Monotone Riemannian metrics on density matrices with non-monotone scalar curvature

Attila Andai†
Department for Mathematical Analysis, Budapest University of Technology and Economics, H-1521 Budapest XI. Sztoczek u. 2, Hungary

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Abstract

The theory of monotone Riemannian metrics on the state space of a quantum system was established by Dénes Petz in 1996. In a recent paper he argued that the scalar curvature of a statistically relevant - monotone - metric can be interpreted as an average statistical uncertainty. The present paper contributes to this subject. It is reasonable to expect that states which are more mixed are less distinguishable than those which are less mixed. The manifestation of this behavior could be that for such a metric the scalar curvature has a maximum at the maximally mixed state. We show that not every monotone metric fulfills this expectation, some of them behave in a very different way. A mathematical condition is given for monotone Riemannian metrics to have a local minimum at the maximally mixed state and examples are given for such metrics.

1 INTRODUCTION

The quantum mechanical Hilbert space formalism gives a mathematical description of particles with spin of $\frac{n-1}{2}$. Concentrating on the spin part of non relativistic particles one can build a proper mathematical model in an $n$ dimensional complex Hilbert space. This is the simplest physical realization of an $n$-level quantum system. The states of an $n$-level system are identified with the set of positive semidefinite self-adjoint $n \times n$ matrices of trace 1. The states form a closed convex set in the space of matrices and its interior, the set of all strictly positive self-adjoint matrices of trace 1 becomes naturally a differentiable manifold.

The idea in mathematical statistics that a statistical or informational distance between probability measures gives rise to a Riemannian metric is due to Rao and was developed by Amari and Streater among others. Let us see how can one measure the statistical distance between the simplest probability distributions in classical case Ref. 4. Assume, that we have two probability distributions $(p_1, 1 - p_1)$ and $(p_2, 1 - p_2)$. Let us now suppose that an experimenter, in making his determination of the value $p_1$, has only $n$ trials. Because of the unavoidable statistical fluctuations

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†andaia@math.bme.hu
associated with a finite sample, the experimenter cannot know \( p_1 \) exactly. After these measurements the experimenter’s uncertainty is the size of a typical fluctuation

\[
\Delta p_1 = \sqrt{\frac{p_1(1-p_1)}{n}}.
\]

We can say that the distributions \((p_1, 1-p_1)\) and \((p_2, 1-p_2)\) are distinguishable in \( n \) trials if the regions of uncertainty do not overlap, that is, if

\[
|p_1 - p_2| \geq \Delta p_1 + \Delta p_2.
\]

Let \( k(n, p_1, p_2) \) denote the number of the probability distributions of the form \((p_i, 1-p_i)\) between \( p_1 \) and \( p_2 \) (that is \( p_1 < p_i < p_2 \)) each of which is distinguishable in \( n \) trials from its neighbors. The statistical distance between the given probability distributions is

\[
d(p_1, p_2) = \lim_{n \to \infty} \frac{k(n, p_1, p_2)}{\sqrt{n}}.
\]

From the previous equations we find that

\[
d(p_1, p_2) = \int_{p_1}^{p_2} \frac{1}{2\sqrt{p(1-p)}} \, dp = \arccos\left(\frac{\sqrt{p_1 p_2} + \sqrt{1-p_1}(1-p_2)}{2}\right).
\]

This distance function was introduced by Fisher in 1922.

The Fisher informational metric is unique in some sense (i.e., it is the only Markovian monotone distance) in the classical case Ref. 5. A family of Riemannian metrics are called monotone if they are decreasing under stochastic mappings (the exact definition is given below). These metrics play the role of Fisher metric in the quantum case. Monotone Riemannian metrics are important for information-theoretical and statistical considerations on the state space. The study of monotone metrics for parametric statistical manifolds was initiated by Chentsov and Morozova6, Petz’s classification theorem7 establishes a correspondence between monotone metrics and operator monotone \( f : [0, \infty] \to \mathbb{R} \) functions, such that \( f(x) = xf(x^{-1}) \) hold for all positive \( x \). In the simplest quantum case, dealing with \( 2 \times 2 \) matrices we can use the Stokes parametrization, that is every state \( D \) can be uniquely written in the

\[
D = \frac{1}{2}(I + x_1 \sigma_1 + x_2 \sigma_2 + x_3 \sigma_3)
\]

form, where \((\sigma_i)_{i=1,2,3}\) are the Pauli matrices and \((x_1, x_2, x_3)\) \( \in \mathbb{R}^3 \) with \( x_1^2 + x_2^2 + x_3^2 \leq 1 \). The interior of the set of states can be identified with the open unit ball in \( \mathbb{R}^3 \) by this parametrization. In this case a monotone Riemannian metric on this manifold can be written in the

\[
ds^2 = \frac{1}{1-r^2} dr^2 + \frac{r^2}{(1+r)f \left( \frac{1-r}{1+r} \right)} d\theta^2 + \frac{r^2 \sin^2 \theta}{(1+r)f \left( \frac{1-r}{1+r} \right)} d\phi^2
\]

form in polar coordinates.

There is strong a connection between the scalar curvature of these manifolds at a given state and statistical distinguishability and uncertainty of the state. If \( D_0 \) is a \( n \times n \) density matrix we call geodesic ball the set

\[
B_r(D_0) = \{ D \, n \times n \text{ density matrix : } d(D_0, D) < r \}.
\]

The volume of this ball is given by

\[
V(B_r(D_0)) = \frac{\sqrt{\pi^{n^2-1} r^{n^2-1}}}{\Gamma \left( \frac{n^2+1}{2} \right)} \left( 1 - \frac{r(D_0)}{6(n^2+1)} r^2 + O(r^4) \right)
\]
where \( r(D_0) \) is the scalar curvature at the point \( D_0 \). According to Ref. 8, the quantity \( V(B_r(D_0)) \) measures the statistical uncertainty and the scalar curvature measures the average statistical uncertainty. A general explicit formula for the scalar curvature was given by Dittmann\(^{10} \) (particular cases have been discussed in Refs. 11 and 12). There are many Riemannian metrics on the state space which are statistically relevant in different ways. The state \( A \) is more mixed than the state \( B \) if for their decreasingly ordered set of eigenvalues \((a_1, \ldots, a_n)\) and \((b_1, \ldots, b_n)\) the inequality

\[
\sum_{l=1}^{k} a_l \leq \sum_{l=1}^{k} b_l
\]

holds for every \( 1 \leq k \leq n \).

