique closed piece of the decomposition, is given by rank 1 density matrices, i.e. pure states.

Definition

Let X be a closed subset of a smooth manifold M. An I-decomposition of X is called a *Whitney stratification* provided each S_i is a smooth embedded submanifold of M and, for all $i \leq j$, Whitney's condition (B) is satisfied:

(B) suppose (x_k) is a sequence of points of S_j and (y_k) a sequence of points of S_i, both converging to some $y \in S_i$, and let ℓ_k be the line through x_k and y_k in some local chart on M. If (ℓ_k) converges to some limiting line ℓ and the tangent spaces $T_{x_k}S_j$ converge to some limiting space τ in the Grassmann bundle of TM, then $\ell \subset \tau$.

We will say that X is a *(Whitney) stratified space*, and call the sets $\{S_i\}$ *strata* of the stratification.

Stratified spaces - decomposition of a topological space

There are three admissible partitions of $\mathfrak{P}_N$

- by the adjoint $SU(N)$ orbits
- by the corresponding orbit types
- by the subsets of density matrices with fixed ranks

Only the last decomposition determines the Whitney stratification. Based on this observation, we establish the connection to our recent paper [3], devoted to the study of the Bures-Fisher metric for rank deficient states, which are non-maximal dimensional strata of the Whitney stratification.

- to derive the Bures metric on each strata $\mathfrak{P}_{N,k}$.
- In detail: the Bures metric for qubit $(N = 2)$ and qutrit $(N = 3)$ in different strata .

[3] M. Bures, A. Khvedelidze and D. Mladenov, Solving the Uhlmann Equation for the Bures-Fisher Metric on the Subset of Rank-Deficient Qudit States, 9th International Conference on Distributed Computing and Grid Technologies in Science and Education, 358-362 (2021)

Geometry of quantum state space

The geometry of the set of density matrices depends on the metric used.

The simplest possible choices exhibit some drawbacks:

- the trace metric, defined by the trace distance

$$D_{\mathrm{Tr}}(\rho,\sigma) = ||\rho-\sigma||_1 := \mathrm{Tr}|\rho-\sigma| = \mathrm{Tr}\sqrt{(\rho-\sigma)^2},$$

  is **monotone, but not Riemannian**, while

- the Hilbert–Schmidt metric, induced by the Hilbert–Schmidt scalar product, $\langle A|B\rangle = \mathrm{Tr} A^\dagger B$ and related to the H–S distance,

$$D_{\mathrm{HS}}(\rho,\sigma) = ||\rho-\sigma||_2 := \sqrt{\mathrm{Tr}[(\rho-\sigma)^2]}\ ,$$

  is **Riemannian but not monotone**.

Other possible metrics and distances in the space of mixed quantum states?

Geometry of quantum state space

- An issue of establishing of Riemannian structures on the quantum counterparts of space of probability measures became a subject of recent investigations.
- Determination of quantum analogues of a well-known, natural Riemannian metric, the so-called Fisher metric.
- Explicit formulae for the Bures metric are known for special cases: e.g. Dittmann has derived several explicit formulae on the manifold of finite-dimensional nonsingular density matrices.
- But: owing to the nontrivial differential geometry of the state space $\mathfrak{P}_N$, studies of its Riemannian structures require a refined analysis for the non maximal rank density matrices.

Geometry of quantum state space

- Let $\mathfrak{P}_{N,k} \subset \mathrm{M}_N(\mathbb{C})$ be a manifold which consists of normalized $N \times N$ density matrices of rank k.
- According to Dittmann (1995), every $\mathfrak{P}_{N,k}$ admits the Bures metric g_B and hence one can consider subspace of fixed rank as the Riemannian manifold $(\mathfrak{P}_{N,k}, \mathrm{g}_B)$.
- The union $\mathfrak{D}_N := \bigcup_{k=1}^{N} \mathfrak{P}_{N,k}$ is not a manifold, but a convex subset of affine space of all normalized Hermitian matrices.

Fidelity and Bures distance

- We will analyse the metric on $\mathfrak{P}_N$, originated from the distance function $d(\varrho_1, \varrho_2)$ between density matrices $\varrho_1, \varrho_2 \in \mathfrak{P}_N$, which is known under different names:
  - Fisher (in statistics)
  - Bures (classical and quantum information theory)
  - Wasserstein metric (optimal transport)

$$d(\varrho_1, \varrho_2) := \sqrt{\operatorname{Tr} \varrho_1 + \operatorname{Tr} \varrho_2 - 2\sqrt{F(\rho_1, \rho_2)}},$$

  where the fidelity is defined as

$$F(\rho_1, \rho_2) = \left[\operatorname{Tr} \sqrt{\sqrt{\rho_A}\rho_B\sqrt{\rho_A}}\right]^2.$$

- This distance function corresponds to the Bures metric which belongs to the special class of the so-called monotone Riemannian metrics.
- It is minimal among all monotone metrics and its extension to pure states is exactly the Fubini–Study metric.

