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The scalar curvature of the Bures metric on the space of density matrices

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Abstract

The Riemannian Bures metric on the space of (normalized) complex positive matrices is used for parameter estimation of mixed quantum states based on repeated measurements just as the Fisher information in classical statistics. It appears also in the concept of purifications of mixed states in quantum physics. Therefore, and also for mathematical reasons, it is natural to ask for curvature properties of this Riemannian metric. Here we determine its scalar curvature and Ricci tensor and prove a lower bound for the curvature on the submanifold of trace-1 matrices. This bound is achieved for the maximally mixed state, a further hint for the statistical meaning of the scalar curvature. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

Let $\mathcal{D}$ denote the space of complex positive $n \times n$-matrices for a fixed n and $\mathcal{D}^1$ the submanifold of trace-1 matrices representing nondegenerate mixed states of an n-dimensional quantum system. The tangent space at $\varrho \in \mathcal{D}$ (resp. $\mathcal{D}^1$) consists of all Hermitian (traceless) matrices. These manifolds carry the so-called Riemannian Bures metric g defined by

$$g_\varrho(X, Y) = \tfrac{1}{2}\mathrm{Tr}\, XG, \quad X, Y \in \mathrm{T}_\varrho\mathcal{D},$$

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where G is the (unique, by the Sylvester–Rosenblum theorem, see [2]) solution of $\varrho G + G\varrho = Y$. It should be mentioned that g is also well defined on manifolds of all $\varrho \geq 0$ of fixed rank, but we will deal only with the maximal rank. This Riemannian metric was introduced by Uhlmann [17–19] in generalizing the Berry phase to mixed states. He was led to this metric by asking for curves on minimal length purifying a given path of densities. Later on this metric appeared also in other contexts, see e.g. [3,14].

The restriction of g to the manifold of trace-1 diagonal matrices, i.e. to the manifold of all probability distributions on an n-point set, is (up to the factor 1/4) just the Fisher metric known from classical statistics, see e.g. [1,10]. Similarly to this case, the Bures metric is related to the statistical distance of quantum states, see [3,4]. Roughly speaking, both metrics give a lower bound for the variance of an optimal parameter estimator. Thus, the Bures metric generalizes the classical Fisher information to the quantum case. Among other generalization, namely the so-called monotone metrics (i.e. metrics decreasing under stochastic mappings) [14], the Bures metric is minimal, and it seems to play a distinguished role also for other reasons, see [7,9]. Partial results concerning the curvature of the Bogoliubov metric, another monotone metric, were obtained in [11].

Several authors, e.g. [13,16], suggested that the scalar curvature has a quantum statistical meaning as a measure of local distinguishability of states in the sense that regions of small curvature require many measurements for distinguishing between neighboring states. But this is still in progress, and up to now, no statistical equation or estimation involving the scalar curvature seems to be available. However, we show that the scalar curvature is minimal for the maximally mixed state $(1/n)\mathbf{1}$ and that it diverges nearby pure states, further hints for the suggested statistical meaning.

We determine here the Ricci tensor and the scalar curvature (Propositions 2 and 3) completing the list of basic local curvature quantities of the Bures metric.

Notation. The eigenvalues of a positive matrix ϱ are denoted by λ_i. Thus, if we assume ϱ to be diagonal, then $\varrho = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Bold letters are used for operators acting on matrices. They will depend on ϱ, so that they actually represent fields of operators called by several authors as superoperators. However, we frequently suppress this dependence for brevity of notation similarly to vector field and other quantities. In particular, $\mathbf{L}_\varrho$ and $\mathbf{R}_\varrho$ denote the operators of left and right multiplication by ϱ and $1/(\mathbf{L} + \mathbf{R})$ is the inverse operator of $\mathbf{L} + \mathbf{R}$ (denoted by $\mathcal{R}_{\hat{\rho}}^{-1}$ in [3]). This operator appears in many of the following formulae and is a serious obstruction for using coordinates in handling the Bures metric which now reads

$$g = \frac{1}{2}\,\mathrm{Tr}\,\mathrm{d}\varrho \frac{1}{\mathbf{L} + \mathbf{R}}(\mathrm{d}\varrho). \tag{1}$$

However, from the theory of matrix equations [2,15], some explicit formulae for this operator and the metric can be derived [8]. Vector fields $X, Y, \ldots$, on $\mathcal{D}$ resp. $\mathcal{D}^1$, we regard as functions $\varrho \mapsto X_\varrho$ with Hermitian (traceless for $\mathcal{D}^1$) matrix values. Quantities with superscript 1 will always refer to $\mathcal{D}^1$.