It is reasonable to expect that the most mixed states are less distinguishable than the less mixed states; for details see Refs. 13 and 14. It means mathematically that in this case the scalar curvature of a Riemann structure should have the following monotonicity property: if \( D_1 \) is more mixed than \( D_2 \) then \( r(D_2) \) should be less then \( r(D_1) \), where \( r(D) \) denotes the scalar curvature of the manifold at the state \( D \). It has been shown that the Bures metric does not have this monotonicity property for the scalar curvature and moreover it has a global minimum at the most mixed state. Actually in Ref. 9 it was proved that for the Bures metric for every \( n \times n \) density matrix \( D \) the inequality

\[
r(D) \geq \frac{(5n^2 - 4)(n^2 - 1)}{4}
\]

holds. If \( n > 3 \), equality holds iff \( D = \frac{1}{n} I \). If \( n = 2 \), then \( r(D) = 24 \). This implies that the Bures metric is (trivially) monotone for \( n = 2 \). Indeed all metrics studied thus far in two level quantum systems have monotone scalar curvature. This means that these metrics are compatible with one’s statistical view. Do all monotone metrics have this property in two level quantum system? The answer is no; in this paper we show a family of monotone metrics with non monotone scalar curvature and we give a condition for monotone metric to have a local minimum at the maximally mixed state.

2 SCALAR CURVATURE ON THE TWO LEVEL QUANTUM SYSTEMS

2.1 The setup

Let \( \mathcal{M}_n^+ \) be the space of all complex self-adjoint positive definite \( n \times n \) matrices of trace 1 and let \( \mathcal{M}_n \) be the real vector space of all self-adjoint traceless \( n \times n \) matrices. The space \( \mathcal{M}_n^+ \) can be endowed with a differentiable structure Ref. 15.

The tangent space \( T_D \) at \( D \in \mathcal{M}_n^+ \) can be identified with \( \mathcal{M}_n \). A map

\[
K : \mathcal{M}_n^+ \times \mathcal{M}_n \times \mathcal{M}_n \to \mathbb{C} \quad (D, X, Y) \mapsto K_D(X, Y)
\]

will be called a Riemannian metric if the following condition hold: For all \( D \in \mathcal{M}_n^+ \) the map

\[
K_D : \mathcal{M}_n \times \mathcal{M}_n \to \mathbb{C} \quad (X, Y) \mapsto K_D(X, Y)
\]

is a scalar product and for all \( X \in \mathcal{M}_n \) the map

\[
K,(X, X) : \mathcal{M}_n^+ \to \mathbb{C} \quad D \mapsto K_D(X, X)
\]

is smooth.
We now use differential geometrical notation to define the scalar curvature of the \((\mathcal{M}_n^+, K)\) Riemannian manifold. In this case the Riemannian metric is a
\[
K : \mathcal{M}_n^+ \to \text{LIN}(\mathcal{M}_n \times \mathcal{M}_n, \mathbb{R}) \quad D \mapsto ((X, Y) \mapsto K_D(X, Y))
\]
map, where \text{LIN}(U, V) denotes the set of linear maps from the vector space \(U\) to the vector space \(V\). The derivative of the metric \(K\) is a map
\[
dK : \mathcal{M}_n^+ \to \text{LIN}(\mathcal{M}_n, \text{LIN}(\mathcal{M}_n \times \mathcal{M}_n, \mathbb{R})) \quad D \mapsto \left(X \mapsto ((Y, Z) \mapsto dK_D(X, Y, Z))\right).
\]
At a given \(D \in \mathcal{M}_n^+\) point for given \(X, Y \in \mathcal{M}_n\) tangent vectors the map
\[
\tau_{D,X,Y} : \mathcal{M}_n \to \mathbb{R} \quad Z \mapsto \frac{1}{2}(dK_D(Y)(X, Z) + dK_D(X)(Z, Y) - dK_D(Z)(X, Y))
\]
is a linear functional. It means that there exists a unique \(V_{D,X,Y} \in \mathcal{M}_n\) tangent vector such that for all \(Z \in \mathcal{M}_n\) vector
\[
K_D(V_{D,X,Y}, Z) = \tau_{D,X,Y}(Z)
\]
holds. One can define the map
\[
\Gamma : \mathcal{M}_n^+ \to \text{LIN}(\mathcal{M}_n \times \mathcal{M}_n \times \mathcal{M}_n, \mathcal{M}_n) \quad D \mapsto ((X, Y) \mapsto V_{D,X,Y})
\]
which is called covariant differentiation. Its derivative is a map
\[
d\Gamma : \mathcal{M}_n^+ \to \text{LIN}(\mathcal{M}_n, \text{LIN}(\mathcal{M}_n \times \mathcal{M}_n \times \mathcal{M}_n, \mathcal{M}_n)) \quad D \mapsto \left(X \mapsto ((Y, Z) \mapsto d\Gamma_D(X, Y, Z))\right).
\]
The Riemann curvature tensor defined to be
\[
R : \mathcal{M}_n^+ \to \text{LIN}(\mathcal{M}_n \times \mathcal{M}_n \times \mathcal{M}_n \times \mathcal{M}_n, \mathbb{R}) \quad (D, X, Y, Z) \mapsto R_D(X, Y, Z),
\]
where
\[
R_D(X, Y, Z) = d\Gamma_D(X)(Y, Z) - d\Gamma_D(Y)(X, Z) + \Gamma_D(X, \Gamma_D(Y, Z)) - \Gamma_D(Y, \Gamma_D(X, Z)).
\]
The map
\[
\alpha : \mathcal{M}_n^+ \times \mathcal{M}_n \times \mathcal{M}_n \to \text{LIN}(\mathcal{M}_n, \mathcal{M}_n) \quad (D, X, Y) \mapsto \alpha_{D,X,Y} = (Z \mapsto R_D(Z, X, Y)),
\]
is needed to define the Ricci tensor
\[
\text{Ric} : \mathcal{M}_n^+ \to \text{LIN}(\mathcal{M}_n \times \mathcal{M}_n, \mathbb{R}) \quad D \mapsto ((X, Y) \mapsto \text{Ric}_D(X, Y)),
\]
where
\[
\text{Ric}_D(X, Y) = \text{Tr} \alpha_{D,X,Y}.
\]
At a given \(D \in \mathcal{M}_n^+\) point for given \(X \in \mathcal{M}_n\) tangent vector the map
\[
\beta_{D,X} : \mathcal{M}_n \to \mathbb{R} \quad Y \mapsto \text{Ric}_D(X, Y)
\]
is a linear functional. It means that there exists a unique \(U_{D,X} \in \mathcal{M}_n\) tangent vector such that for all \(Y \in \mathcal{M}_n\) vector
\[
K_D(U_{D,X}, Y) = \beta_{D,X}(Y)
\]
holds. From the map 
\[ \rho : \mathcal{M}_n^+ \to \text{LIN}(\mathcal{M}_n, \mathcal{M}_n) \quad D \mapsto \rho_D = \left((X) \mapsto U_{D,X} \right) \]
we get the scalar curvature of the manifold 
\[ \text{Scal} : \mathcal{M}_n^+ \to \mathbb{R} \quad D \mapsto \text{Tr} \rho_D. \]

