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UNIVERSITÄT LEIPZIG

Naturwissenschaftlich-Theoretisches

Zentrum

On the Riemannian Metric
on the Space of Density Matrices

by

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Preprint-Nr. 12/1995

Abstract

The concept of purification of mixed states of quantum systems leads naturally to an interesting Riemannian metric on the space of normalized density matrices $\mathcal{D}_n$. More precisely, this Riemannian metric introduced by Uhlmann is defined on submanifolds (of all hermitean matrices) $\mathcal{D}_{nk}$ of density matrices of fixed rank k , but not for vectors transversal to this submanifolds (at least using definitions known in the literature). A natural question is, whether there exists a manifold M of dimension $\dim \mathcal{D}_{nn} = n^2 - 1$, which contains $\bigcup_{k=1}^n \mathcal{D}_{nk}$ as a topological subspace such that $\mathcal{D}_{nk}$, $k = 1, \dots, n$, is isometrically embedded. For $n = 2$ this is true, as Uhlmann observed. We show that for higher n such a manifold does not exist, because the sectional curvature at $\varrho \in \mathcal{D}_{nn}$ diverges if ϱ tends to a state of rank less than $n - 1$. Roughly speaking, the metrics on the manifolds $\mathcal{D}_{nk}$ cannot be glued together, because $\mathcal{D}_{nn}$ contains geodesically complete submanifolds, which look like conical singularities in the neighbourhood of $\partial\mathcal{D}_{nn}$.

1 Preliminaries

1.1 The Riemannian metric

In connection with the generalization of the Berry phase ([1]) to mixed states Uhlmann introduced a Riemannian metric on density matrices ([8]-[10]). This metric is highly distinguished not only by its natural geometric definition, but also by its minimality among monotone metrics ([7]). The nice picture obtained in the 2×2 -case ([10], see also [4]) was a motivation for considering the general case. In [5] it was shown, that the space of nonsingular $n \times n$ density matrices equipped with this Riemannian metric is not locally symmetric for $n > 2$. It is the aim of this paper to investigate this metric in the neighbourhood of singular states. First we introduce some basic notations and already known results.

We denote by $\mathcal{D}_{nk} \subset \mathcal{M}_{nn}(\mathbb{C})$ the space of normalized $n \times n$ -density matrices of rank k and by $\mathcal{D}_n$ the union of the manifolds $\mathcal{D}_{nk}$. $\mathcal{D}_n$ is not a manifold, but a convex subset of the affine space $\mathcal{A}$ of normalized hermitean matrices. The inner points of $\mathcal{D}_n$ are the nondegenerate states $\varrho \in \mathcal{D}_{nn}$.

An operator $w \in \mathcal{M}_{nn}(\mathbb{C})$ is called a purification of a mixed state $\varrho \in \mathcal{D}_n$ iff $\varrho = \pi(w)$, where

$$\pi : S \rightarrow \mathcal{D}_n \subset \mathcal{A}, \quad \pi(w) := w w^*, \quad (1)$$

maps the unit sphere S of $\mathcal{M}_{nn}(\mathbb{C})$ w. r. to the Hilbert-Schmidt metric $\text{Tr}(\cdot)(\cdot)^*$ onto $\mathcal{D}_n$. The mapping π preserves the rank and using the polar decomposition and an ansatz by block matrixes we obtain

$$\text{im } \pi_{*w} = T_\varrho \mathcal{D}_{nk}, \quad (2)$$

where $\varrho = w w^*$ and $k = \text{rank } \varrho$. The Riemannian metric g on $\mathcal{D}_{nk}$ can now be defined by

$$g_\varrho(Y_\varrho, Y_\varrho) := \inf \{ \text{Tr } V V^* \mid V \in TS, \pi_*(V) = Y_\varrho \} ; \quad Y_\varrho \in T_\varrho \mathcal{D}_{nk}. \quad (3)$$

Since the Hilbert-Schmidt metric is invariant under the right $U(n)$ -multiplication, it is sufficient to take vectors V tangent to S at $\sqrt{\varrho}$:

$$g_\varrho(Y_\varrho, Y_\varrho) = \inf \{ \text{Tr } V V^* \mid \sqrt{\varrho} V^* + V \sqrt{\varrho} = Y_\varrho \} . \quad (4)$$