2. Ricci tensor and scalar curvature

The following calculations are based on results which appeared as a brief communication in [6]. Proofs and more details can be found in [5]. In particular, we obtained the following proposition.

Proposition 1. *The Riemannian curvature tensor field of the Bures metric on $\mathcal{D}$ resp. $\mathcal{D}^1$ is given by*

$$\begin{aligned}\mathcal{R}(W,Z,X,Y) &= 2g\left(\mathrm{i}\mathbf{LR}\left[\frac{1}{\mathbf{L}+\mathbf{R}}X,\frac{1}{\mathbf{L}+\mathbf{R}}Y\right],\mathrm{i}\left[\frac{1}{\mathbf{L}+\mathbf{R}}W,\frac{1}{\mathbf{L}+\mathbf{R}}Z\right]\right)\\ &\quad+g\left(\mathrm{i}\mathbf{LR}\left[\frac{1}{\mathbf{L}+\mathbf{R}}Z,\frac{1}{\mathbf{L}+\mathbf{R}}Y\right],\mathrm{i}\left[\frac{1}{\mathbf{L}+\mathbf{R}}W,\frac{1}{\mathbf{L}+\mathbf{R}}X\right]\right)\\ &\quad-g\left(\mathrm{i}\mathbf{LR}\left[\frac{1}{\mathbf{L}+\mathbf{R}}Z,\frac{1}{\mathbf{L}+\mathbf{R}}X\right],\mathrm{i}\left[\frac{1}{\mathbf{L}+\mathbf{R}}W,\frac{1}{\mathbf{L}+\mathbf{R}}Y\right]\right),\\ \mathcal{R}^1(W,Z,X,Y) &= \mathcal{R}(W,Z,X,Y)+g(Y,Z)\,g(X,W)-g(X,Z)\,g(Y,W),\end{aligned}$$

where the commutator is pointwise the usual matrix commutator, $[X,Y]_\varrho := X_\varrho Y_\varrho - Y_\varrho X_\varrho$.

We mention that for $n=2$ the Riemannian manifold $(\mathcal{D}^1, g)$ is isometric to an open half 3-sphere of radius 1/2 [19]. The geometry for $n>2$ is much more complicated, e.g. $\mathcal{D}^1$ is not locally symmetric [5].

Now we first determine the curvature mapping, which we denote in accordance with [12] also by $\mathcal{R}$. It is given by $g(\mathcal{R}(X,Y)Z, W) = \mathcal{R}(W,Z,X,Y)$ and we have to separate W in the above equations as a single argument of g. We will treat simultaneously the normalized and the unnormalized case including in brackets additional terms corresponding to the normalized case. Using the definition of g and the self-adjointness of $\mathbf{L}$ and $\mathbf{R}$ w.r.t. the Hilbert–Schmidt product, we find after a straightforward calculation:

$$\begin{aligned}\mathcal{R}^{(1)}(X,Y)Z &= 2\left[\frac{1}{\mathbf{L}+\mathbf{R}}Z,\frac{\mathbf{LR}}{\mathbf{L}+\mathbf{R}}\left[\frac{1}{\mathbf{L}+\mathbf{R}}Y,\frac{1}{\mathbf{L}+\mathbf{R}}X\right]\right]\\ &\quad+\left[\frac{1}{\mathbf{L}+\mathbf{R}}X,\frac{\mathbf{LR}}{\mathbf{L}+\mathbf{R}}\left[\frac{1}{\mathbf{L}+\mathbf{R}}Y,\frac{1}{\mathbf{L}+\mathbf{R}}Z\right]\right]\\ &\quad+\left[\frac{1}{\mathbf{L}+\mathbf{R}}Y,\frac{\mathbf{LR}}{\mathbf{L}+\mathbf{R}}\left[\frac{1}{\mathbf{L}+\mathbf{R}}Z,\frac{1}{\mathbf{L}+\mathbf{R}}X\right]\right]\\ &\quad+(g(Y,Z)X-g(X,Z)Y).\end{aligned}$$