For further differential geometry details see, for example, Ref. 16.

Let \( M_n(\mathbb{C}) \) denote the set of complex \( n \times n \) matrices and \( M_k(M_n) \) denote the set of \( k \times k \) matrices with entries \( M_n(\mathbb{C}) \). If \( T : M_n(\mathbb{C}) \to M_m(\mathbb{C}) \) is a linear map, it induces a linear map \( T^{(k)} : M_k(M_n) \to M_k(M_m) \) by 
\[ T^{(k)}([A_{ij}]) = [T(A_{ij})]. \]
The map \( T \) is called positive if it takes positive operators to positive operators. Say that \( T \) is \( k \)-positive if \( T^{(k)} \) is positive and \( T \) is completely positive if it is \( k \)-positive for all \( k \geq 1 \).

A linear mapping \( T : M_n(\mathbb{C}) \to M_m(\mathbb{C}) \) is defined to be stochastic if \( T \) is completely positive and trace preserving. For more information on completely positive and stochastic maps see Ref. 13 and 14.

Let \( (K^m)_{m \in \mathbb{N}} \) be a family of metrics, such that \( K^m \) is a Riemannian metric on \( \mathcal{M}_m^+ \) for all \( m \). This family of metrics defined to be monotone if 
\[ K^{m}_{T(D)}(T(X), T(X)) \leq K^m_B(\mathcal{D}, \mathcal{D}) \]
for every stochastic mapping \( T : M_n(\mathbb{C}) \to M_m(\mathbb{C}) \), for every \( D \in \mathcal{M}_n^+ \) and for all \( X \in \mathcal{M}_n \) and for all \( m, n \in \mathbb{N} \).

**Theorem 2.1. Petz classification theorem\textsuperscript{7}**: There exists a bijective correspondence between the monotone family of metrics \( (K^n)_{n \in \mathbb{N}} \) and operator monotone \( f : \mathbb{R}^+ \to \mathbb{R} \) functions such that \( f(x) = xf(x^{-1}) \) hold for all positive \( x \). The metric is given by 
\[ K^n_B(X, Y) = \text{Tr} \left( X \left( R^\frac{x^2}{(1+x)^2} D(L_n_D R^{-1}_n D) R^\frac{x^2}{(1+x)^2} \right)^{-1}(Y) \right) \]  
(1)
for all \( n \in \mathbb{N} \) where \( L_{n,D}(X) = DX, R_{n,D}(X) = XD \) for all \( D, X \in M_n(\mathbb{C}) \).

A Riemannian metric \( K \) is said to be monotone if there is a monotone family of metrics \( (K^m)_{m \in \mathbb{N}} \) such that \( K = K^n \) for an \( n \). We use the normalization condition for the function \( f \) in the previous theorem \( f(1) = 1 \). Here are some examples of operator monotone functions which generate monotone metrics from Refs. 17 and 18:
\[
\begin{align*}
1 + x & \quad 2x \quad x - 1 \quad 2(x-1)^2 \quad 2(x-1) \sqrt{x} \quad 2x^{\alpha+1/2} \quad \beta(1 - \beta)(x - 1)^2 \quad 2x^{\alpha} \quad (x^\beta - 1)(x^{1-\beta} - 1),
\end{align*}
\]
where \( 0 \leq \alpha \leq 1/2 \) and \( 0 < |\beta| < 1 \).

**2.2 Curvature and eigenvalues on \( \mathcal{M}_2^+ \)**

There is an explicit formula for scalar curvature in a given \( D \in \mathcal{M}_2^+ \) state using a monotone metric coming from a suitable \( f \) function defined by Eq. (1). To use that result to build up a more explicit formula to our \( \mathcal{M}_2^+ \) manifold, first introduce the Morozova-Chentsov function related to the monotone function \( f \) defined by
\[ c(x, y) := \frac{1}{y f(x/y)}, \]  
(2)
Let us denote by \( \partial_1 c(x, y) \) the partial derivative of \( c(x, y) \) with respect to its first variable. Define four new functions (as in Ref. 10)

\[
\begin{align*}
  h_1(x, y, z) &:= \frac{c(x, y) - zc(x, z)c(y, z)}{(x - z)(y - z)c(x, z)c(y, z)} \\
  h_2(x, y, z) &:= \frac{(c(x, z) - c(y, z))^2}{(x - y)^2c(x, y)c(x, z)c(y, z)} \\
  h_3(x, y, z) &:= \frac{z}{x - y} \left( \partial_1 \left( \log c(z, x) - \partial_1 \left( \log c(z, y) \right) \right) \right) \\
  h_4(x, y, z) &:= z\partial_1 \left( \log c(z, x) \right) \partial_1 \left( \log c(z, y) \right).
\end{align*}
\]