Definition through the purification of a mixed state

- A mixed quantum state can be either understood as a statistical mixture of pure quantum states, or as being part of a higher-dimensional, pure state – a *purification* of the mixed state.
- For every mixed state $\rho_A \in \mathcal{H}_A$, it is possible to find a pure state $|\psi\rangle$ in a larger system $\mathcal{H}_A \otimes \mathcal{H}_B$ such that when we trace out the purification system $\mathcal{H}_B$, we recover the original state: $\rho_A = \mathrm{Tr}_B |\psi\rangle \langle\psi|$.

Fidelity and Bures distance through purification

- **Fidelity** • The fidelity between the density operators ϱ_1 and ϱ_2 is definite by the maximum over all possible purifications ψ_{ϱ_1} and ψ_{ϱ_1} of states

$$F(\varrho_1\,,\varrho_2) = \max_{over\ \ purification} |\langle \psi_{\varrho_1} \,|\, \psi_{\varrho_2} \rangle|$$

- **Bures metric** • Bures distance is defined as

$$d(\varrho_1\,,\varrho_2) = \min_{over\ \ purification} ||\psi_{\varrho_1} - \psi_{\varrho_2}||\,,$$

where the minimum is again taken over all possible purifications $|\psi_{\varrho_1}\rangle$ and - $|\psi_{\varrho_2}\rangle$, of the states ϱ_1 and ϱ_2.

Bures vs. Hilbert-Schmidt distance for a qubit

It is instructive to compare the geometry induced by the Bures and the Hilbert-Schmidt metric. [4]

- Any $N = 2$ density matrix ρ may be expressed in the Bloch representation

$$\rho = \frac{1}{2}\left(\mathbb{I} + \vec{\tau} \cdot \vec{\sigma}\right)$$

  where $\vec{\sigma}$ denotes a vector of three Pauli matrices, $\{\sigma_x, \sigma_y, \sigma_z\}$, while the Bloch vector $\vec{\tau} = \{x, y, z\}$ belongs to $\mathbb{R}^3$.
- With respect to the HS metric the set of mixed states $\mathcal{M}_2$ forms the Bloch ball B^3 with the set of all pure states at its boundary, called *Bloch sphere*.
- The H–S distance between any mixed states of a qubit is proportional to the Euclidean distance inside the ball, so the H–S metric induces the flat geometry in $\mathcal{M}_2$.

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[4] Bures volume of the set of mixed quantum states, HJ Sommers, K Zyczkowski, Journal of Physics A: Mathematical and General 36 (39), 10083.

Bures vs. Hilbert-Schmidt distance for a qubit

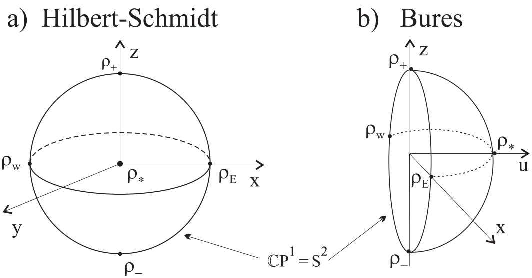

Figure: Geometry of the set of the mixed states for $N = 2$: a) – the 3-ball embedded in $\mathbb{R}^3$ induced by the Hilbert-Schmidt distance, b) – hemisphere of $\mathbf{S}^3$ embedded in $\mathbb{R}^4$, (shown as a cross-section of R^4 taken at $y = 0$), induced by the Bures distance. The maximally mixed state ρ_* is located at the center of the ball (a), and at the hyper-pole of $\mathbf{S}^3$ (b). The set of pure states is represented by the Bloch sphere $\mathbf{S}^2$ (a) and by the Uhlmann equator $\mathbf{S}^2 \in \mathbf{S}^3$ (b). The cross-section of $\mathcal{M}_2$ with the plane $z = 0$ produces a full circle in the equatorial plane (a), or a half of a hyper-meridian joining the states ρ_W and ρ_E (b).

Bures metric on rank deficiency states

- Let ϱ be an element of $\mathfrak{P}_{N,k}$, where $\mathfrak{P}_{N,k}$ is a set comprising of normalized $N \times N$ density matrices of rank k. For a given ϱ consider the equation

$$\varrho\,\mathrm{G}_\varrho + \mathrm{G}_\varrho\,\varrho = \mathrm{d}\varrho$$

  for an unknown 1-form G_ϱ.

