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Brief Communication

Some properties of the Riemannian Bures metric on mixed states

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We consider the Riemannian geometry of the space of nonsingular density matrices $\mathscr{D}$ equipped with the Bures metric g. This space is of certain physical relevance on the background of generalization of the Berry phase to mixed states. The main result is the determination of the covariant derivative and the curvature tensor field related to the Levi-Cività connection of $(\mathscr{D}, g)$. It turns out that $\mathscr{D}$ is not a space of constant curvature and even not a locally symmetric space in contrast to the suggestions one gets from the case of two-dimensional density matrices. Moreover, we give a local description of $\mathscr{D}$ and explicit formulae for g in terms of natural matrix operations containing ρ and $d\rho$ only.

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1. Introduction

The space $\mathscr{D}$ of nonsingular, normalized $n\times n$ density matrices ρ carries an interesting and quite natural Riemannian metric g called the Riemannian Bures metric [1]. It appears on the background of purification of mixed states in larger systems and of generalization of the Berry phase in this context (see refs. [2–4] and references therein). So it is natural to ask for the differential geometric properties of $(\mathscr{D}, g)$.

The metric g is the infinitesimal version of the distance function [5,6]

$$d(\rho, \mu)=\sqrt{2-2\,\mathrm{Tr}(\rho^{1/2}\mu\rho^{1/2})^{1/2}}\ .$$

More precisely, g_ρ is the Hessian of the function $\mathscr{D}\ni\mu\mapsto\frac{1}{2}(d(\rho,\mu))^2$ at the point $\mu:=\rho$. Equivalently g is defined as follows: The bundle space $\mathscr{P}$ of the principal $\mathrm{U}(n)$-bundle $\mathrm{gl}(n,\mathbb{C})\supset\mathscr{P}:=\pi^{-1}(\mathscr{D})\to\mathscr{D}$, where $\pi(w):=ww^*$, has the metric induced from the real part of the Hilbert–Schmidt metric $\langle X, Y\rangle=\mathrm{Tr}\,XY^*$ on $\mathrm{gl}(n,\mathbb{C})$. The vectors orthogonal to the fibres form the horizontal subspaces of a certain connection on $\mathscr{P}$. This connection and the metric on $\mathscr{P}$ induce the

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Riemannian metric g on the base space $\mathscr{D}$ we are interested in. It turns out that it is given by

$$g=\tfrac{1}{2}\mathrm{Tr}\,\mathrm{d}\rho\, G\,, \tag{1}$$

where $\rho G+G\rho=\mathrm{d}\rho$, $\rho\in\mathscr{D}$, is the implicit definition of the hermitean matrix valued one-form G (see ref. [4]). The connection above was first considered by Uhlmann [10]. He observed that the horizontality requirement for a lift of a path $t\mapsto\gamma(t)\in\mathscr{D}$ to $\mathscr{P}$ is an appropriate generalization of the Berry condition for mixed states.

In order to motivate the results presented later let us briefly explain some basic features of $(\mathscr{D},g)$ in the case $n=2$ [1]. The mapping $\mathrm{S}^3_+\ni(x_\alpha)\mapsto\frac{1}{2}(\mathbb{1}+x_\alpha\sigma^\alpha)\in\mathscr{D}$, where σ^α are the Pauli matrices, is a diffeomorphism of the upper half-shell of the unit three-sphere onto $\mathscr{D}$. Moreover, using $\rho^2-\rho+|\rho|\mathbb{1}=0$ one obtains $G=\frac{1}{2}\rho^{-1}(\mathrm{d}\rho+[\rho,\mathrm{d}\rho])=\mathrm{d}\rho+\frac{1}{2}\rho^{-1}\mathrm{d}|\rho|$. This yields for the Bures metric [1,7]

$$g=\tfrac{1}{2}\mathrm{Tr}\,\mathrm{d}\rho\,\mathrm{d}\rho+\mathrm{d}\sqrt{|\rho|}\,\mathrm{d}\sqrt{|\rho|}=\tfrac{1}{4}\mathrm{d}x_\alpha\,\mathrm{d}x^\alpha\,. \tag{2}$$

We see that $(\mathscr{D},g)$ is isometric to an open half-shell of a three-sphere of radius $\frac{1}{2}$. It is a space of constant curvature with $\mathrm{o}(4)$ as the Lie algebra of Killing fields. Up to this case no "nice" embedding of $\mathscr{D}$ into a flat space is known to the author. Moreover, it is interesting that the gauge field corresponding to Uhlmann's connection mentioned above satisfies the source-free Yang–Mills equation $D{*}F=0$ in the case $n=2$ [8].

These observations for $n=2$ lead to some suggestions for arbitrary finite nondegenerate normalized density matrices. One of the problems in studying this space is the implicitness in the definition of g. The aim of this communication is to answer the following questions:

1. How can one obtain formulae analogous to (2) for the Bures metric involving ρ, its invariants, "d" and natural matrix operations only?
2. What is the covariant derivative and the curvature tensor of the Levi-Cività connection on $\mathscr{D}$? Is $\mathscr{D}$ a space of constant curvature or, at least, a locally symmetric space?
3. What does the space $\mathscr{D}$ look like in the neighbourhood of a generic point?

A detailed discussion and proofs can be found in ref. [9].

