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 one matrices. This bound is achieved for the maximally mixed state, a further hint for the statistical meaning of the scalar curvature.

PACS Numbers 03.65.Bz, 02.40.-k, 02.40.Ky

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Typeset using REVTEX
I. 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 one matrices. $\mathcal{D}^1$ represents the space of nondegenerate mixed states of a $n$-dimensional quantum system. The tangent space at $\rho \in \mathcal{D}$ (resp. $\mathcal{D}^1$) consists of all Hermitian (traceless) matrices. These manifolds carry the so called Riemannian Bures metric $g$ defined by

$$g_\rho(X, Y) = \frac{1}{2} \text{Tr} \ X G, \quad X, Y \in T_\rho \mathcal{D},$$

where $G$ is the (unique, by the Sylvester-Rosenblum theorem, see [5]) solution of $\rho G + G \rho = Y$. It should be mentioned, that $g$ is also well defined on manifolds of all $\rho \geq 0$ of fixed rank, but we will deal only with the maximal rank. This Riemannian metric was introduced by Uhlmann in generalizing the Berry phase to mixed states, [6–8]. 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. [9,10].

The restriction of $g$ to the manifold of trace one diagonal matrices, i. e. to the manifold of all probability distributions on a $n$-point set, is (up to the factor $1/4$) just the Fisher metric known from classical statistics, see e. g. [2,3]. Similarly to this case the Bures metric is related to the statistical distance of quantum states, see [9,10]. 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), [13], the Bures metric is minimal, and it seems to play a distinguished role also for other reasons, see [17,18]. Partial results concerning the curvature of the Bogoliubov metric, another monotone metric, were obtained in [14].

Several authors, e. g. [15,16], 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 $\frac{1}{n} I$ 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.

Notations: The eigenvalues of a positive matrix $\rho$ are denoted by $\lambda_i$. Thus, if we assume $\rho$ to be diagonal, then $\rho = \text{diag}(\lambda_1, \ldots, \lambda_n)$. Bold letters are used for operators acting on matrices. They will depend on $\rho$, so that they actually represent fields of operators called by several authors superoperators. However, we frequently suppress this dependence for brevity of notation similarly to vector field and other quantities. In particular, $L_\rho$ and $R_\rho$ denote the operators of left and right multiplication by $\rho$ and $\rho^{-1}_{L+R}$ is the inverse operator of $L + R$ (denoted by $R^{-1}_\rho$ in [7]). 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

$$g = \frac{1}{2} \text{Tr} d\rho \frac{1}{L + R}(d\rho).$$
However, from the theory of matrix equations,\cite{4,5}, some explicit formulae for this operator and the metric can be derived,\cite{19}.

II. THE RIEMANNIAN CURVATURE TENSOR

In this section we explain some results concerning the Riemannian curvature tensor of the Bures metric and introduce on this occasion some further notations. A brief communication of this results appeared in\cite{11}. Proofs and more details can be found in\cite{12}.

The manifold $D$ is an open subset of the space of Hermitian matrices and all tangent spaces $T_{\varrho}D$ are identified with this real vector space. Thus we regard vector fields $X,Y,\ldots$ on $D$ as functions $\varrho \mapsto X_{\varrho}$ on $D$ with Hermitian (traceless for $D^{1}$) values. The flat covariant derivative $\nabla f$ on $D$ inherited from the affine structure of the Hermitian matrices is simply the derivation along straight lines; $(\nabla f X)_{\varrho} = \lim_{t \to 0} (Y_{\varrho} + tX_{\varrho} - Y_{\varrho})/t$. In particular, $\nabla f_{\varrho} N = X$, where $N$ is the vector field defined by $N_{\varrho} := \varrho$. It is perpendicular w. r. to the Bures metric to the submanifold $D^{1}$. This allows for determining curvature quantities of $D^{1}$ from that of $D$ by the Gauss equation. Quantities with superscript 1 will always refer to $D^{1}$.

We denote by $\nabla$ resp. $\nabla^{1}$ the covariant derivative of the Levi-Civita connection of the Bures metric on $D$ resp. $D^{1}$. In\cite{12} it was shown that

$$\nabla X Y = \nabla X Y - \frac{1}{L+R}(X)N \frac{1}{L+R}(Y) - \frac{1}{L+R}(Y)N \frac{1}{L+R}(X)$$

$$\nabla^{1} X Y = \nabla X Y + 2g(X,Y)N,$$

where on the right hand side of (1.3) appears the usual product of matrix valued functions. Of course, in order to apply (1.1) one must extend the vector fields $X$ and $Y$ on $D^{1}$ to a neighborhood of $D^{1}$, but the result will not depend on this extension. (1.1) corresponds to the well known equation

$$\nabla_{\varrho}(a^{i}) \partial_{j} = \partial_{i}(a^{j}) \partial_{j} + a^{i} \Gamma_{ij}^{k} \partial_{k},$$

which relates the covariant derivative to the flat derivative induced by a local parametrization.

The calculations of the next section are based on the following Proposition derived from (1).