In order to find the Ricci tensor:

$$\mathrm{Ricci}(Y,Z) := \mathbf{Tr}\,\{X\mapsto \mathcal{R}(X,Y)Z\},$$

we eliminate the argument X in $\mathcal{R}^{(1)}(X, Y)Z$,

$$\begin{aligned}\mathrm{Ricci}^{(1)}(Y, Z) = \mathbf{Tr}\bigg\{&2\mathbf{ad}\frac{1}{\mathbf{L}+\mathbf{R}}Z \circ \frac{\mathbf{LR}}{\mathbf{L}+\mathbf{R}} \circ \mathbf{ad}\frac{1}{L+R}Y \circ \frac{1}{\mathbf{L}+\mathbf{R}} \\ &+ \mathbf{ad}\frac{\mathbf{LR}}{\mathbf{L}+\mathbf{R}}\left[\frac{1}{\mathbf{L}+\mathbf{R}}Z, \frac{1}{\mathbf{L}+\mathbf{R}}Y\right] \circ \frac{1}{\mathbf{L}+\mathbf{R}} \\ &+ \mathbf{ad}\frac{1}{\mathbf{L}+\mathbf{R}}Y \circ \frac{\mathbf{LR}}{\mathbf{L}+\mathbf{R}} \circ \mathbf{ad}\frac{1}{\mathbf{L}+\mathbf{R}}Z \circ \frac{1}{\mathbf{L}+\mathbf{R}}\bigg\} \\ &+ ((n^2-2)g(Y, Z)). \end{aligned} \tag{2}$$

This equation requires some comments. $\mathbf{ad}V$ denotes the usual commutation operator, $\mathbf{ad}V(W) := [V, W]$, and we have to do with compositions of operators. The trace should be regarded, originally, as the trace of operators acting on the real tangent spaces, that means on the space of Hermitian matrices, traceless for Ricci[1]. Clearly, the additional term in the normalized case is the trace of $X \mapsto g(Y, Z)X - g(X, Z)Y$ on the (n^2-1)-dimensional tangent space. For the common term there is no need for distinguishing between the spaces, since the normal direction generated by ϱ does not give any contribution to the trace of $X \mapsto \mathcal{R}(X, Y)Z$. Indeed, $\mathcal{R}(X, Y)Z$ vanishes for $X_\varrho := \varrho$, because $(\mathbf{L}+\mathbf{R})^{-1}(\varrho) = \frac{1}{2}\mathbf{1}$. Finally, complexification does not change the trace. Therefore, we can regard (2) as the trace of a complex operator acting on all complex $n \times n$-matrices.

To continue the determination of the Ricci tensor we notice that the second term in (2) vanishes, because $\mathbf{Tr}\,\mathbf{ad}V \circ (\mathbf{L}+\mathbf{R})^{-1} = 0$ for all V. Indeed, we can suppose that ϱ is diagonal. Then the standard matrices are eigenvectors of $\mathbf{L}$ and $\mathbf{R}$,

$$f(L, R)(\mathrm{E}_{ij}) = f(\lambda_i, \lambda_j)\,\mathrm{E}_{ij}$$

for any function f, and we get

$$\mathbf{Tr}\,\mathbf{ad}V \circ \frac{1}{\mathbf{L}+\mathbf{R}} = \sum_{i,j}\left\langle \mathrm{E}_{ij}, \left[V, \frac{1}{\mathbf{L}+\mathbf{R}}\mathrm{E}_{ij}\right]\right\rangle = \sum_{i,j}\frac{1}{\lambda_i+\lambda_j}\langle \mathrm{E}_{ii} - \mathrm{E}_{jj}, V\rangle = 0.$$