2. Results

Let L_ρ (R_ρ) be the operator of left (right) multiplication of matrices by $\rho\in\mathscr{D}$ and denote by L (R) the related operator valued function on $\mathscr{D}$. Then eqs. (1) read as

$$g = \tfrac{1}{2}\mathrm{Tr}\, \mathrm{d}\rho \frac{1}{L+R}(\mathrm{d}\rho) = \tfrac{1}{2}\mathrm{Tr}\, \mathrm{d}\rho\, \widetilde{\mathrm{d}\rho}\,, \qquad G = \frac{1}{L+R}(\mathrm{d}\rho) =: \widetilde{\mathrm{d}\rho}\,, \tag{3}$$

where tilde denotes for simplicity the application of $(L+R)^{-1}$. Of course, g can be extended by (3) to a metric on all (not normalized) nonsingular density matrices, which we also denote by g. We regard vector fields X, Y, W and Z as matrix valued functions and $[X, Y] := XY - YX$ denotes the commutator of such functions. Moreover, let N denote the function given by $N_\rho := \rho$.

2.1. ALGEBRAIC FORMULAE FOR THE METRIC

For $n=3$ we get, using the Hamilton–Cayley theorem $-\rho^3+\rho^2-\sigma_2\rho+\sigma_3\mathbb{1}=0$, the identity

$$\frac{L-R}{L+R} = \frac{1}{\sigma_2-\sigma_3}(\mathrm{Id}-L)\circ(\mathrm{Id}-R)\circ(L-R)\,, \tag{4}$$

which leads to a new formula for the Bures metric on nonsingular 3×3-density matrices,

$$g = \frac{1}{4(\sigma_2-\sigma_3)}\{2\,\mathrm{Tr}(\mathrm{d}\rho-\rho\,\mathrm{d}\rho)^2 - \mathrm{d}\sigma_2\,\mathrm{d}\sigma_2 + 4\mathrm{d}\sqrt{\sigma_3}\,\mathrm{d}\sqrt{\sigma_3}\}\,. \tag{5}$$

Verifying (4) for a diagonal ρ and common eigenvectors E_{ij} of L and R it is not difficult to see how to obtain algebraic formulae analogous to (4) and (5) for general n. One has to extend $1/(L+R)$ by a polynomial of $L+R$, such that the denominator becomes an invariant of ρ. Since the coefficients of the characteristic polynomial of $L+R$ are invariants of ρ this really can be achieved and, finally, one gets g in the desired form.

2.2. THE LEVI-CIVITÀ CONNECTION

Let ∇^{f} denote the flat covariant derivative on matrices, ∇ the covariant derivative of the Levi-Cività connection on $(\mathscr{D}, g)$ and $\mathscr{R}$ its curvature tensor. The following result allows one to determine differential-geometric quantities of $(\mathscr{D}, g)$.

Theorem.

$$\nabla_X Y = \nabla^{\mathrm{f}}_X Y - \tilde{X}N\tilde{Y} - \tilde{Y}N\tilde{X} + 2g(X, Y)\cdot N\,, \tag{6}$$

$$\begin{aligned}\mathscr{R}(W, Z, X, Y) = {} & 2g(\mathrm{i}N[\tilde{X}, \tilde{Y}]N, \mathrm{i}[\tilde{W}, \tilde{Z}]) + g(\mathrm{i}N[\tilde{Z}, \tilde{Y}]N, \mathrm{i}[\tilde{W}, \tilde{X}]) \\ & - g(\mathrm{i}N[\tilde{Z}, \tilde{X}]N, \mathrm{i}[\tilde{W}, \tilde{Y}]) \\ & + g(Y, Z)g(X, W) - g(X, Z)g(Y, W)\,. \end{aligned} \tag{7}$$

Considering for example the sectional curvature $\mathscr{K}$ we get:

Corollary. *$\mathscr{K}(p) \geqslant 1$ for all planes p. The space $(\mathscr{D}, g)$ is not of constant curvature and not even locally symmetric for $n \geqslant 3$.*

The last statement is in contradiction to suggestions coming from $n=2$. However, it should not disappoint, because the property of local symmetry means that locally there is no essential difference between going along a geodesic in a direction X_ρ and in the opposite direction $-X_\rho$. But this should not be true for mixed states.

2.3. LOCAL STRUCTURE

For a generic $\rho \in \mathscr{D}$ we have the decomposition $\rho = u\mu^2 u^*$, where $\lambda := \mu^2$ is diagonal with different eigenvalues only and $u \in \mathrm{U}(n)/\mathrm{T}^n$. Then the Bures metric splits as follows:

$$g = \mathrm{Tr}\, \mathrm{d}\mu\, \mathrm{d}\mu + \tfrac{1}{2}\mathrm{Tr}\{[u^*\mathrm{d}u, \lambda] \frac{1}{L_\lambda + R_\lambda} ([u^*\mathrm{d}u, \lambda])\} . \qquad (8)$$

Thus, in a generic point ρ the Riemannian manifold $(\mathscr{D}, g)$ is locally isometric to $\mathrm{S}^{n-1} \times \mathrm{U}(n)/\mathrm{T}^n$, where the $\mathrm{U}(n)$-invariant metric on the homogeneous space $\mathrm{U}(n)/\mathrm{T}^n$ given by the second term of (8) depends on the parameter $\lambda \in \mathrm{S}^{n-1}$.

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