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ON THE CURVATURE OF A CERTAIN RIEMANNIAN SPACE OF MATRICES

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Abstract. Positive definite matrices of trace 1 describe the state space of a finite quantum system. This manifold can be endowed by the physically very relevant Bogoliubov-Kubo-Mori inner product as a Riemannian metric. In the paper the curvature tensor and the scalar curvature are computed.

1. Introduction

The state space of a finite quantum system is identified with the set of positive semidefinite matrices of trace 1. The set of all strictly positive definite matrices of trace 1 becomes naturally a differentiable manifold and the Bogoliubov-Kubo-Mori scalar product defines a Riemannian structure on it. Reference [4] tells about the relation of this metric to the von Neumann entropy functional. Shortly speaking, the von Neumann entropy is a concave functional on the above space of matrices and its negative Hessian is a positive definite inner product knowns as Bogoliubov-Kubo-Mori scalar product (or canonical correlation). For the physical background of the Bogoliubov-Kubo-Mori inner product, [2] is a good source.

The objective of the paper is to compute the scalar curvature in the Riemannian geometry of the Bogoliubov-Kubo-Mori scalar product. Earlier this was obtained in [7] for the 2×2 matrices and some sectional curvatures were computed in [4] for larger matrices. In this paper, we consider the space of real density matrices which is a geodetic submanifold in the space of complex density matrices. Our study is strongly motivated by the conjectures formulated in [4] and [5]. It was conjectured that the scalar curvature takes its maximum when all eigenvalues of the density matrix are equal, and more generally the scalar curvature is monotone with respect to the majorization relation of matrices. Although we obtain an explicit formula for the scalar curvature, the conjecture remains unproven. (Nevertheless, a huge number of numerical examples are still supporting the conjecture.) The method of computation of the Ricci and scalar curvature is inspired by [3]. First we use a basis in the tangent space to express the scalar curvature and then we get rid of the basis by means of linear algebra.

When this paper was nearly finished we received the preprint [1] where the scalar curvature is computed for arbitrary monoton metrics in the complex case by a different method. Our aim is to find a formula for the scalar curvature which depends only on easily computable quantities of matrices. The scalar curvature turns out to be a rather complicated function of the eigenvalues and we express it in terms of some symmetric functions of pairs and triplets of the eigenvalues.

2. The Bogoliubov-Kubo-Mori scalar product on the space of positive definite matrices

2.1. The setup. Let $\mathcal{S} = \mathcal{S}(n)$ be the space of all real selfadjoint $(n \times n)$-matrices, $\mathcal{S}_+ = \mathcal{S}_+(n)$ be the open subspace of positive definite matrices. Then $\mathcal{S}_+$ is a manifold with tangent bundle

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$T\mathcal{S}_+ = \mathcal{S}_+ \times \mathcal{S}$. We shall consider the following Riemannian metric on $\mathcal{S}_+$, where $D \in \mathcal{S}_+$ and $X, Y \in T_D\mathcal{S}_+ = \mathcal{S}$:

$$G_D(X,Y) = \int_0^\infty \mathrm{Tr}\,\big((D+t)^{-1}X(D+t)^{-1}Y\big)\,dt.$$

Because

$$\Big|\mathrm{Tr}\,\big((D+t)^{-1}X(D+t)^{-1}Y\big)\Big| \le nt^{-2}\|X\|\,\|Y\|$$

the integral is finite. We shall identify $\mathcal{S}$ with its dual $\mathcal{S}^*$ by the standard (i.e., Hilbert-Schmidt) inner product $\langle X, Y\rangle = \mathrm{Tr}\,(XY)$. Then we can view the Riemannian metric G also as a mapping

$$G_D : T_D\mathcal{S}_+ = \mathcal{S} \to T^*_D\mathcal{S}_+ = \mathcal{S}^* \cong \mathcal{S},$$
$$G_D(X) = \int_0^\infty (D+t)^{-1}X(D+t)^{-1}\,dt,$$

which is symmetric with respect to $\langle X, Y\rangle = \mathrm{Tr}\; XY$. (Note that G_D is the Frechet derivative of $\log D$.) Now let $D \in \mathcal{S}_+$ and choose a basis of $\mathbb{R}^n$ such that $D = \sum_i \lambda_i E_{ii}$ is diagonal, where (E_{ij}) is the usual system of matrix units, then the selfadjoint matrices

$$F_{kl} \equiv E_{kl} + E_{lk} \qquad (k \le l)$$

are a complete system of eigenvectors of $G_D : \mathcal{S} \to \mathcal{S}$. This means that $(F_{ij})_{1\le i\le j\le n}$ is an orthogonal basis of $(T_D\mathcal{S}, G_D)$ with

$$G_D(F_{ij}, F_{kl}) = \begin{cases} 0 & \text{for } (i,j) \ne (k,l) \\ 2m_{ij} & \text{for } i = k < j = l \\ 4m_{ii} & \text{for } i = j = k = l \end{cases}$$

where

$$\int_0^\infty (\lambda_k + t)^{-1}(\lambda_l + t)^{-1}\,dt = \frac{\log\lambda_l - \log\lambda_k}{\lambda_l - \lambda_k} =: m_{kl}\,.$$

The expression m_{kl} is a symmetric function of the eigenvalues λ_k and λ_l. In fact $1/m_{kl}$ is the logarithmic mean of λ_k and λ_l. This implies that

$$m_{kl} = \frac{1}{\lambda_k} \qquad \text{whenever} \qquad \lambda_k = \lambda_l,$$

in particular, $m_{kk} = 1/\lambda_k$. Note that $G_D(F_{ij}) = m_{ij}F_{ij}$ for all $i \le j$.