The terms like \( h_i(x, y, z) \) can be computed as

\[
\lim_{y \to x} h_i(x, y, z)
\]

limit. We will need a linear combination of these functions

\[
h(x, y, z) = h_1(x, y, z) - \frac{1}{2} h_2(x, y, z) + 2 h_3(x, y, z) - h_4(x, y, z).
\]

**Theorem 2.2.** (see Ref. 10) Let \( \sigma(D) \) be the spectrum of the state \( D \in \mathcal{M}_n^+ \). Then for the scalar curvature one has the expression

\[
r(D) = \sum_{x, y, z \in \sigma(D)} h(x, y, z) - \sum_{x \in \sigma(D)} h(x, x, x) + \frac{1}{4} \left( n^2 - 1 \right) \left( n^2 - 2 \right).
\]

**Corollary 2.1.** The scalar curvature at the state \( D \in \mathcal{M}_n^+ \) with eigenvalues \( \lambda_1, \lambda_2 \) is given by

\[
r(D) = h(\lambda_1, \lambda_1, \lambda_2) + h(\lambda_1, \lambda_2, \lambda_1) + h(\lambda_2, \lambda_1, \lambda_1) + h(\lambda_2, \lambda_2, \lambda_1) + h(\lambda_1, \lambda_2, \lambda_2) + h(\lambda_1, \lambda_2, \lambda_2) + \frac{3}{2}.
\]

**Theorem 2.3.** Let \( D \in \mathcal{M}_n^+ \) and \( a = 2\lambda_1 - 1 \) where \( \lambda_1 \) is an eigenvalue of \( D \) and assume that the monotone metric of \( \mathcal{M}_n^+ \) comes from a function \( f \). Then the scalar curvature at \( D \) is

\[
r(a) = \frac{14(a - 1) \left( f' \left( \frac{1-a}{1+a} \right) \right)^2}{(1 + a)^3} + \frac{8(1-a) f'' \left( \frac{1-a}{1+a} \right)}{(1 + a)^3} \\
+ \frac{2(1+a) f \left( \frac{1-a}{1+a} \right)}{a^2} - \frac{3a^3 + 5a^2 + 8a - 4}{2(1+a)a^2}.
\]

**Proof.** Through the computation we will use the identities \( f'(1) = \frac{1}{2} \) and \( 2f^{(3)}(1) + 3f^{(2)}(1) = 0 \) which come from the equations \( f(x) = x f(1/x) \) and \( f(1) = 1 \). It is easy to recognize that \( h_i(y, x, x) = h_i(x, y, x) \) for \( i = 1, 2, 3, 4 \). First let us note the following identities

\[
\begin{align*}
  c(x, x) &= \frac{1}{x}, & c(x, y) &= c(y, x), & c(x, y) &= tc(tx, ty), & \forall t \in \mathbb{R}^+, \\
  \partial_1 c(x, x) &= -\frac{1}{2x^2}, & \partial_1^k \partial_2 c(x, y) &= \partial_1^k \partial_2 c(y, x), & c(x, y) &= -x \partial_1 c(x, y) - y \partial_2 c(x, y)
\end{align*}
\]

which will be used through the computation.

The \( h_i(x, y, x) \) and \( h_i(x, y, x) \) like limit functions can be computed. For example:

\[
\begin{align*}
  h_1(x, y, x) &= \lim_{q \to x} h_1(x, q, y) = \lim_{q \to x} \frac{c(x, q) - yc(x, y)c(q, y)}{(x - q)(q - y)c(x, y)c(q, y)} = c(x, y) - y \left( c(x, y) \right)^2, \\
  h_4(x, y, x) &= \lim_{q \to x} h_4(x, y, q) = \lim_{q \to x} \frac{\partial_1 c(q, x) \partial_1 c(q, y) c(q, x)}{c(q, x) c(q, y)} = \frac{2 \partial_1 c(x, x) \partial_1 c(x, y) c(x, x)}{c(x, x) c(x, y)}.
\end{align*}
\]
After taking into account the identities (6) these limit functions can be simplified:

\[
\begin{align*}
    h_1(x, x, y) &= \frac{1 - xy [c(x, y)]^2}{x(x - y)^2 [c(x, y)]^2} \\
    h_1(x, y, x) &= -\frac{1}{2} \frac{c(x, y) + 2x \partial_1 c(x, y)}{(x - y)c(x, y)} \\
    h_2(x, x, y) &= x \left( \frac{\partial_1 c(x, y)}{c(x, y)} \right)^2 \\
    h_2(x, y, x) &= \frac{1}{x} \left( \frac{1 - xc(x, y)}{(x - y)c(x, y)} \right)^2 \\
    h_3(x, x, y) &= -\frac{y^2 c(x, y) [\partial_1 c(y, x)]^2}{c(x, y)^2} + 2yc(x, y)\partial_1 c(y, x) + xy\partial_1 c(x, y)\partial_1 c(y, x) \\
    h_3(x, y, x) &= -\frac{c(x, y) + 2x \partial_1 c(x, y)}{2(x - y)c(x - y)} \\
    h_4(x, x, y) &= y \left( \frac{\partial_1 c(y, x)}{c(x, y)} \right)^2 \\
    h_4(x, y, x) &= -\frac{1}{2} \frac{\partial_1 c(x, y)}{c(x, y)}.
\end{align*}
\]