- The solution determines the Bures metric on $\mathfrak{P}_{N,k}$ as [5]

$$\mathrm{g}_B = (\mathrm{d}\varrho\,, G_\varrho)\,.$$

[5] Armin Uhlmann, Geometric Phases and Related Structures, Rep. Math. Phys., **36** 461-481, (1995)

• **Qubit Bures metric for rank**$(\varrho) = 2$ **states** •

$$g_2^{k=2} = \frac{(\mathrm{d}r_1)^2}{2r_1} + \frac{(\mathrm{d}r_2)^2}{2r_2} + 2|\Omega_{12}|^2 \frac{(r_1 - r_2)^2}{r_1 + r_2}$$

where Ω is given in terms of left invariant 1-forms ω_1 and ω_2 on the coset $SU(2)/U(1)$:

$$\Omega_{12} = \frac{\imath}{2}(\omega_1 - \imath\omega_2)$$

Using expressions for 1-forms in terms of the Euler angles

$$\omega_1 = \sin\beta\cos\gamma\mathrm{d}\alpha - \sin\gamma\mathrm{d}\beta \qquad \omega_2 = \sin\beta\sin\gamma\mathrm{d}\alpha + \cos\gamma\mathrm{d}\beta$$

and taking into account that $r_1 + r_2 = 1$ we have

$$g_2^{k=2} = \frac{1}{2(1-r^2)}(\mathrm{d}r)^2 + \frac{1}{2}r^2\left[\sin^2\beta(\mathrm{d}\alpha)^2 + (\mathrm{d}\beta)^2\right] \ ,$$

where $r = r_1 - r_2$.

• **Qubit Bures metric for rank**$(\varrho) = 1$ **states** •

For pure qubit states the metric reads

$$g_2^{k=1} = 2|\Omega_{12}|^2 = \frac{1}{2}\left[\sin^2\beta(\mathrm{d}\alpha)^2 + (\mathrm{d}\beta)^2\right] .$$

Explicit solutions - qutrit

• **Bures metric for rank**$(\varrho) = 3$ **qutrit states** •

Fixed rank decomposition for qutrit state space

$$\mathfrak{P}_3 = \mathfrak{P}_3^3 \cup \mathfrak{P}_3^2 \cup \mathfrak{P}_3^1 \,,$$

For the generic non-singular set of density matrices $\dim(\mathfrak{P}_3) = 8$

$$\mathrm{g}_B^{k=3}$$

• Bures metric for rank(ϱ) $= 3$ qutrit states •
We use the Euler parameterization,

$$U = e^{\frac{\imath\alpha}{2}\lambda_3} V(\alpha,\beta,\gamma) \exp\left(i\theta\lambda_5\right) V(a,b,c) \exp\left(i\phi\lambda_8\right) \;,$$

where the left and right factors V denote two copies of the $SU(2)$ group embedded in $SU(3)$:

$$V(a,b,c) = \exp\left(i\frac{a}{2}\lambda_3\right) \exp\left(i\frac{b}{2}\lambda_2\right) \exp\left(i\frac{c}{2}\lambda_3\right) \;.$$

The decomposition angles $\Omega_3 = \{\alpha,\beta,\gamma,a,b,c,\theta,\phi\}$ take values from the intervals

$$\alpha, a \in [0,2\pi]; \quad \beta, b \in [0,\pi]; \quad \gamma, c \in [0,4\pi];$$
$$\theta \in [0,\pi/2]; \quad \phi \in [0,\sqrt{3}\pi] \,.$$

• **Bures metric for rank**$(\varrho) = 2$ **qutrit states** •

$$g_B^{k=1} = \frac{(\mathrm{d}r_1)^2}{2r_1} + \frac{(\mathrm{d}r_2)^2}{2r_2} + 2\frac{(r_1 - r_2)^2}{r_1 + r_2}|\Omega_{12}|^2 + 2\left(r_1|\Omega_{13}|^2 + r_2|\Omega_{23}|^2\right)$$

Here $\Omega_{12}\,, \Omega_{13}$ and Ω_{23} are the components of the Cartan left-invariant form

$$U^\dagger \mathrm{d}U = \frac{\imath}{2}\sum_{a=1}^{8} \omega_a \lambda_a$$

on the coset $SU(3)/T^2$.

$$\Omega_{12} = \omega_1 - \imath\omega_2\,, \qquad \Omega_{13} = \omega_4 - \imath\omega_5\,, \qquad \Omega_{23} = \omega_6 - \imath\omega_7\,,$$

• **Bures metric for rank**$(\varrho) = 1$ **qutrit states** •

$$g_B^{k=2} = \frac{(\mathrm{d}r_1)^2}{2r_1} + (1 + r_1)\left(|\Omega_{12}|^2 + |\Omega_{13}|^2\right)$$
$$= \frac{(\mathrm{d}r_1)^2}{2r_1} + (1 + r_1)\left(\omega_1^2 + \omega_2^2 + \omega_4^2 + \omega_5^2\right)$$

Now Ω_{12} and Ω_{13} denote the components of the Cartan form $U^\dagger \mathrm{d}U$ evaluated at the coset $SU(3)/S(U(2) \times U(1))$.