$\text{Tr } V V^*$ takes its infimum iff V is orthogonal to the kernel of π_* at $\sqrt{\varrho}$ and one gets

$$g_\varrho(Y_\varrho, Y_\varrho) = \frac{1}{2} \text{Tr } Y_\varrho \mathbf{G}_\varrho, \quad (5)$$

where $\mathbf{G}_\varrho \in \mathcal{M}_{nn}(\mathbb{C})$ is any solution of the equation

$$\varrho \mathbf{G}_\varrho + \mathbf{G}_\varrho \varrho = Y_\varrho. \quad (6)$$

To see this, let ϱ be diagonal of the form $\varrho = \lambda_1 E_{11} + \dots + \lambda_r E_{rr}$ and make, again, an ansatz for Y_ϱ and V as block matrices. Finally, we get for arbitrary arguments

$$g_\varrho(X_\varrho, Y_\varrho) = \frac{1}{2} \text{Tr } X_\varrho \mathbf{G}_\varrho, \quad X_\varrho, Y_\varrho \in T_\varrho \mathcal{D}_{nk}, \quad (7)$$

where $\mathbf{G}_\varrho$ is any solution of (6). This is the Riemannian metric on density matrices $\mathcal{D}_{nk}$ introduced by Uhlmann. It is the infinitesimal version of the Bures distance ([2])

$$d_B(\varrho, \mu) = \sqrt{2 - 2 \operatorname{Tr} \left(\varrho^{\frac{1}{2}} \mu \varrho^{\frac{1}{2}} \right)^{\frac{1}{2}}} . \quad (8)$$

Notice that equation (6) has a solution $\mathbf{G}_\varrho$ for a traceless hermitean right hand side Y iff $Y \in T_\varrho \mathcal{D}_{nk}$, where $k = \operatorname{rank} \varrho$. Therefore, equation (7) defines a Riemannian metric on every $\mathcal{D}_{nk}$, as mentioned above.

In this paper we are interested in the behaviour of the metric on $\mathcal{D}_{nn}$ if we get close to singular states. For $\varrho > 0$ equation (6) has exactly one solution for every right hand side. Indeed, the operator $L_\varrho + R_\varrho$ (L_ϱ and R_ϱ denote left resp. right multiplication by ϱ) is invertible, because its spectrum $\{\lambda_i + \lambda_j \mid \lambda_i, \lambda_j - \text{eigenvalues of } \varrho\}$ is positive. For simplicity we will denote this solution by $\tilde{Y}_\varrho$;

$$\tilde{Y}_\varrho := \mathbf{G}_\varrho(Y_\varrho) = (L_\varrho + R_\varrho)^{-1} (Y_\varrho) . \quad (9)$$

Using this notation (7) reads as

$$g = \frac{1}{2} \operatorname{Tr} d\varrho \frac{1}{L+R} (d\varrho) = \frac{1}{2} \operatorname{Tr} d\varrho \tilde{d}\varrho . \quad (10)$$

1.2 Geodesics

The metric g on $\mathcal{D}_{nn}$ appears verry naturally in the following bundle picture: Let $S \supset \mathcal{P} := \pi^{-1}(\mathcal{D}_{nn})$. Then $\mathcal{P} \xrightarrow{\pi} \mathcal{D}_{nn}$ is a principal bundle w. r. to the right $U(n)$ -multiplication on $\mathcal{P}$. Moreover, $\mathcal{P}$ is equipped with the Riemannian metric $\operatorname{ReTr}(\cdot)(\cdot)^*$. The vectors V orthogonal to the fibres ($\operatorname{ReTr} w a V^* = 0, \forall a \in \mathfrak{u}(n)$) form the horizontal subspaces of Uhlmann's connection on this bundle ([8],[3]). This connection and the metric on $\mathcal{P}$ induce a Riemannian metric on $\mathcal{D}_{nn}$ by horizontal lifting of vectors tangent to $\mathcal{D}_{nn}$. Obviously, it coincides with the metric defined by (3).

A vector $V \in T_w \mathcal{P}$ is horizontal w. r. to this connection iff

$$w^* V = V^* w . \quad (11)$$

A piece of a great circle c on S ,

$$c(s) := \cos(s)w + \sin(s)V , \quad s \in (-\epsilon, \epsilon) ,$$

starting at $w \in \mathcal{P}$ with a horizontal, normalized velocity $V \in T_w \mathcal{P}$,

$$\operatorname{Tr} (w V^* + V w^*) = 0, \quad w^* V = V^* w, \quad \operatorname{Tr} V V^* = 1 ,$$

is a horizontal path, that means, c satisfies the horizontality condition (11):

$$c^* \dot{c} = \dot{c}^* c .$$

Therefore, $\gamma := \pi \circ c$ is a geodesic on $\mathcal{D}_{nn}$ and every geodesic is of this kind. Moreover, any geodesic has at most the length of a half unit circle.