Another symmetric expression

$$\int_0^\infty (\lambda_i + t)^{-1}(\lambda_j + t)^{-1}(\lambda_k + t)^{-1}\,dt = \frac{m_{jk} - m_{ij}}{\lambda_i - \lambda_k} =: m_{ijk}$$

will appear below. The identity

$$\frac{1}{m_{kl}}\left(\frac{m_{kkl}}{m_{kk}} + \frac{m_{kll}}{m_{ll}}\right) = 1$$

is easily computed and will be used later.

2.2. The Christoffel symbol. Since we have a global chart we can express the Levi-Civita connection by one Christoffel symbol:

$$(\nabla_\xi \eta)|_D = d\eta(D).\xi(D) - \Gamma_D(\xi(D), \eta(D))$$

where $\xi,\eta:\mathcal{S}_+\to\mathcal{S}$ are smooth vector fields. The Christoffel symbol is then given by

$$G_D(\Gamma_D(X,Y),Z)=\tfrac12 dG(D)(Z)(X,Y)-\tfrac12 dG(D)(X)(Z,Y)-\tfrac12 dG(D)(Y)(X,Z),$$

where the derivative of the metric

$$\begin{aligned}dG(D)(Z)(X,Y)=\int_0^\infty \operatorname{Tr}\Big(&-(D+t)^{-1}Z(D+t)^{-1}X(D+t)^{-1}Y-\\&-(D+t)^{-1}X(D+t)^{-1}Z(D+t)^{-1}Y\Big)\,dt\end{aligned}$$

is visibly symmetric in the entries Z,X,Y.

The Christoffel form is given by

$$\begin{aligned}G_D(\Gamma_D(X,Y))&=-\tfrac12 dG(D)(X)(Y)\\&=\tfrac12\int_0^\infty (D+t)^{-1}\Big(X(D+t)^{-1}Y+Y(D+t)^{-1}X\Big)(D+t)^{-1}\,dt,\\ \Gamma_D(X,\quad)&=-\tfrac12 G_D^{-1}.dG(D)(X)\\ &.\end{aligned}$$

Since

$$G_D^{-1}(X)=\int_0^1 D^uXD^{1-u}\,du\,,$$

we can express the Christoffel form as an integral formula. The derivative is

$$d\Gamma(D)(X)(Y,Z)=-\tfrac12 d(G^{-1})(D)(X).dG(D)(Y)(Z)+\tfrac12 G_D^{-1}\ d^2G(D)(X,Y)(Z).$$

2.3. When $D=\sum_i\lambda_iE_{ii}$ is diagonal, then

$$dG(D)(Z)(X)=-\sum_{ijk}m_{ijk}\big(E_{ii}ZE_{jj}XE_{kk}+E_{ii}XE_{jj}ZE_{kk}\big).$$

In particular,

$$dG(D)(F_{ij})(F_{kl})=-\delta_{jk}m_{ilj}F_{il}-\delta_{jl}m_{ikj}F_{ik}-\delta_{il}m_{jki}F_{jk}-\delta_{ik}m_{jli}F_{jl},$$

and

$$\Gamma_D(F_{ij},F_{kl})=-\delta_{jk}\frac{m_{ilj}}{m_{il}}F_{il}-\delta_{jl}\frac{m_{ikj}}{m_{ik}}F_{ik}-\delta_{il}\frac{m_{jki}}{m_{jk}}F_{jk}-\delta_{ik}\frac{m_{jli}}{m_{jl}}F_{jl}$$

2.4. The curvature. The Riemannian curvature $R(\xi,\eta)\zeta=(\nabla_\xi\nabla_\eta-\nabla_\eta\nabla\xi-\nabla_{[\xi,\eta]})\zeta$ is then determined in terms of the Christoffel form by

$$\begin{aligned}R_D(X,Y)Z=&-d\Gamma(D)(X)(Y,Z)+d\Gamma(D)(Y)(X,Z)+\\&+\Gamma_D(X,\Gamma_D(Y,Z))-\Gamma_D(Y,\Gamma_D(X,Z)).\end{aligned}$$

If we insert the expressions from 2.2 we get after some computation

$$\begin{aligned}R_D(X,Y)Z&=\tfrac14 d(G^{-1})(D)(X).dG(D)(Y)(Z)-\tfrac14 d(G^{-1})(D)(Y).dG(D)(X)(Z)\\&=-\tfrac14 G_D^{-1}.dG(D)(X).G_D^{-1}.dG(D)(Y)(Z)\\&\quad+\tfrac14 G_D^{-1}.dG(D)(Y).G_D^{-1}.dG(D)(X)(Z)\end{aligned}$$