What remains in (2) has the shape of $2(Z, Y) + (Y, Z) + ((n^2-2)g(Y, Z))$ and the symmetry of the Ricci tensor implies the symmetry of the bilinear form $(\ ,\ )$. Hence (2) reduces to

$$\begin{aligned}\mathrm{Ricci}^{(1)}(Y, Z) = 3\,\mathbf{Tr}\,&\mathbf{ad}\frac{1}{\mathbf{L}+\mathbf{R}}Y \circ \frac{\mathbf{LR}}{\mathbf{L}+\mathbf{R}} \circ \mathbf{ad}\frac{1}{\mathbf{L}+\mathbf{R}}Z \circ \frac{1}{\mathbf{L}+\mathbf{R}} \\ &+ ((n^2-2)g(Y, Z)). \end{aligned} \tag{3}$$

The Ricci tensor can be represented as $\mathrm{Ricci}(Y, Z) = g(Y, \mathbf{F}_{\mathrm{Ricci}}(Z))$, where the Ricci mapping $\mathbf{F}_{\mathrm{Ricci}}$ is a field of operators self-adjoint w.r.t. the Bures metric and whose trace is the scalar curvature. We cannot expect that Ricci is a simple quadratic form like the Killing form or that $\mathbf{F}_{\mathrm{Ricci}}$ is a simple expression in terms of $\mathbf{L}$ and $\mathbf{R}$, e.g. like $\mathbf{LR}(\mathbf{L}+\mathbf{R})^{-1}$. Indeed, for diagonal ϱ, Eq. (3) yields using the standard basis:

$$\mathrm{Ricci}(Y,Z)=3\sum_{i,j,k}\frac{Y_{ji}\lambda_k Z_{ij}}{(\lambda_i+\lambda_j)(\lambda_i+\lambda_k)(\lambda_k+\lambda_j)}-\frac{3}{2}\sum_{i,j}\frac{Y_{ii}Z_{jj}}{(\lambda_i+\lambda_j)^2}$$

and

$$\mathbf{F}_{\mathrm{Ricci}}(Z)=6\sum_{i,j,k}\frac{\lambda_k}{(\lambda_i+\lambda_k)(\lambda_k+\lambda_j)}Z_{ij}\mathrm{E}_{ij}-6\sum_{i,j}\frac{\lambda_i}{(\lambda_i+\lambda_j)^2}Z_{jj}\mathrm{E}_{ii}. \tag{4}$$

To express the Ricci mapping for a general ϱ we need the following natural mappings:

$$\mathrm{m},\mathrm{m}_{\mathrm{o}}:\mathcal{A}\otimes\mathcal{A}\longrightarrow\mathcal{A},\qquad \Delta:\mathcal{A}\longrightarrow\mathcal{A}\otimes\mathcal{A},\qquad \mathcal{A}:=\mathrm{M}_{n\times n}(\mathbb{C}),$$

where m is the usual multiplication, m_{o} the opposite multiplication, $\mathrm{m}_{\mathrm{o}}(X\otimes Y)=YX$, and Δ is the dual of m if we identify $\mathcal{A}$ and $\mathcal{A}^*$ via $A\mapsto\langle A,\cdot\rangle$. Explicitly,

$$\Delta(\mathrm{E}_{ij})=\sum_k \mathrm{E}_{ik}\otimes\mathrm{E}_{kj}.$$

It is obvious that m, m_{o} and Δ are invariant under the adjoint action of the unitary group, e.g. $\Delta=(\mathbf{Ad}u\otimes\mathbf{Ad}u)\circ\Delta\circ\mathbf{Ad}u^*$. Our first result is the following proposition.