Of course, $\gamma(s)$ may be singular for some s . Then it is at least problematic to call these paths geodesics on $\mathcal{D}_n$, although it is reasonable to call them minimal. This was one of the motivations to ask, whether the metrics on the manifolds $\mathcal{D}_{nk}$ can be glued together, or not.

Let us consider this case in more detail. For this purpose let

$$(s_0 - \epsilon, s_0 + \epsilon) \ni s \mapsto \gamma(s) := \pi(c(s))$$

be a geodesic on $\mathcal{D}_{nn}$ for $s \neq s_0$ and $\gamma(s_0) \in \mathcal{D}_{nk}$, $k < n$. Suppose that the one-dimensional space $L_s := \mathbb{R} \dot{\gamma}(s) \subset \mathcal{M}(n, n)$ exists for $s \rightarrow s_0$. Then L_{s_0} is tangent or transversal to $\mathcal{D}_{nk}$ (It can be shown that both cases occur). In the second case $\dot{\gamma}(s_0)$ must be zero because of (2). This shows that one cannot define the length $\|X\|$ of a vector transversal to a manifold of singular states by putting $\|\dot{\gamma}(s_0)\| = \|X\|$, where $s \mapsto \gamma(s)$ is a minimal path sent from $\mathcal{D}_{nn}$ to the singular state with $L_{s_0} = \mathbb{R}X$.

To avoid this problem one could, roughly speaking, try to change the differentiable structure in the transversal direction, so that the derivative of such a minimal path will not be zero at a singular state. This is, essentially, what can be done in the case of 2×2 -density matrices (see 2.3). To consider the general case we need the knowledge of the curvature of $\mathcal{D}_{nn}$.

1.3 Covariant derivative and curvature

The covariant derivative ∇ of the Levi-Cevita connection of $(\mathcal{D}_{nn}, g)$ and the corresponding curvature tensor field $\mathcal{R}$ were given in [5]. For vector fields X and Y on $\mathcal{D}_{nn}$ regarded as matrix valued functions we obtained

$$\nabla_X Y = \nabla_X^f Y - \widetilde{X}N\widetilde{Y} - \widetilde{Y}N\widetilde{X} + 2g(X, Y)N, \quad (12)$$

where $\nabla_X^f Y$ is the covariant derivative of the underlying flat affine structure on density matrices and N is the normal vector field given by $N_\varrho := \varrho$. The fields $\widetilde{X}$ and $\widetilde{Y}$ are given by (9), the multiplication is the pointwise matrix multiplication.

Moreover, for the curvature we have

$$\begin{aligned} \mathcal{R}(X, Y, X, Y) &= -3g(N[\widetilde{X}, \widetilde{Y}]N, [\widetilde{X}, \widetilde{Y}]) \\ &\quad + g(X, X)g(Y, Y) - g(X, Y)g(X, Y), \end{aligned} \quad (13)$$

where $[\cdot, \cdot]$ is the pointwise matrix commutator. Here, g is the $\mathbb{C}$ -linear extension of (7) to all complex matrices, so that the first term of the right hand side of (13) is in fact nonnegative (the arguments are antihermitean).

2 Results

2.1 The unbounded sectional curvature

From (13) we get for the sectional curvature on $\mathcal{D}_{nn}$

$$\mathcal{K}(X \wedge Y) = 1 + 3 \frac{g(iN[\tilde{X}, \tilde{Y}]N, i[\tilde{X}, \tilde{Y}])}{g(X, X)g(Y, Y) - g(X, Y)g(X, Y)} \geq 1. \quad (14)$$

Our basic observation is the following

Theorem: *Let $n \geq 3$. Then the sectional curvature on the manifold of nonsingular $n \times n$ -normalized density matrices $\mathcal{D}_{nn}$ is unbounded in any neighbourhood of a singular state of rank less than $n - 1$. This means, for every $\varrho_0 \in \mathcal{D}_{nk}$ with $k < n - 1$, and all $C, \epsilon \in \mathbb{R}_+$ there exist a $\varrho \in \mathcal{D}_{nn}$ and vectors $X_\varrho, Y_\varrho \in T_\varrho \mathcal{D}_{nn}$ such that*

$$d_B(\varrho_0, \varrho) < \epsilon \quad \text{and} \quad \mathcal{K}_\varrho(X_\varrho \wedge Y_\varrho) > C. \quad (15)$$