The Ricci curvature is then given by the following trace

$$\operatorname{Ric}_D(X,Z)=\operatorname{Tr}_{\mathcal{S}}\left(Y\mapsto R_D(X,Y)Z\right),$$

and the scalar curvature is

$$\operatorname{Scal}(D) = \operatorname{Tr}_{\mathcal{S}}(X \mapsto G_D^{-1}.\operatorname{Ric}_D(X, \quad)).$$

Next we compute the traces in a concrete basis. Let A_s be an orthonormal basis with respect to the inner product $\langle X, Y\rangle = \operatorname{Tr}(XY)$ on $\mathcal{S}$. Then

$$\operatorname{Ric}_D(X, Z) = \sum_s \langle R_D(X, A_s)Z, A_s\rangle$$

and

$$\begin{aligned}\operatorname{Scal}(D) &= \sum_t \langle G_D^{-1}.\operatorname{Ric}_D(A_t, \quad), A_t\rangle = \sum_t \langle \operatorname{Ric}_D(A_t, \quad), G_D^{-1}A_t\rangle \\ &= \sum_t \operatorname{Ric}_D(A_t, G_D^{-1}A_t) = \sum_t \sum_s \langle R_D(A_t, A_s)G_D^{-1}A_t, A_s\rangle\,.\end{aligned}$$

3. The submanifold of normalized matrices

3.1. The submanifold of trace 1 matrices. We consider the affine submanifold of $\mathcal{S}_+$ of all positive definite real selfadjoint matrices with trace 1 and its tangent bundle:

$$\begin{aligned}\mathcal{S}_1 &= \{D \in \mathcal{S}_+ : \operatorname{Tr}(D) = 1\}, \\ T\mathcal{S}_1 &= \mathcal{S}_1 \times \mathcal{S}_0, \text{ where } \mathcal{S}_0 = \{X \in \mathcal{S} : \operatorname{Tr}(X) = 0\}.\end{aligned}$$

Lemma.

(1) *The unit normal field n along the submanifold $\mathcal{S}_1$ with respect to the Riemannian metric G from 2.1 is given by $n(D) = (D, D)$.*

(2) *The G-orthonormal projection $P_D : \mathcal{S} = T_D\mathcal{S}_+ \to T_D\mathcal{S}_1 = \mathcal{S}_0$ is given by $P_D(X) = X - \operatorname{Tr}(X)n(D) = X - \operatorname{Tr}(X)D$ for $D \in \mathcal{S}_1$ and $X \in \mathcal{S}_)$.*

(3) *The Christoffel form for the covariant derivative ∇^1 of the induced Riemannian metric $\mathcal{S}_1, G^1$ is given by*

$$\Gamma^1_D(X, Y) = P_D\Gamma_D(X, Y) = \Gamma_D(X, Y) - \operatorname{Tr}(\Gamma_D(X, Y)).D, \quad D \in \mathcal{S}_1,\ X, Y \in \mathcal{S}_0,$$

and the second fundamental form is given by

$$\begin{aligned}S_D &: T_D\mathcal{S}_1 \times T_D\mathcal{S}_1 = \mathcal{S}_0 \times \mathcal{S}_0 \to \mathbb{R} \\ S_D(X, Y) &= \operatorname{Tr}(\Gamma_D(X, Y)) \\ &= \int_0^\infty \operatorname{Tr}\Big((D+t)^{-1}X(D+t)^{-1}Y \\ &\qquad - \tfrac{1}{2}D(D+t)^{-2}X(D+t)^{-1}Y \\ &\qquad - \tfrac{1}{2}D(D+t)^{-2}Y(D+t)^{-1}X\Big)\,dt.\end{aligned}$$

Proof. If $X \in \mathcal{S}$ commutes with D we get

$$\begin{aligned}G_D(X, Y) &= \int_0^\infty \operatorname{Tr}((D+t)^{-1}X(D+t)^{-1}Y)dt = \int_0^\infty \operatorname{Tr}((D+t)^{-2}XY)dt = \\ &= [-\operatorname{Tr}((D+t)^{-1}XY)]_{t=0}^{t=\infty} = \operatorname{Tr}(D^{-1}XY)\end{aligned}$$

Thus for $Y \in \mathcal{S}_0$ we have $G_D(D, Y) = \operatorname{Tr}(Y) = 0$. Moreover for $D \in \mathcal{S}_1$ we have $G_D(D, D) = \operatorname{Tr}(D) = 1$, so (1) follows. The remaining assertions are standard facts from Riemannian geometry.