**Proposition 1:**

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

$$\mathcal{R}(W, Z, X, Y) := g(\nabla X \nabla Y - \nabla Y \nabla X - \nabla[X,Y], W)$$

$$= 2g \left( iLR \left[ \frac{1}{L+R}X, \frac{1}{L+R}Y \right], i \left[ \frac{1}{L+R}W, \frac{1}{L+R}Z \right] \right)$$

$$+ g \left( iLR \left[ \frac{1}{L+R}Z, \frac{1}{L+R}Y \right], i \left[ \frac{1}{L+R}W, \frac{1}{L+R}X \right] \right)$$

$$- g \left( iLR \left[ \frac{1}{L+R}Z, \frac{1}{L+R}X \right], i \left[ \frac{1}{L+R}W, \frac{1}{L+R}Y \right] \right),$$

(2a)

$$\mathcal{R}^{1}(W, Z, X, Y) = \mathcal{R}(W, Z, X, Y) + g(Y,Z)g(X,W) - g(X,Z)g(Y,W).$$

(2b)

Note the different meaning of commutators in the equations above. In (2a) it is pointwise the usual matrix commutator, $[X,Y]_{\varrho} := X_{\varrho}Y_{\varrho} - Y_{\varrho}X_{\varrho}$. All further commutators will be understood in this sense. An immediate consequence of Proposition 1 is
Corollary 1:
Let \( p \) be the plane generated by two tangent vectors \( X \) and \( Y \). Then the sectional curvature is given by

\[
K(p) := \frac{\mathcal{R}(X, Y, X, Y)}{g(X, X)g(Y, Y) - g(X, Y)^2}
= \frac{3g \left( iLR \left[ \frac{1}{L+R} X, \frac{1}{L+R} Y \right], i \left[ \frac{1}{L+R} W, \frac{1}{L+R} Z \right] \right)}{g(X, X)g(Y, Y) - g(X, Y)^2} - g(X, Y)^2
\]

\[\mathcal{K}^1(p) = K(p) + 1.\]

Finally we mention that for \( n = 2 \) the Riemannian manifold \((D^1, g)\) is isometric to an open half 3-sphere of radius \( 1/2 \), [8]. The geometry for \( n > 2 \) is much more complicated, e. g. \( D^1 \) is not locally symmetric, [12].

III. RICCI TENSOR AND SCALAR CURVATURE

In order to determine the Ricci tensor and the scalar curvature we have to calculate traces of the curvature given by Proposition 1. For clarity we will distinguish in the notation between the trace of matrices and the trace of operators acting on matrices. We will treat simultaneously the normalized and the unnormalized case. For brevity we include in brackets additional terms corresponding to the normalized case.

First we determine the curvature mapping, also denoted by \( \mathcal{R} \), which is given by

\[
\mathcal{R}^{(1)}(X, Y)Z = 2 \left[ \frac{1}{L+R} Z, L \left[ \frac{1}{L+R} X, \frac{1}{L+R} Y \right] \right] + \left[ \frac{1}{L+R} X, L \left[ \frac{1}{L+R} Y, \frac{1}{L+R} Z \right] \right] + \left[ \frac{1}{L+R} Y, L \left[ \frac{1}{L+R} Z, \frac{1}{L+R} X \right] \right] + \left( g(Y, Z)X - g(X, Z)Y \right).
\] (4)

The Ricci tensor is defined by

\[
Ricci(Y, Z) := \text{Tr} \left\{ X \mapsto \mathcal{R}(X, Y)Z \right\}.
\]

Eliminating \( X \) in (4) yields

\[
Ricci^{(1)}(Y, Z) = \text{Tr} \left\{ 2 \text{ad}_{\frac{1}{L+R} Z} \circ \frac{L}{L+R} \circ \text{ad}_{\frac{1}{L+R} Y} \circ \frac{1}{L+R} + \text{ad}_{\frac{L}{L+R} \left[ \frac{1}{L+R} Z, \frac{1}{L+R} Y \right]} \circ \frac{1}{L+R} + \text{ad}_{\frac{1}{L+R} Y} \circ \frac{L}{L+R} \circ \text{ad}_{\frac{1}{L+R} Z} \circ \frac{1}{L+R} \right\} + \left( n^2 - 2 \right) g(Y, Z).
\] (5)

This equation requires some comments. \( \text{ad} V \) denotes the usual commutation operator, \( \text{ad} V(W) := [V, W] \), and we have to do with compositions of operators. The trace should
be regarded, originally, on the real tangent spaces, that means on the Hermitian matrices, traceless or not. But the normal direction generated by \( \varrho \) does not give any contribution to the trace in \( \text{Ricci}(Y, Z) \) because \( R(X, Y)Z \) vanishes for \( X_\varrho := \varrho \). 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 space of traceless Hermitian matrices. Finally, the trace of a real operator equals the trace of its complexification. Therefore we can take the trace in (5) on all complex \( n \times n \)-matrices.