Introducing the suitable sum-functions for \( h_i (i = 1, 2, 3, 4) \)

\[
sh_i(x, y) := h_i(x, x, y) + 2h_i(x, y, x) + h_i(y, y, x) + 2h_i(y, x, y)
\]

we get that

\[
\begin{align*}
    sh_1(x, y) &= \frac{(x + y)(1 - xy [c(x, y)]^2)}{xy(x - y)^2 [c(x, y)]^2} - \frac{4x \partial_1 c(x, y) + 2c(x, y)}{(x - y)c(x, y)} \\
    sh_2(x, y) &= \frac{x [\partial_1 c(x, y)]^2 + y [\partial_1 c(y, x)]^2}{[c(x, y)]^2} + 2 \left( \frac{x + y + xy(x + y)}{xy(x - y)^2 [c(x, y)]^2} - \frac{4yc(x, y)}{xy(x - y)^2 [c(x, y)]^2} \right) \\
    sh_3(x, y) &= \frac{(x + y)(c(x, y) [\partial_1 c(x, y)]^2 - \partial_1 c(x, y)\partial_1 c(y, x))}{[c(x, y)]^2} - \frac{4x \partial_1 c(x, y) + 2c(x, y)}{(x - y)c(x, y)} \\
    sh_4(x, y) &= \frac{x [\partial_1 c(x, y)]^2 + y [\partial_1 c(y, x)]^2}{[c(x, y)]^2} - \frac{\partial_1 c(x, y) + \partial_1 c(y, x)}{c(x, y)}.
\end{align*}
\]
These sum-functions can be expressed by the operator monotone function $f(x)$:

$$sh_1(x, y) = \frac{1}{(x - y)^2} \left( \frac{y(x + y)}{x} [f(x/y)]^2 + y - 3x + \frac{4x(x - y)}{y} \frac{f'(x/y)}{f(x/y)} \right)$$

$$sh_2(x, y) = \frac{x}{y^2} \left( \frac{f'(x/y)}{f(x/y)} \right)^2 + \frac{y^3}{x^4} \left( \frac{f(x/y)f'(y/x)}{[f(y/x)]^2} \right)^2 + \frac{2y(x + y)}{x(x - y)^2} [f(x/y)]^2$$

$$- \frac{8y}{(x - y)^2} f(x/y) + \frac{2(x + y)}{(x - y)^2}$$

$$sh_3(x, y) = \frac{-2x(x + y)}{y^3} \left( \frac{f'(x/y)}{f(x/y)} \right)^2 - \frac{(x + y)}{x^2} \frac{f'(x/y)f'(y/x)}{[f(x/y)]^2} + \frac{2(x^2 + 2xy - y^2)}{y^2(x - y)^2} \frac{f'(x/y)}{f(x/y)}$$

$$+ \frac{x(x + y)}{y^3} \frac{f''(x/y)}{f(x/y)} - \frac{2}{x - y}$$

$$sh_4(x, y) = \frac{x}{y^2} \left( \frac{f'(x/y)}{f(x/y)} \right)^2 + \frac{y^3}{x^4} \left( \frac{f(x/y)f'(y/x)}{[f(y/x)]^2} \right)^2 + \frac{1}{y} \frac{f'(x/y)}{f(x/y)} + \frac{y}{x^2} \frac{f(x/y)f'(y/x)}{[f(y/x)]^2}.$$

The scalar curvature is given by the linear combination of the functions $sh_i(x, y)$:

$$r(D) = sh_1(x, y) - \frac{1}{2} sh_2(x, y) + 2sh_3(x, y) - sh_4(x, y).$$

The result is the following:

$$r(D) = 2\frac{yf(x/y) - 1}{(x - y)^2} + 6 \frac{xf'(x/y) - yf(x/y)}{y(x - y)f(x/y)} - \frac{x(8 + 3y)}{2} \frac{(f'(x/y))^2}{y^3} - \frac{3y}{2x^2} \left( \frac{f'(y/x)}{f(y/x)} \right)^2$$

$$+ \frac{(3 + x)f''(x/y)}{y^2f(x/y)} + 2 \frac{xf''(x/y)}{y^2f(x/y)} - \frac{f'(y/x)^2}{xf(y/x)} - 2 \frac{f'(x/y)f'(y/x)}{x^2 [f(y/x)]^2} + \frac{3}{2}.$$ (11)

The eigenvalues of $D$ can be expressed by $a$ as

$$\lambda_1 = \frac{1 + a}{2}, \quad \lambda_2 = \frac{1 - a}{2}.$$ Substituting these into the previous formula and collecting the terms we get Eq. (10). 

Since the scalar curvature formula Eq. (9) is a rather complicated one it is worth mentioning that there is a completely different proof (which is based on the subsection 2.1) for Theorem 2.3.

**Proof 2.** There is another parametrization of the state as it was mentioned in the introduction. Let us use the following parametrization for the $2 \times 2$ density matrices:

$$\frac{1}{2} \begin{pmatrix} 1 + r \cos \theta & (r \sin \theta \cos \phi) + i(r \sin \theta \sin \phi) \\ (r \sin \theta \cos \phi) - i(r \sin \theta \sin \phi) & 1 - r \cos \theta \end{pmatrix},$$

where $(r, \theta, \phi)$ denote the spherical coordinates, but now $0 \leq r < 1$. In this case the metric is:

$$ds^2 = \frac{1}{1 - r^2} dr^2 + \frac{r^2}{(1 + r) f \left(\frac{1 + r}{r}\right)} d\theta^2 + \frac{r^2 \sin^2 \theta}{(1 + r) f \left(\frac{1 + r}{r}\right)} d\phi^2.$$
Let us use the order \((r, \theta, \phi)\) for the coordinates. (For example \(\partial_2 t(r, \theta, \phi)\) denotes the partial derivative of \(t(r, \theta, \phi)\) with respect to \(\theta\).) The \(g_{ik}\) metric can be written in the form \(g_{ik} = \delta_{ik} \alpha_i (r, \theta, \phi)\).