For the explicit expression of the second fundamental form we proceed as follows. For $D \in \mathcal{S}_1$ the Weingarten mapping is given by

$$\begin{aligned} L_D :& T_D\mathcal{S}_1 = \mathcal{S}_0 \to \mathcal{S}_0 = T_D\mathcal{S}_1, \\ L_D(X) :=& \nabla_{(D,X)} n = dn(D).X - \Gamma_D(X, n(D)) = X - \Gamma_D(X, D), \end{aligned}$$

and the second fundamental form is then given by

$$\begin{aligned} S_D :& T_D\mathcal{S}_1 \times T_D\mathcal{S}_1 = \mathcal{S}_0 \times \mathcal{S}_0 \to \mathbb{R} \\ S_D(X,Y) :=& G_D(L_D(X), Y) = G_D(X - \Gamma_D(X,D), Y) \\ =& G_D(X,Y) + \tfrac{1}{2} dG(D)(X)(D,Y) \\ =& \int_0^\infty \operatorname{Tr}\big((D+t)^{-1}X(D+t)^{-1}Y \\ &\quad - \tfrac{1}{2}D(D+t)^{-2}X(D+t)^{-1}Y - \tfrac{1}{2}D(D+t)^{-2}Y(D+t)^{-1}X\Big)\, dt. \end{aligned}$$

Another formula for the second fundamental form is

$$\begin{aligned} S_D(X,Y) :=& \operatorname{Tr}(\Gamma_d(X,Y)) = \operatorname{Tr}(-\tfrac{1}{2}G_D^{-1}\, dG(X)(Y)) \\ =& \tfrac{1}{2}\int_o^1 \int_0^\infty \operatorname{Tr}\big(D^u(D+t)^{-1}X(D+t)^{-1}Y(D+t)^{-1}D^{1-u} + \\ &\quad + D^u(D+t)^{-1}Y(D+t)^{-1}X(D+t)^{-1}D^{1-u}\Big)\, dt\, du. \quad \square \end{aligned} \tag{4}$$

3.2. The curvature via the Gauß equation. The Gauß equation expresses the curvature R of $\mathcal{S}_+$ and the curvature R^1 of $\mathcal{S}_1$ for $D \in \mathcal{S}_1$ and $X, Y, Z, U \in \mathcal{S}_0$ by

$$G_D(R(X,Y)Z, U) = G_D(R^1(X,Y)Z, U) + S_D(X,Z)S_D(Y,U) - S_D(Y,Z)S_D(X,U).$$

The Ricci curvature of the submanifold $\mathcal{S}_1$ is then given by the following trace

$$\operatorname{Ric}^1_D(X,Z) = \operatorname{Tr}_{\mathcal{S}_0}\big(Y \mapsto R^1_D(X,Y)Z\big),$$

and the scalar curvature is

$$\operatorname{Scal}^1(D) = \operatorname{Tr}_{\mathcal{S}_0}(X \mapsto G_D^{-1}.\operatorname{Ric}^1_D(X, \quad)).$$

Next we compute the traces in a concrete basis in case of a diagonal $D = \sum_i \lambda_i E_{ii} \in \mathcal{S}_1$. Let A_s be an orthonormal basis with respect to the inner product G_D on $\mathcal{S}_0$. Then

$$\operatorname{Ric}^1_D(X,Z) = \sum_s G_D(R^1_D(X,A_s)Z, A_s)$$

and

$$\begin{aligned} \operatorname{Scal}^1(D) &= \sum_t G_D(G_D^{-1}.\operatorname{Ric}^1_D(A_t, \quad), A_t) = \sum_t \langle \operatorname{Ric}^1_D(A_t, \quad), A_t\rangle \\ &= \sum_t \operatorname{Ric}^1_D(A_t, A_t) = \sum_t \sum_s G_D(R^1_D(A_t, A_s)A_t, A_s) \\ &= \sum_{t,s} \Big(G_D(R_D(A_t,A_s)A_t,A_s) - S_D(A_t,A_t)S_D(A_s,A_s) - S_D(A_s,A_t)S_D(A_t,A_s)\Big) \end{aligned}$$

4. Computation of the scalar curvature

Our aim is to have an explicit formula for the scalar curvature $\mathrm{Scal}^1(D)$ in terms of eigenvalues of the D, which we assume to be a diagonal matrix. As in the previous section, let A_s be an orthonormal basis with respect to the inner product G_D on $\mathcal{S}_0$. We assume that some of the basis elements are diagonal (like D) and the others are normalized symmetrized matrix units.

4.1. The first term. We decompose the sum

$$\sum_{t,s} G_D(R_D(A_t, A_s)A_t, A_s)$$

into three subsums and we compute them separately. First we consider the case when both A_t and A_s are offdiagonal, that is, they are in the form $F_{ij}/\sqrt{2m_{ij}}$.

Offdiagonal-offdiagonal.

$$\begin{aligned}\sum \frac{1}{4m_{ij}m_{kl}} G_D(R_D(F_{ij}, F_{kl})F_{ij}, F_{kl}) &= \sum \frac{1}{4m_{ij}} \langle R_D(F_{ij}, F_{kl})F_{ij}, F_{kl}\rangle \\ = -\sum \frac{1}{16m_{ij}} &\langle G_D^{-1}.d(G)(D)(F_{ij}).G_D^{-1}.dG(D)(F_{kl})(F_{ij}), F_{kl}\rangle \\ + \sum_{ijkl} \frac{1}{16m_{ij}} &\langle G_D^{-1}.d(G)(D).(F_{kl}).G_D^{-1}.dG(D)(F_{ij})(F_{ij}), F_{kl}\rangle,\end{aligned}$$

where summation is over $i < j$ and $k < l$. We continue with the first term and calculate in an elementary way:

$$-\sum \frac{1}{16m_{ij}} \langle G_D^{-1}.d(G)(D)(F_{ij}).G_D^{-1}.dG(D)(F_{kl})(F_{ij}), F_{kl}\rangle$$
$$\frac{12}{16} \sum_{u<v<w} \frac{m_{uvw}^2}{m_{uv}m_{vw}m_{uw}} + \frac{2}{16} \sum_{i<j} \frac{m_{iij}^2}{m_{ij}^2 m_{ii}} + \frac{2}{16} \sum_{i<j} \frac{m_{ijj}^2}{m_{ij}^2 m_{jj}}$$