Proof: Let ϱ , X_ϱ and Y_ϱ be given by $\varrho := \lambda_1 E_{11} + \lambda_2 E_{22} + \dots + \lambda_n E_{nn}$ with $\lambda_1 + \lambda_2 + \dots + \lambda_n = 1$ and $\lambda_i \neq 0$, $X_\varrho := E_{12} + E_{21}$ and $Y_\varrho := i(E_{12} - E_{21})$. Then we get

$$\tilde{X}_\varrho = \frac{1}{\lambda_1 + \lambda_2} (E_{12} + E_{21}), \quad \tilde{Y}_\varrho = \frac{i}{\lambda_1 + \lambda_2} (E_{12} - E_{21}),$$

and by (7)

$$g_\varrho(X_\varrho, X_\varrho) = g_\varrho(Y_\varrho, Y_\varrho) = \frac{1}{\lambda_1 + \lambda_2}, \quad g_\varrho(X_\varrho, Y_\varrho) = 0.$$

Moreover, we obtain

$$\begin{aligned} [\tilde{X}_\varrho, \tilde{Y}_\varrho] &= \frac{2i}{(\lambda_1 + \lambda_2)^2} (-E_{11} + E_{22}), \\ \varrho [\tilde{X}_\varrho, \tilde{Y}_\varrho] \varrho &= \frac{2i}{(\lambda_1 + \lambda_2)^2} (-\lambda_1^2 E_{11} + \lambda_2^2 E_{22}), \\ g_\varrho(i\varrho[\tilde{X}_\varrho, \tilde{Y}_\varrho]\varrho, i[\tilde{X}_\varrho, \tilde{Y}_\varrho]) &= \frac{1}{(\lambda_1 + \lambda_2)^3} \end{aligned}$$

and, finally, using (14)

$$\mathcal{K}_\varrho(X_\varrho \wedge Y_\varrho) = 1 + \frac{3}{\lambda_1 + \lambda_2}. \quad (16)$$

Now, let there be given a singular state ϱ_0 of rank less than $n - 1$, $\varrho_0 \sim \mu_3 E_{33} + \dots + \mu_n E_{nn}$, and two positive numbers C and ϵ . To ensure $d_B(\varrho_0, \varrho) < \epsilon$, we have to choose $\lambda_3, \dots, \lambda_n$ sufficiently close to $\mu_3, \dots, \mu_n$. This leads by (16) to arbitrarily large sectional curvature. $\square$

2.2 Noncompatibility of the metrics

As a consequence of our Theorem we get the following negative answer to the question formulated above, the metrics on $\mathcal{D}_{nk}$ are not compatible in the following sense:

Corollary:

For $n \geq 3$ there does not exist a continuous mapping $\Phi : \mathcal{D}_n \longrightarrow M$ into a Riemannian manifold M of dimension $\dim \mathcal{D}_{nn} = n^2 - 1$, such that the restrictions of Φ to the Riemannian manifolds $\mathcal{D}_{nk}$, $k = 1, \dots, n$, are isometric embeddings.

Proof: If such a manifold M existed, the sectional curvature on M would be locally bounded, in contradiction to the Theorem. $\square$

It would be interesting to know, whether, at least, the metrics on $\mathcal{D}_{nn}$ and $\mathcal{D}_{nn-1}$ can be glued together in the above sense as for $n = 2$. Notice that $\dim \mathcal{D}_{nn-1} = \dim \mathcal{D}_{nn} - 1$ and, moreover, the Theorem is not an obstruction in this case.

In the Corollary we could replace the condition on the dimension of M by the requirement that $\Phi(\mathcal{D}_{nn})$ is a geodesically complete submanifold of M . In 2.4 we will give a geometric interpretation of the Theorem and the Corollary. For this purpose we briefly explain the known case of two dimensional density matrices.