The identities
\[
\partial_2 \alpha_1 = \partial_3 \alpha_1 = 0, \quad \partial_2 \alpha_2 = \partial_3 \alpha_2 = 0, \quad \partial_3 \alpha_3 = 0
\]
will simplify the computation. The Christoffel symbols of the second kind for this Riemannian manifold is
\[
\Gamma_{ij}^m = \sum_{k=1}^{3} \frac{1}{2} g^{km} (\partial_i g_{jk} + \partial_j g_{ik} - \partial_k g_{ij}),
\]
where \(g^{ij}\) denotes the inverse matrix of \(g_{ij}\). Since \(\Gamma_{ij}^m = \Gamma_{ji}^m\), there are only seven nonzero independent Christoffel symbols in this case
\[
\Gamma_{1,1}^1 = \frac{r}{1 - r^2}, \quad \Gamma_{2,2}^2 = \frac{-r(1-r)}{2(1+r)^2 f(c(r))} \left( r^2 + 3r + 2 + 2r \frac{f'(c(r))}{f(c(r))} \right), \quad \Gamma_{3,3}^3 = \sin^2 \theta \Gamma_{2,2}^2,
\]
\[
\Gamma_{1,2}^1 = \frac{-f(c(r))}{r^2(1-r)} \Gamma_{2,2}^2, \quad \Gamma_{3,3}^2 = -\sin \theta \cos \theta, \quad \Gamma_{1,3}^2 = \Gamma_{1,2}^1, \quad \Gamma_{2,3}^2 = \frac{\cos \theta}{\sin \theta}.
\]

The Riemannian curvature tensor is given by the equation
\[
R_{ijkl} = \sum_{n=1}^{3} \sum_{m=1}^{3} g_{in} \left( \partial_j \Gamma_{mk}^n - \partial_j \Gamma_{mn}^k + \sum_{m=1}^{3} (\Gamma_{mk}^n \Gamma_{im}^m - \Gamma_{mk}^m \Gamma_{im}^n) \right).
\]

Since \(R_{ijkl} = -R_{jikl}, R_{i,jkl} = -R_{ijlk}\) and \(R_{ijkl} = R_{kl}ij\), there are only three nonzero independent element of the curvature tensor:
\[
R_{1212} = \frac{-r}{(1+r)^4(1-r^2)f(c(r))} \left( 2r(1-r) \frac{f''(c(r))}{f(c(r))} - 3r(1-r) \left( \frac{f'(c(r))}{f(c(r))} \right)^2 \right) + (1+r)(3r - 2) \frac{f'(c(r))}{f(c(r))} + \frac{(r^2 + r + 4)(1+r)^2}{4}
\]
\[
R_{1313} = \sin^2 \theta \ R_{1212}
\]
\[
R_{2323} = \frac{r^2(1-r) \sin^2 \theta}{(1+r)^4 [f(c(r))]^2} \left( r(r+2) \frac{f'(c(r))}{f(c(r))} + \frac{r^2}{1+r} \left( \frac{f'(c(r))}{f(c(r))} \right)^2 - \frac{(1+r)^3}{1-r} \frac{f(c(r))}{f(c(r))} \right) + \frac{(1+r)(2+r)^2}{4}
\]

The Ricci curvature tensor is
\[
\text{Ric}_{ij} = \sum_{k,l=1}^{3} g^{kl} R_{iklj}.
\]
It is symmetric $R_{ij} = R_{ji}$, and it has three nonzero elements:

$$R_{1,1} = \frac{1}{(1+r)^4} \left( 4 \frac{f''(c(r))}{f(c(r))} - 6 \left( \frac{f'(c(r))}{f(c(r))} \right)^2 + \frac{2(1+r)(3r-2)}{1-r} \frac{f'(c(r))}{f(c(r))} \right)$$

$$+ \frac{(r^2 + r + 4)(1+r)^2}{2r(1-r)}$$

$$R_{2,2} = \frac{r^2(1-r)}{(1+r)^4 f(c(r))} \left( 2 \frac{f''(c(r))}{f(c(r))} - 4 \left( \frac{f'(c(r))}{f(c(r))} \right)^2 + \frac{(1+r)(r^2 + 4r - 4)}{r(1-r)} \frac{f'(c(r))}{f(c(r))} \right)$$

$$+ \frac{(1+r)^4}{r^2(1-r)} f(c(r)) + \frac{(r^3 + 2r^2 + 2r - 2)(1+r)^2}{2r^2(1-r)}$$

$$R_{3,3} = \sin^2 \theta \ R_{2,2}.$$  

The scalar curvature at point $D$ is

$$r(D) = \sum_{i,j=1}^{3} g^{ij} R_{ij}.$$  

Computing $r(D)$ we get Eq. (18). The state $D$ is maximally mixed if its eigenvalues are equal, in this case $a = 0$. So the scalar curvature has local minimum or maximum at the maximally mixed state if and only if the function $r(a)$ has local minimum or maximum at the origin.

### 2.3 Curvature formula at the origin and Radon measures

To find an operator monotone function $f$ such that the scalar curvature has local minimum at the origin we start from the following representation theorem in Ref. 19.

The map $\mu \mapsto f$ defined by

$$f(x) = \int_{0}^{\infty} \frac{x(1+t)}{x+t} d\mu(t) \quad \text{for} \quad x > 0$$

establishes an affine isomorphism from the class of positive Radon measures $[0, \infty]$ onto the class of operator monotone functions.

We use a modified version of the previous theorem Ref. 20.

**Theorem 2.4.** The map $\mu \mapsto f$, defined by

$$f(x) = \int_{0}^{1} \frac{x}{(1-t)x+t} d\mu(t), \quad \text{for} \quad x > 0,$$

establishes a bijection between the class of positive Radon measures on $[0, 1]$ and the class of operator monotone functions.

From this representation we get that

$$xf(x^{-1}) = \int_{0}^{1} \frac{x}{(1-t)x+t} d\mu(t) = \int_{0}^{1} \frac{x}{(1-t)x+t} d\mu(1-t).$$
Thus \( f(x) = xf(x^{-1}) \) holds iff \( \mu([0,t]) = \mu([1-t,1]) \) for all \( t \in [0,1] \) and the \( f(1) = 1 \) normalization means that \( \mu([0,1]) = 1 \). Let \( T \) denote the set of all positive Radon measures on the \([0,1] \) interval such that \( \mu(X) = \mu(1-X) \) for every measurable \( X \) subset of \([0,1] \) and \( \mu([0,1]) = 1 \). Theorem 2.1 and 2.4 imply that there is bijective correspondence between monotone metrics and \( T \).