For the second term we use $dG(D)(F_{ij})(F_{ij}) = -m_{iij}F_{ii} - m_{ijj}F_{jj}$ and get

$$\begin{aligned}&+ \sum_{i<j,k<l} \frac{1}{16m_{ij}} \langle G_D^{-1}.d(G)(D).(F_{kl}).G_D^{-1}.dG(D)(F_{ij})(F_{ij}), F_{kl}\rangle \\ &= \frac{1}{2} \sum_{u<v<w} \frac{m_{uuv}m_{uuw}}{m_{uv}m_{uw}m_{uu}} + \frac{1}{2} \sum_{u<v<w} \frac{m_{vvw}m_{uvv}}{m_{vw}m_{uv}m_{vv}} + \frac{1}{2} \sum_{u<v<w} \frac{m_{uww}m_{vww}}{m_{uw}m_{vw}m_{ww}} \\ &\qquad + \frac{1}{4} \sum_{i<j} \frac{m_{iij}^2}{m_{ij}^2 m_{ii}} + \frac{1}{4} \sum_{i<j} \frac{m_{ijj}^2}{m_{ij}^2 m_{jj}}\end{aligned}$$

Offdiagonal-diagonal. Next we compute the sum

$$\sum_{t,s} G_D(R_D(A_t, A_s)A_t, A_s)$$

when $A_t = \sum_i a_i^t E_{ii}$ are diagonal, G_D-orthogonal to D, and orthonormalized, and where the A_s are still offdiagonal. This means that

$$G_D(D, A_t) = \sum_i m_{ii}\lambda_i a_i^t = \sum_i a_i^t = 0 \quad \text{and} \quad G_D(A_t, A_{t'}) = \sum_i m_{ii}a_i^t a_i^{t'} = \sum_i \frac{a_i^t a_i^{t'}}{\lambda_i} = \delta_{t,t'}.$$

We also have

$$dG(D)(F_{kl})(A_t) = dG(D)(A_t)(F_{kl}) = -(m_{kkl}a_k^t + m_{kll}a_l^t)F_{kl}, \quad dG(D)(A_t)(A_{t'}) = -D^{-2}A_tA_{t'},$$
$$dG(D)(F_{kl})(F_{kl}) = -\delta_{kl}(m_{llk} + m_{kkl})F_{kl} - m_{kkl}F_{kk} - m_{llk}F_{ll}, \quad \text{and } G_D^{-1}A_t = DA_t$$

since D, A_t, and $A_{t'}$ commute. We get

$$\begin{aligned}
&\sum_{t,k<l} \frac{1}{2m_{kl}} G_D(R_D(A_t,F_{kl})A_t,F_{kl}) \\
&= -\sum_{t,k<l} \frac{1}{8m_{kl}} \langle dG(D)(A_t).G_D^{-1}.dG(D)(F_{kl})(A_t),F_{kl}\rangle \\
&\quad + \sum_{t,k<l} \frac{1}{8m_{kl}} \langle dG(D)(F_{kl}).G_D^{-1}.dG(D)(A_t)(A_t),F_{kl}\rangle = \\
&= -\sum_{t,k<l} \frac{1}{8m_{kl}} \langle G_D^{-1}.dG(D)(F_{kl})(A_t), d(G)(D)(A_t)(F_{kl})\rangle \\
&\quad + \sum_{t,k<l} \frac{1}{8m_{kl}} \langle G_D^{-1}.dG(D)(A_t)(A_t), dG(D)(F_{kl})(F_{kl})\rangle = \\
&= -\sum_{t,k<l} \frac{1}{8m_{kl}} \langle \frac{1}{m_{kl}}(-m_{kkl}a_k^t - m_{kll}a_l^t)F_{kl}, (-m_{kkl}a_k^t - m_{kll}a_l^t)F_{kl}\rangle \\
&\quad + \sum_{t,k<l} \frac{1}{8m_{kl}} \langle -\sum_p \frac{1}{\lambda_p}(a_p^t)^2 E_{pp}, (-m_{kkl}F_{kk} - m_{llk}F_{ll})\rangle = \\
&= -\sum_{t,k<l} \frac{1}{4m_{kl}^2}(m_{kkl}a_k^t + m_{kll}a_l^t)^2 \\
&\quad + \sum_{t,k<l} \frac{1}{4m_{kl}} \left(m_{kkl}\frac{1}{\lambda_k}(a_k^t)^2 + m_{llk}\frac{1}{\lambda_l}(a_l^t)^2 \right) =: Q
\end{aligned}$$