Proposition 2.

$$\mathrm{Ricci}^{(1)}(Y,Z)=g(Y,\mathbf{F}^{(1)}_{\mathrm{Ricci}}(Z)),$$

where

$$\mathbf{F}^{(1)}_{\mathrm{Ricci}}=6(\mathrm{m}-\mathrm{m}_{\mathrm{o}})\circ\left(\frac{\mathbf{LR}}{\mathbf{L}+\mathbf{R}}\otimes\frac{1}{\mathbf{L}+\mathbf{R}}+\frac{1}{\mathbf{L}+\mathbf{R}}\otimes\frac{\mathbf{LR}}{\mathbf{L}+\mathbf{R}}\right)\circ\Delta\circ\frac{1}{\mathbf{L}+\mathbf{R}} +((n^2-2)\,\mathbf{Id}). \tag{5}$$

Proof. If ϱ is diagonal the last equation follows by comparing it with (4). For general ϱ it is sufficient to show that $\mathbf{F}$ given by the right-hand side of (5) is $\mathrm{U}(n)$-invariant, i.e.

$$\mathbf{F}_{u\varrho u^*}=\mathbf{Ad}u\circ\mathbf{F}_\varrho\circ\mathbf{Ad}u^*.$$

But this follows from the invariance of the operators involved in (5). □

Now we proceed with the scalar curvature $\mathcal{S}=\mathbf{Tr}\,\mathbf{F}_{\mathrm{Ricci}}$. Again, the normal direction does not contribute to the trace and we can take it on all complex matrices. Using some obvious algebraic relations between the multiplication operators, e.g.

$$\mathrm{m}\circ(\mathbf{L}\otimes\mathbf{Id})=\mathbf{L}\circ\mathrm{m}\circ(\mathbf{Id}\otimes\mathbf{Id}),\qquad \mathrm{m}\circ(\mathbf{R}\otimes\mathbf{Id})=\mathrm{m}\circ(\mathbf{Id}\otimes\mathbf{L}),$$
$$\mathrm{m}_{\mathrm{o}}\circ(\mathbf{R}\otimes\mathbf{Id})=\mathbf{R}\circ\mathrm{m}_{\mathrm{o}}\circ(\mathbf{Id}\otimes\mathbf{Id}),\qquad \mathrm{m}_{\mathrm{o}}\circ(\mathbf{L}\otimes\mathbf{Id})=\mathrm{m}_{\mathrm{o}}\circ(\mathbf{Id}\otimes\mathbf{R}),$$

Eq. (5) yields

$$\begin{aligned}\mathcal{S}&=\mathbf{Tr}\,\mathbf{F}_{\mathrm{Ricci}}\\&=6\,\mathbf{Tr}(\mathbf{L}+\mathbf{R})\circ\{\mathrm{m}\circ(\mathbf{R}\otimes\mathbf{Id})-\mathrm{m}_{\mathrm{o}}\circ(\mathbf{Id}\otimes\mathbf{R})\}\circ\left(\frac{1}{\mathbf{L}+\mathbf{R}}\otimes\frac{1}{\mathbf{L}+\mathbf{R}}\right)\circ\Delta\circ\frac{1}{\mathbf{L}+\mathbf{R}}\end{aligned}$$

$$= 6\,\mathbf{Tr}\{\mathfrak{m} \circ (\mathbf{R}\otimes\mathbf{Id}) - \mathfrak{m}_0 \circ (\mathbf{Id}\otimes\mathbf{R})\} \circ \left(\frac{1}{\mathbf{L}+\mathbf{R}} \otimes \frac{1}{\mathbf{L}+\mathbf{R}}\right) \circ \Delta. \tag{6}$$

The evaluation of this trace yields our second result as follows.