2.3 The case $n = 2$

For the case of 2×2 -density matrices Uhlmann gave a nice realization of $\mathcal{D}_2$ as a three-hemisphere of radius one half as follows ([10]):

Let $\varrho := \frac{1}{2}(\mathbb{1} + x_1\sigma_1 + x_2\sigma_2 + x_3\sigma_3)$. Then $\varrho \geq 0$ iff $x_1^2 + x_2^2 + x_3^2 \leq 1$. Hence, $\mathcal{D}_2$ is topologically a three-ball with pure states sitting on the boundary $\mathcal{D}_{21} \approx S^2$. Define

$$\Phi : \mathcal{D}_2 \rightarrow S^3 \subset \mathbb{R}^4 \quad \text{by} \quad \Phi(\varrho) := \frac{1}{2} \left(x_1, x_2, x_3, \sqrt{1 - x_1^2 - x_2^2 - x_3^2} \right), \quad (17)$$

where S^3 is the three-sphere of radius $\frac{1}{2}$. The mapping Φ homeomorphically blows up the disk $\mathcal{D}_2$ to the upper hemisphere, but it is not differentiable in the direction transversal to the pure states. The restrictions of Φ to $\mathcal{D}_{22}$ and $\mathcal{D}_{21}$ are embeddings and, moreover, isometries. We may identify $\mathcal{D}_2$ with $S^3/\sim$, where $\sim$ means the identification of points with opposite x_4 -coordinates. Then the projections of geodesics on S^3 correspond to the minimal paths in $\mathcal{D}_2$ mentioned in 1.2.

2.4 Geometric interpretation

The above Theorem has a nice geometric interpretation. A. Uhlmann informed me, that the unboundedness of the sectional curvature of $\mathcal{D}_{nn}$ is related to the existence of geodesically complete submanifolds, which look like conical singularities. A submanifold N of a Riemannian manifold M is geodesically complete iff the second fundamental form of the submanifold vanishes (see [6]). That means, for all vector fields X, Y tangent to N the covariant derivative $\nabla_X Y$ w. r. to M is tangent to N , too. In this case the sectional curvature w. r. to M of a plane tangent to N coincides with the sectional curvature w. r. to the induced metric on N . Now, let $B \subset \mathcal{D}_{nn}$ be a submanifold of block-diagonal matrices for a fixed block structure. Then B is geodesically complete. Indeed, vectors tangent to B are block-diagonal and all operations involved in (12) maintain this block structure. By the same argument the submanifolds

$$\mathcal{C}_\lambda := \left\{ \varrho_\lambda = \begin{pmatrix} \lambda \varrho & 0 \\ 0 & \frac{1-\lambda}{n-2} \mathbb{1} \end{pmatrix} \in \mathcal{D}_{nn} \mid \varrho \in \mathcal{D}_{22} \right\} \approx S_+^3; \quad \lambda \in (0, 1), \quad (18)$$

and $\mathcal{C} := \bigcup_{\lambda} \mathcal{C}_{\lambda}$ are geodesically complete. By (7) and **2.3** the manifold $\mathcal{C}_{\lambda}$ is isometric to an open three-hemisphere of radius $\frac{\sqrt{\lambda}}{2}$ and for the induced metric on $\mathcal{C} \approx \mathcal{D}_{22} \times (0, 1)$ one gets

$$g_c = \lambda g_2 + \frac{1}{4\lambda(1-\lambda)} (d\lambda)^2, \quad (19)$$

where g_2 is the Riemannian metric on $\mathcal{D}_{22}$. The Riemannian manifold $(\mathcal{C}, g_c)$ can be isometrically embedded into $\mathbb{R}^5$ (see the picture) by

$$j : \mathcal{C} \approx \mathcal{D}_{22} \times (0, 1) \longrightarrow \mathbb{R}^4 \times \mathbb{R}; \quad j(\varrho, \lambda) := (\sqrt{\lambda} \Phi(\varrho), f(\lambda)), \quad (20)$$

where Φ is given by (17) and the real function f by

$$f(\lambda) := \frac{1}{4} \int_{\lambda_0}^{\lambda} \sqrt{\frac{3+x}{x(1-x)}} dx. \quad (21)$$

Indeed, a simple calculation shows that the pullback of the standard metric on $\mathbb{R}^5$ via j is just g_c .

Thus, the Riemannian manifold $(\mathcal{C}, g_c)$ looks like a cone and contains arbitrarily small hemispheres as geodesically complete submanifolds, what leads to the unboundedness of the sectional curvature on $\mathcal{D}_{nn}$.

Acknowledgement

I would like to thank A. Uhlmann for helpful discussions, especially for his hint concerning the above geometric interpretation.

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