Denoting by Q this seemingly basis dependent quantity we transform the sums in Q as follows:

$$\sum_{t,k<l}(\dots) = \frac{1}{2}\left(\sum_{t,k,l}(\dots) - \sum_{t,k=l}(\dots) \right).$$

Summing for $k = l$ indexes we obtain:

$$\begin{aligned}
&-\sum_{t,k=l} \frac{1}{4m_{kl}^2}(m_{kkl}a_k^t + m_{kll}a_l^t)^2 = -\sum_{t,k} \frac{m_{kkk}^2}{m_{kk}^2}(a_k^t)^2 = -\frac{1}{4}\sum_{t,k}\frac{1}{\lambda_k^2}(a_k^t)^2, \\
&\sum_{t,k=l} \frac{1}{4m_{kl}} \left(m_{kkl}\frac{1}{\lambda_k}(a_k^t)^2 + m_{llk}\frac{1}{\lambda_l}(a_l^t)^2 \right) = \sum_{t,k} \frac{1}{4m_{kk}} \frac{2m_{kkk}}{\lambda_k}(a_k^t)^2 = \frac{1}{4}\sum_{t,k}\frac{1}{\lambda_k^2}(a_k^t)^2.
\end{aligned}$$

The two terms turned out to be equal, so

$$Q = \frac{1}{8}\left[-\sum_{t,k,l}\frac{1}{m_{kl}^2}(m_{kkl}a_k^t + m_{kll}a_l^t)^2 + \sum_{t,k,l}\frac{1}{m_{kl}}\left(\frac{m_{kkl}}{\lambda_k}(a_k^t)^2 + \frac{m_{llk}}{\lambda_l}(a_l^t)^2 \right) \right].$$

We start to deal with the first sum. Let

$$b_k^t = \frac{a_k^t}{\sqrt{\lambda_k}}, \quad \Lambda_k = \sqrt{\lambda_k} \qquad (1 \le k \le n).$$

Then $\Lambda, b^1, b^2, \dots, b^{(n-1)}$ is an orthonormal basis in $\mathbb{R}^n$. We define a linear mapping $\mathcal{K}$ from $\mathbb{R}^n$ to the space of all real $n \times n$ matrices (endowed with the standard Hilbert-Schmidt inner product).

$$\mathcal{K}c = \sum_{k,l}\frac{1}{m_{kl}}\left[m_{kkl}\sqrt{\lambda_k}c_k + m_{kll}\sqrt{\lambda_l}c_l \right]E_{kl} \qquad (c \in \mathbb{R}^n).$$

Then

$$\|\mathcal{K}b^t\|^2 = \sum_{k,l} \frac{1}{m_{kl}^2} \left[m_{kkl}a_k^t + m_{kll}a_l^t\right]^2$$

which is a term in Q. Hence

$$\sum_{t,k,l} \frac{1}{m_{kl}^2}(m_{kkl}a_k^t + m_{kll}a_l^t)^2 = \sum_t \|\mathcal{K}b^t\|^2 = \operatorname{Tr}\mathcal{K}^*\mathcal{K} - \|\mathcal{K}\Lambda\|^2.$$

Since

$$\|\mathcal{K}\Lambda\|^2 = \sum_{k,l} \frac{[m_{kkl}\lambda_k + m_{kll}\lambda_l]^2}{m_{kl}^2} = \sum_{k,l} 1 = n^2$$

and

$$\begin{aligned}\operatorname{Tr}\mathcal{K}^*\mathcal{K} &= \sum_i \|\mathcal{K}e_i\|^2 = \sum_{i,l} 2\frac{m_{iil}^2\lambda_i}{m_{il}^2} + 2\sum_i \frac{m_{iii}^2\lambda_i}{m_{ii}^2} \\ &= 2\sum_{k,l} \frac{m_{kkl}^2\lambda_k}{m_{kl}^2} + \frac{1}{2}\sum_i \lambda_i^{-1}\end{aligned}$$

we have

$$\sum_{t,k,l} \frac{1}{m_{kl}^2}(m_{kkl}a_k^t + m_{kll}a_l^t)^2 = 2\sum_{k,l} \frac{m_{kkl}^2\lambda_k}{m_{kl}^2} + \frac{1}{2}\sum_i \lambda_i^{-1} - n^2.$$

The other terms of Q are similarly computed as traces.

$$\begin{aligned}\sum_{t,k,l} \frac{1}{m_{kl}} \left(\frac{m_{kkl}}{\lambda_k}(a_k^t)^2 + \frac{m_{llk}}{\lambda_l}(a_l^t)^2\right) &= \sum_{k,l} \frac{m_{kkl} + m_{kll}}{m_{kl}} - \sum_{k,l} \frac{m_{kkl}\lambda_k + m_{kll}\lambda_l}{m_{kl}} \\ &= \sum_{k,l} \frac{m_{kkl} + m_{kll}}{m_{kl}} - n^2\end{aligned}$$

Finally, we obtain a basis independent expression for Q:

$$Q = -\sum_{k,l} \frac{m_{kkl}^2\lambda_k}{4m_{kl}^2} - \frac{1}{16}\sum_i \lambda_i^{-1} + \sum_{k,l} \frac{m_{kkl} + m_{kll}}{8m_{kl}}$$

Diagonal-offdiagonal. This case is completely similar (in fact, symmetric) and yields the same Q.