Proposition 3. *The scalar curvature on $\mathcal{D}$ resp. $\mathcal{D}^1$ equals*

$$\mathcal{S}_\varrho^{(1)} = 6\,\mathrm{Tr}\,\varrho \frac{\chi'_\varrho(-\varrho)^2}{\chi_\varrho(-\varrho)^2} - \frac{3}{2}\,\mathrm{Tr}\,\varrho^{-1} + ((n^2-1)(n^2-2)), \tag{7a}$$

$$= \mathrm{Tr}\,h_\varrho(\varrho) + ((n^2-1)(n^2-2)), \tag{7b}$$

where χ_ϱ is the characteristic polynomial of ϱ, χ'_ϱ its derivative and h_ϱ the function given by

$$h_\varrho(t) := 6t\left(\mathrm{Tr}\,\frac{1}{\varrho + t\mathbf{1}}\right)^2 - \frac{3}{2t}.$$

Remark. *$\chi_\varrho(-\varrho)$ is, in fact, invertible since $\chi_\varrho(-t) = \prod(\lambda_i + t)$ implies $\chi_\varrho(-\lambda_j) > 0$ for all eigenvalues.*

Proof. It is sufficient to prove the assertion for diagonal ϱ. For such ϱ it is easy to calculate the trace in (6),

$$\mathcal{S}_\varrho = 6\sum_{i,j,k} \frac{\lambda_k}{(\lambda_i+\lambda_k)(\lambda_k+\lambda_j)} - \frac{3}{2}\sum_i \frac{1}{\lambda_i}$$

$$= 6\sum_k \lambda_k \left(\sum_i \frac{1}{\lambda_i + \lambda_k}\right)^2 - \frac{3}{2}\,\mathrm{Tr}\,\varrho^{-1}. \tag{8}$$

This is in accordance with formulae (7a) and 7(b). The additional term in the normalized case is obvious by (5). □

The scalar curvature depends only on the invariants of ϱ. In order to express it in terms of invariants, we introduce the following matrix depending on ϱ:

$$\mathcal{E} := [\mathcal{E}_{ij}]_{i,j=1}^n,$$
$$\mathcal{E}_{ij} := 1 \quad \text{for } i+1 = j,$$
$$\mathcal{E}_{ij} := (-1)^{n-j} e_{n+1-j} \quad \text{for } i = n,$$
$$\mathcal{E}_{ij} := 0 \quad \text{otherwise},$$

where e_i is the elementary invariant of degree i of ϱ, i.e. $\chi(t) = \sum_{i=0}^n e_{n-i}(-t)^i$. Since $\mathcal{E}_\varrho$ has the same characteristic polynomial as ϱ both matrices are conjugate provided the eigenvalues of ϱ are different. Thus, at least for such points, we get from Proposition 3 the following corollary.

Corollary 4.

$$\mathcal{S}^{(1)} = 6\,\mathrm{Tr}\,\mathcal{E}\,\frac{\chi'(-\mathcal{E})^2}{\chi(-\mathcal{E})^2} - \frac{3}{2}\,\mathrm{Tr}\,\mathcal{E}^{-1} + ((n^2-1)(n^2-2)), \tag{9a}$$

$$= \mathrm{Tr}\,h_{\mathcal{E}}(\mathcal{E}) \quad + ((n^2-1)(n^2-2)), \tag{9b}$$

where

$$h_{\mathcal{E}}(t) := 6t\left(\mathrm{Tr}\,\frac{1}{\mathcal{E}+t\mathbf{1}}\right)^2 - \frac{3}{2t}.$$

Since the set of ϱ with different eigenvalues is dense, the corollary is true for all points by continuity of the curvature.

A further consequence of Proposition 3 is the following lower bound for the scalar curvature in the normalized case.

Corollary 5.

$$\mathcal{S}^1_\varrho \geq \frac{(5n^2-4)(n^2-1)}{2}. \tag{10}$$

For $n > 2$ equality holds iff $\varrho = (1/n)\mathbf{1}$. For $n = 2$ the scalar curvature equals 24 *for all ϱ.*