## 3 SCALAR CURVATURE

### 3.1 Scalar curvatures with local minimum at the origin

For detailed verification of Theorem 3.1 and 3.3 the Maple program was used. The Maple worksheet, containing these proofs is available at Ref. 21.

**Theorem 3.1.** The series expansion of \( r(a) \) at the origin leads to the

\[
 r(a) = (6 + 36f''(1)) + a^2 \left( \frac{100}{3}f^{(4)}(1) - 140f''(1) - 120f'''(1)^2 \right) + a^4 \left( 352f''(1)^3 \right) + O(a^6)
\]

Proof. From Eq. 15 one may expect that the \( 1/a \) and \( 1/a^2 \) type divergences occur in this expansion but the behavior derivatives of \( f \) not allow this. It is obvious that \( r(a) = r(-a) \) from symmetric reasons (not from the formula!) this means that the coefficient of \( a^{2n+1} \) will be zero for all \( n \in \mathbb{N} \). We proof this series expansion only up to the order \( O(a^4) \) because the coefficient of \( a^4 \) can be derived in a similar way, but it needs more complicated formulas. Through the computation we will use the identities

\[
 f'(1) = \frac{1}{2}, \quad f''(1) = \frac{3}{2}f'(1), \quad f'''(1) = -\frac{15f^{(4)}(1) + 60f''(1) + 60f''(1)^3}{2}
\]

which come from the equations \( f(x) = xf(1/x) \) and \( f(1) = 1 \). We consider the scalar curvature as a sum of five functions according to the Eq. 16. The series expansion of the summands can be computed in elementary way, but the intermediate formulas are rather complicated. The series expansions of the five summands from Eq. 16 after simplifications are the following.

1st: \( -\frac{7}{2} + 7 \left( 4f''(1) + 1 \right) a - 7 \left( 8f''(1)^2 + 4f''(1) + 1 \right) a^2 \)

2nd: \( -6 \cdot \frac{1}{a} + (24f''(1) + 13) - (28f''(1) + 12) a + (16f^{(4)}(1) - 48f''(1)^2 - 52f''(1) + 12) a^2 \)

3rd: \( 8f''(1) + (16f^{(4)}(1) - 16f''(1)^2 - 56f''(1)) a^2 \)

4th: \( 2 \cdot \frac{1}{a^2} + 4f''(1) + (\frac{4}{3}f^{(4)}(1) - 4f''(1)) a^2 \)

5th: \( -2 \cdot \frac{1}{a^3} + 6 \cdot \frac{1}{a} - 5 + 5 a - 5 a^2 \)

The sum of these expansions leads to Eq. (5) in this theorem.

Combining Eqs. 19 and 20 we conclude that the scalar curvature has local minimum at the origin if

\[
 12 \left( \int_0^1 t(1-t) \, d\mu(t) \right)^2 - \int_0^1 t(t-1)(20t^2 - 40t + 13) \, d\mu(t) < 0
\]

(21)
holds for a \( \mu \in T \). The scalar curvature at the origin is given by

\[
6 + 72 \int_0^1 (t^2 - t) \, d\mu(t).
\]

It has maximum when \( \mu = (1/2)\delta_0 + (1/2)\delta_1 \), the corresponding operator monotone function is \( f(x) = \frac{1}{x+1} \) and then \( r(0) = 6 \). It has minimum when \( \mu = \delta_{1/2} \), the corresponding operator monotone function is \( f(x) = \frac{2x}{1+x} \) and then \( r(0) = -12 \).

The measure \( \mu \in T \) can be transformed into a probability measure \( \mu' \) on the \([0,1]\) interval such that:

\[
\int_0^1 t(1-t) \, d\mu(t) = \frac{1}{8} \int_0^1 x \, d\mu'(x)
\]

because the \( 4t(1-t) \) function maps the \( 2\mu|_{[0,1/2]} \) measure into a probability measure on \([0,1]\). If \( \lambda \) denotes the Lebesgue-measure and \( \mu(t)|_{[0,1/2]} = \rho(t) \, d\lambda(t) + \sum a_i \delta_{p_i} \), then

\[
\mu'(x) = \frac{1}{2} \rho \left( \frac{1-\sqrt{1-x}}{x} \right) \frac{1}{\sqrt{1-x}} \, d\lambda(x) + \sum 2a_i \delta_{4p_i(1-p_i)}.
\]

There is one to one correspondence between probability measures on \([0,1]\) and \( T \). Let \( m_\mu \) denote the expectation \( \sigma_\mu^2 \) the variance and \( E_{n,\mu} \) the \( n \)-th momentum of the \( \mu' \) measure. Using Eq. (19) and the previous notation one can check the following equalities

\[
f''(1) = -\frac{m_\mu}{2} \quad f^{(4)}(1) = -3m_\mu + \frac{3}{2} E_{2,\mu} \quad f^{(6)}(1) = -90m_\mu - \frac{45}{4} E_{3,\mu} + 90E_{2,\mu}
\]

Substituting this into the approximation Eq. (20) one get the following theorem.

**Theorem 3.2.** If for a measure \( \mu \in T \) the inequality

\[
m_\mu(3 - 2m_\mu) < 5\sigma_\mu^2
\]

holds or if

\[
m_\mu(3 - 2m_\mu) = 5\sigma_\mu^2 \quad \text{and} \quad -44m_\mu^3 + 70m_\mu^2 + 114m_\mu < 98E_{3,\mu}
\]

then the scalar curvature of the metric induced by the measure \( \mu \) by the Eq. (19) has local minimum at the origin.

We give examples for monotone metrics which satisfies the previous conditions so the scalar curvature of them has local minimum at the maximally mixed state.