Diagonal-diagonal. Now we compute the sum

$$\sum_{t,s} G_D(R_D(A_t, A_s)A_t, A_s)$$

when A_t and A_s are both diagonal, G_D-orthogonal to D, and orthonormalized. We get

$$\begin{aligned}&\sum_{t,s} G_D(R_D(A_t, A_s)A_t, A_s) \\ &= -\sum_{t,s} \frac{1}{4}\langle d(G)(D)(A_t).G_D^{-1}.dG(D)(A_s)(A_t), A_s\rangle \\ &\quad + \sum_{t,s} \frac{1}{4}\langle d(G)(D)(A_s).G_D^{-1}.dG(D)(A_t)(A_t), A_s\rangle = \\ &= -\sum_{t,s} \frac{1}{4}\langle G_D^{-1}.dG(D)(A_s)(A_t), d(G)(D)(A_t)(A_s)\rangle \\ &\quad + \sum_{t,s} \frac{1}{4}\langle G_D^{-1}.dG(D)(A_t)(A_t), d(G)(D)(A_s)(A_s)\rangle = \\ &= -\sum_{t,s} \frac{1}{4}(\langle -D^{-1}A_tA_s, -D^{-2}A_tA_s\rangle - \langle -D^{-1}(A_t)^2, -D^{-2}(A_s)^2\rangle) = 0\end{aligned}$$

4.2. The second term. We start the computation of

$$-\sum_{t,s} S_D(A_t, A_t) S_D(A_s, A_s).$$

We use first the formula from 3.1.(4), and use also 2.3.

$$\begin{aligned}
S_D(F_{ij}, F_{kl}) &= \operatorname{Tr}\left(-\tfrac{1}{2} G_D^{-1}\, dG(F_{ij})(F_{kl})\right) \\
&= \operatorname{Tr}\left(-\tfrac{1}{2} G_D^{-1}(-\delta_{jk} m_{ilj} F_{il} - \delta_{jl} m_{ikj} F_{ik} - \delta_{il} m_{jki} F_{jk} - \delta_{ik} m_{jli} F_{jl})\right) \\
&= \tfrac{1}{2} \operatorname{Tr}\left(\delta_{jk} \frac{m_{ilj}}{m_{il}} F_{il} + \delta_{jl} \frac{m_{ikj}}{m_{ik}} F_{ik} + \delta_{il} \frac{m_{jki}}{m_{jk}} F_{jk} + \delta_{ik} \frac{m_{jli}}{m_{jl}} F_{jl}\right) \\
&= \delta_{jk}\delta_{il} \frac{m_{ilj}}{m_{il}} + \delta_{jl}\delta_{ik} \frac{m_{ikj}}{m_{ik}} + \delta_{il}\delta_{jk} \frac{m_{jki}}{m_{jk}} + \delta_{ik}\delta_{jl} \frac{m_{jli}}{m_{jl}}
\end{aligned}$$

We observe that for $(i<j) \neq (k<l)$ we get $S_D(F_{ij}, F_{kl}) = 0$. Furthermore, for $i<j$ we have

$$\begin{aligned}
S_D(F_{ij}, F_{ij}) &= \frac{m_{iij}}{m_{ii}} + \frac{m_{ijj}}{m_{jj}} \\
S_D(F_{ii}, F_{kk}) &= 4\delta_{ik} \frac{m_{iki}}{m_{ik}} \\
S_D(F_{ii}, F_{kl}) &= \delta_{ik}\delta_{il} \frac{m_{ili}}{m_{il}} + \delta_{il}\delta_{ik} \frac{m_{iki}}{m_{ik}} + \delta_{il}\delta_{ik} \frac{m_{iki}}{m_{ik}} + \delta_{ik}\delta_{il} \frac{m_{ili}}{m_{il}} \\
&= 0 \text{ if } k<l.
\end{aligned}$$

First we take summation when both A_t and A_s are offdiagonal:

$$\begin{aligned}
&-\sum_{t,s} S_D(A_t, A_t) S_D(A_s, A_s) = \\
&= -\sum_{i<j,k<l} S_D\left(\frac{1}{\sqrt{2m_{ij}}} F_{ij}, \frac{1}{\sqrt{2m_{ij}}} F_{ij}\right) S_D\left(\frac{1}{\sqrt{2m_{kl}}} F_{kl}, \frac{1}{\sqrt{2m_{kl}}} F_{kl}\right) \\
&= -\sum_{i<j,k<l} \frac{1}{4 m_{ij} m_{kl}} \left(\frac{m_{iij}}{m_{ii}} + \frac{m_{ijj}}{m_{jj}}\right)\left(\frac{m_{kkl}}{m_{kk}} + \frac{m_{kll}}{m_{ll}}\right) \\
&= -\frac{1}{4} \sum_{i<j,k<l} 1 = -\frac{n^2(n-1)^2}{16}.
\end{aligned}$$

Next we assume that A_t is diagonal and A_s is offdiagonal.

$$S_D(A_t, A_t) = \frac{1}{2} \sum_p (a_p^t)^2 \lambda_p^{-1} = \frac{1}{2},$$

and

$$-\sum_{t,s} S_D(A_t, A_t) S_D(A_s, A_s) = -\frac{1}{2}(n-1) \sum_{k<l} \frac{1}{4 m_{kl}} \left(\frac{m_{kkl}}{m_{kk}} + \frac{m_{kll}}{m_{ll}}\right) = -\frac{n(n-1)^2}{16}.$$

Note that this contribution is symmetric in t and s and we should take it twice.