Proof. The eigenvalues of $\varrho \in \mathcal{D}^1$ satisfy $\sum \lambda_i = 1$ and we have

$$\sum_k \lambda_k \left(\sum_i \frac{1}{\lambda_i+\lambda_k}\right)^2 - \frac{1}{4}\sum_k \frac{1}{\lambda_k} = \sum_k \lambda_k \left(\sum_{\substack{i\\ i\neq k}} \frac{1}{\lambda_i+\lambda_k}\right)^2 + \sum_{i\neq k} \frac{1}{\lambda_i+\lambda_k}$$

$$\geq \left(\sum_{i\neq k} \frac{\lambda_k}{\lambda_i+\lambda_k}\right)^2 + \sum_{i\neq k}\frac{1}{\lambda_i+\lambda_k} \geq \frac{n^2(n-1)^2}{4} + \frac{n^2(n-1)}{2}$$

$$= \frac{n^2(n^2-1)}{4}.$$

Here we used the Schwartz inequality, the relation

$$\sum_{i\neq k} \frac{\lambda_k}{\lambda_i+\lambda_k} = \sum_{i,k} \frac{\lambda_k}{\lambda_i+\lambda_k} - \frac{n}{2} = \frac{n^2}{2} - \frac{n}{2} = \frac{n(n-1)}{2}$$

and the fact that the arithmetic mean of all $1/(\lambda_i+\lambda_k)$, $i \neq k$, is greater than or equal to the harmonic mean which equals $n/2$. Hence, Eqs. (7a), (7b) and (8) imply

$$\mathcal{S}^1_\varrho \geq \frac{3}{2}n^2(n^2-1) + (n^2-1)(n^2-2) = \frac{(5n^2-4)(n^2-1)}{2}.$$

Moreover, the bound is achieved for $\varrho = (1/n)\mathbf{1}$. Finally, we note that for $n = 2$ the above estimations are, in fact, equations ($\mathcal{S}^1 = 24$). For higher n this can hold only iff all $\lambda_i + \lambda_k$, $i \neq k$, are equal, i.e. iff $\lambda_i = 1/n$. Hence, $\varrho = (1/n)\mathbf{1}$ is the only minimal point. □

There is no upper bound for $n > 2$. Indeed, by (8) the scalar curvature equals up to a constant the sum of all $6\lambda_k/((\lambda_i+\lambda_k)(\lambda_k+\lambda_j))$, where not all indices are equal. Therefore, $\mathcal{S}^1$ tends to infinity iff at least two eigenvalues become small, or, equivalently, iff e_{n-1} tends to zero, because e_{n-1} is the sum of all products $\lambda_{i_1}\cdots\lambda_{i_{n-1}}, i_1 < i_2 < \cdots < i_{n-1}$. Roughly speaking $\mathcal{S}^1$ diverges if we get close to density matrices of rank $k < n-1$, in particular, if we get close to a pure state.

Example. We consider the scalar curvature on $\mathcal{D}^1$ for $n = 3$ using Corollary 2: we have to set $e_1 = 1$. Then

$$\chi(t) = -t^3 + t^2 - e_2 t + e_3, \qquad \mathcal{E} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ e_3 & -e_2 & 1 \end{pmatrix},$$

$$\chi(-\mathcal{E}) = 2\begin{pmatrix} e_3 & 0 & 1 \\ e_3 & e_3-e_2 & 1 \\ e_3 & e_3-e_2 & 1+e_3-e_2 \end{pmatrix},$$

$$\chi'(-\mathcal{E}) = \begin{pmatrix} -e_2 & -2 & -3 \\ -3e_3 & 2e_2 & -5 \\ -5e_3 & 5e_2-3e_3 & 2e_2-5 \end{pmatrix},$$

and we obtain

$$\mathcal{S}^1 = 6\,\mathrm{Tr}\,\mathcal{E}\,\chi'(-\mathcal{E})^2\chi(-\mathcal{E})^{-2} - \frac{3}{2}\,\mathrm{Tr}\,\mathcal{E}^{-1} + 56 = 2\,\frac{28\,e_3 - 49\,e_2 - 9}{e_3 - e_2}.$$

Similarly for $n = 4$:

$$\mathcal{S}^1 = 6\,\frac{63\,e_4 + 35\,e_3^2 - 43\,e_2e_3 - 7\,e_3 - 3\,e_2^2}{e_4 + e_3^2 - e_2e_3}.$$

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