**Theorem 3.3.** Let

\[
\frac{7 - \sqrt{7}}{14} < p \leq \frac{1}{2}
\]

and

\[
h(p) = \frac{\sqrt{14p^2 - 14p + 4 + \sqrt{-64p^4 + 1280p^3 - 880p^2 + 240p + 9}}}{2\sqrt{7}}
\]

(22)

and \( 0 \leq q < \frac{1}{2} - h(p) \). Then the scalar curvature of the \( \mathcal{M}_2^+ \) manifold coming from the operator monotone function

\[
f(x) = \frac{x}{4} \left( \frac{1}{px + 1 - p} + \frac{1}{(1-p)x + p} + \frac{1}{qx + 1 - q} + \frac{1}{(1-q)x + q} \right)
\]

(23)

has local minimum at the origin.
Proof. First one can try to find a $\mu \in T$ measure such that Eq. (21) holds in

$$\mu_p = \frac{1}{2}\delta_p + \frac{1}{2}\delta_{1-p}$$

form where $\delta_p$ is a Dirac-measure. Let

$$t_\mu := 12 \left( \int_0^1 t(1-t) \, d\mu(t) \right)^2 - \int_0^1 t(t-1)(20t^2 - 40t + 13) \, d\mu(t)$$

and $t(p) = t_{\mu_p}$. We get that

$$t(p) = p(1-p)(8p^2 - 8p + 3).$$

For all $p \in [0, 1/2]$ we have $t(p) > 0$. This means that the scalar curvature has local maximum at the origin for all $\mu_p$ measures.

Let $p \in [0, 1/2], q \in [p, 1/2]$ and

$$\mu_{p,q} = \frac{1}{4}\delta_p + \frac{1}{4}\delta_q + \frac{1}{4}\delta_{1-p} + \frac{1}{4}\delta_{1-q}.$$  \hspace{1cm} (26)

Let $t(p, q) = t_{\mu_{p,q}}$ then

$$t(p, q) = -7(p^4 + q^4) + 14(p^3 + q^3) - 6pq(p + q - pq - 1) - \frac{17}{2}(p^2 + q^2) + \frac{3}{2}(p + q).$$  \hspace{1cm} (27)

After substituting into Eq. (27) the

$$p = \frac{v + \sqrt{v^2 - 4u}}{2} \quad q = \frac{v - \sqrt{v^2 - 4u}}{2}$$

formulas one derives that

$$t(u, v) = -8u^2 + (28v^2 - 48v + 23)u - \left(7v^4 - 14v^3 + \frac{17}{2}v^2 - \frac{3}{2}v\right).$$  \hspace{1cm} (29)

The equation $t(u, v) = 0$ has two solutions for a given $v$. Taking into account that $u = pq$ we get the condition $0 < u < \frac{1}{4}$. The only solution of the equation $t(u, v) = 0$ which fulfills this condition is

$$u(v) = \frac{7}{4}v^2 - 3v + \frac{23}{16} - \frac{1}{16}\sqrt{560v^4 - 2240v^3 + 3320v^2 - 2160v + 529}. \hspace{1cm} (30)$$

If the parameter $p$ is given then $q$ can be computed from the equation $u(p + q) = pq$. There are four solutions for $q$ but only one of them is admissible

$$q(p) = \frac{1}{2} - \frac{1}{14}\sqrt{84p^2 - 84p + 28 + 7\sqrt{-640p^4 + 1280p^3 - 880p^2 + 240p + 9}} \hspace{1cm} (31)$$

because of the conditions for $q$. This equation gives positive parameter $q$ if

$$\frac{7 - \sqrt{7}}{14} < p \leq \frac{1}{2}.$$  

One can check that if $0 < q < q(p)$ then the function $t(p, q)$ is negative. Then we use Eq. (10) defining a desired $f(z)$ operator monotone function from the $\mu_{p,q}$ measures.
If we choose $\frac{7 - \sqrt{7}}{14} < p \leq \frac{1}{2}$ arbitrary and $q = 0$ in the previous theorem then we get, that the scalar curvature coming from the operator monotone function

$$f(x) = \frac{x}{4} \left( \frac{1}{(1-p)x + p} + \frac{1}{px + 1 - p} + \frac{1}{x} + 1 \right)$$

has local minimum at the origin. In this case series expansion of the scalar curvature at the origin is

$$r(a) = \left( \frac{9}{2} - 36p(1-p) \right) - 20p(1-p)(14p^2 - 14p + 3) \cdot a^2 + O(a^4).$$

One can prove that the minimum at the origin is not only local but global for these functions. The greatest value of the scalar curvature in this case is

$$r(1) = \frac{7}{2} + \frac{1}{p(1-p)}.$$

Here some other examples for operator monotone functions, such that the scalar curvature derived from them has local, but not global minimum at the maximally mixed state.

$$f(x) = \frac{x}{4} \left( \frac{4}{x + 1} + \frac{50}{x + 49} + \frac{50}{49x + 1} \right), \quad f(x) = \frac{250x}{999x + 1} + \frac{250x}{x + 999} + \frac{x}{x + 1}.$$

Numerical computations suggest that the scalar curvature of the Riemannian metric of a three level quantum system induced by the second function has local minimum at the maximally mixed state.

### 4 CONCLUSIONS

The Riemannian metrics so far studied on the manifold $M_n^+$ come from special operator monotone functions according to Theorem 2.1. The metric carries all differential geometrical properties of the manifold, this means that from a suitable function $f$ one can derive all geometrical quantities of the manifold. One of the basic phenomenological problem is to give physical interpretation of differential geometrical quantities.

One can expect that the greatest statistical uncertainty should belong to the most mixed states. This expectation means that the scalar curvature of a Riemannian metrics should have a global maximum at the maximally mixed state. We gave several examples for suitable operator monotone functions such that the derived scalar curvatures do not fulfill this expectations and have even a local minimum at the maximally mixed state.

The Kubo-Mori (or Bogoliubov) metric comes from the function $f(x) = \frac{e^{-1}}{\log x}$. This is one of the statistically most relevant metrics. It was conjectured in Ref. 17 that the scalar curvature of this metric is monotone in the following sense. If $D_1, D_2 \in M_n^+$ and $D_1$ is more mixed than $D_2$ then $r(D_1) \geq r(D_2)$.

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