Now it easily follows the value of the sum when both A_t and A_s are diagonal:

$$-\sum_{t,s} S_D(A_t, A_t) S_D(A_s, A_s) = -\sum_{t,s} \frac{1}{2} \cdot \frac{1}{2} = -\frac{1}{4}(n-1)^2$$

4.3. The third term. Now we have to deal with

$$-\sum_{t,s} S_D(A_t,A_s)S_D(A_s,A_t) = -\sum_{t,s} S_D(A_t,A_s)^2$$

By the formulas from 4.2 we have that it suffices to sum when both A_t and A_s are diagonal and both of them are offdiagonal. Hence

$$-\sum_{t,s} S_D(A_t,A_s)S_D(A_s,A_t) = -\frac{n-1}{4} - \sum_{k<l}\frac{1}{4m_{kl}^2}\left(\frac{m_{kkl}}{m_{kk}}+\frac{m_{kll}}{m_{ll}}\right)^2 = -\frac{n-1}{4} - \frac{n(n-1)}{8}.$$

4.4. The scalar curvature formula.

$$\begin{aligned}R = \quad & \frac{3}{4}\sum_{u<v<w}\frac{m_{uvw}^2}{m_{uv}m_{vw}m_{wu}} + \frac{1}{2}\sum_{u<v<w}\frac{m_{vvw}m_{vvu}}{m_{vu}m_{vv}m_{vw}} \\ & + \frac{1}{2}\sum_{u<v<w}\frac{m_{wwu}m_{wwv}}{m_{wu}m_{wv}m_{ww}} + \frac{1}{2}\sum_{u<v<w}\frac{m_{uuv}m_{uuw}}{m_{uu}m_{uv}m_{uw}} \\ & + \frac{3}{8}\sum_{i<j}\frac{m_{iij}^2}{m_{ij}^2 m_{ii}} + \frac{3}{8}\sum_{i<j}\frac{m_{ijj}^2}{m_{ij}^2 m_{jj}} \\ & - \sum_{k,l}\frac{m_{kkl}^2\lambda_k}{2m_{kl}^2} - \frac{1}{8}\sum_i \lambda_i^{-1} + \sum_{k,l}\frac{m_{kkl}+m_{kll}}{4m_{kl}} \\ & - \frac{n^2(n-1)^2}{16} - \frac{n(n-1)^2}{8} - \frac{1}{4}(n-1)^2 - \frac{n-1}{4} - \frac{n^2(n-1)^2}{16}\end{aligned}$$

Some further simplification:

$$\frac{3}{8}\sum_{i<j}\frac{m_{iij}^2}{m_{ij}^2 m_{ii}} + \frac{3}{8}\sum_{i<j}\frac{m_{ijj}^2}{m_{ij}^2 m_{jj}} = \frac{3}{16}\sum_{i,j}\frac{m_{iij}^2\lambda_i + m_{ijj}^2\lambda_j}{m_{ij}^2} - \frac{3}{2}\sum_i \frac{1}{\lambda_i}$$

$$-\frac{1}{2}\sum_{k,l}\frac{m_{kkl}^2\lambda_k}{m_{kl}^2} = -\frac{1}{4}\sum_{k,l}\frac{m_{kkl}^2\lambda_k + m_{kll}^2\lambda_l}{m_{kl}^2}$$

Hence

$$\begin{aligned}R = \quad & \frac{3}{4}\sum_{u<v<w}\frac{m_{uvw}^2}{m_{uv}m_{vw}m_{wu}} \\ & + \frac{1}{2}\sum_{u<v<w}\frac{m_{vvw}m_{vvu}}{m_{vu}m_{vv}m_{vw}} + \frac{1}{2}\sum_{u<v<w}\frac{m_{wwu}m_{wwv}}{m_{wu}m_{wv}m_{ww}} + \frac{1}{2}\sum_{u<v<w}\frac{m_{uuv}m_{uuw}}{m_{uu}m_{uv}m_{uw}} \\ & - \frac{1}{16}\sum_{k,l}\frac{m_{kkl}^2\lambda_k + m_{kll}^2\lambda_l}{m_{kl}^2} - \frac{13}{2}\sum_i \frac{1}{\lambda_i} + \sum_{k,l}\frac{m_{kkl}+m_{kll}}{4m_{kl}} + \frac{n(n-1)}{4}(n^2-n+1).\end{aligned}$$

Although this formula is rather explicit, it is difficult to analyse it. When the given density matrix is replaced by a more mixed one then some of the terms increase and some of them decrease. Unfortunately, we could not conclude anything for the monotonicity conjecture.

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