To continue the determination of the Ricci tensor we notice that the second term of the trace in (5) vanishes, because \( \text{Tr ad} V \circ (L + R)^{-1} = 0 \) for all \( V \). Indeed, we can suppose that \( \varrho \) is diagonal. Then

\[
\text{Tr ad} V \circ \frac{1}{L + R} = \sum_{i,j} \langle E_{ij}, [V, \frac{1}{L + R} E_{ij}] \rangle = \sum_{i,j} \frac{1}{\lambda_i + \lambda_j} \langle E_{ii} - E_{jj}, V \rangle = 0.
\]

The remaining expression in (5) must be symmetric in \( Y \) and \( Z \), since the Ricci tensor is symmetric. Hence (5) reduces to

\[
\text{Ricci}^{(1)}(Y, Z) = 3 \text{Tr ad} \frac{1}{L + R} Y \circ \frac{LR}{L + R} \circ \text{ad} \frac{1}{L + R} Z \circ \frac{1}{L + R} + \left( (n^2 - 2)g(Y, Z) \right).
\]

The Ricci tensor can be represented as \( \text{Ricci}(Y, Z) = g\langle Y, \text{F Ricci}(Z) \rangle \), where the Ricci mapping \( \text{F Ricci} \) is a field of operators self-adjoint w. r. to the Bures metric and whose trace is the scalar curvature. We cannot expect that \( \text{F Ricci} \) is a simple expression in terms of \( L \) and \( R \), e. g. like \( LR(L + R)^{-1} \). Indeed, if \( \varrho \) is diagonal we obtain from (6) using the standard basis after a simple calculation

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

and

\[
\text{F Ricci}(Z) = 6 \sum_{i,j,k} \frac{\lambda_k}{(\lambda_i + \lambda_k)(\lambda_k + \lambda_j)} Z_{ij} E_{ij} - 6 \sum_{i,j} \frac{\lambda_i}{(\lambda_i + \lambda_j)^2} Z_{jj} E_{ii}
\]

for \( Y, Z \in T_\varrho \mathcal{D} \). To express the Ricci mapping for a general \( \varrho \) we need the following natural mappings:

\[
m, m_\circ : \mathcal{A} \otimes \mathcal{A} \rightarrow \mathcal{A}, \quad \Delta : \mathcal{A} \rightarrow \mathcal{A} \otimes \mathcal{A}, \quad \mathcal{A} := M_{n \times n}(\mathbb{C}),
\]

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

\[
\Delta(E_{ij}) = \sum_k E_{ik} \otimes E_{kj}.
\]

It is obvious that these mappings are equivariant w. r. to the adjoint action of the unitary group, e. g. \( \Delta(uXu^*) = (Adu \otimes Adu) \Delta(X) \). Using these mappings we have:
Proposition 2:

\[ \text{Ricci}^{(1)}(Y, Z) = g \left(Y, F^{(1)}_{\text{Ricci}}(Z) \right), \]  

(8a)

where

\[ F^{(1)}_{\text{Ricci}} = 6(m - m_o) \circ \left( \frac{LR}{L+R} \otimes \frac{1}{L+R} + \frac{1}{L+R} \otimes \frac{LR}{L+R} \right) \circ \Delta \circ \frac{1}{L+R} + \left( n^2 - 2 \right) \text{Id}. \]  

(8b)

Proof: We prove the unnormalized case, the additional term in the normalized one is clear from (7). If \( \varrho \) is diagonal the last equation follows by comparing (8) with (7a). For general \( \varrho \) it is sufficient to remark that the right hand side of (8b) is a (1,1)-tensor field on \( D \) invariant under the \( U(n) \)-conjugation. This implies the invariance of the right hand side of (8a). \( \square \)

Now we proceed with the scalar curvature \( S = \text{Tr} F_{\text{Ricci}} \). Again, the normal direction does not give a contribution to the trace and we can take it on all complex matrices. We will use some obvious algebraic relations between the multiplication operators, e.g.

\[ m \circ (L \otimes \text{Id}) = L \circ m \circ (\text{Id} \otimes L), \]

\[ m \circ (R \otimes \text{Id}) = m \circ (\text{Id} \otimes L), \]

\[ m_o \circ (R \otimes \text{Id}) = R \circ m_o \circ (\text{Id} \otimes L), \]

\[ m_o \circ (L \otimes \text{Id}) = m_o \circ (\text{Id} \otimes R), \]

and obtain from (8b)

\[ S = \text{Tr} F_{\text{Ricci}} \]

\[ = 6 \text{Tr} (L + R) \circ \left\{ m \circ (R \otimes \text{Id}) - m_o \circ (\text{Id} \otimes R) \right\} \circ \left( \frac{1}{L+R} \otimes \frac{1}{L+R} \right) \circ \Delta \circ \frac{1}{L+R} \]

\[ = 6 \text{Tr} \left\{ m \circ (R \otimes \text{Id}) - m_o \circ (\text{Id} \otimes R) \right\} \circ \left( \frac{1}{L+R} \otimes \frac{1}{L+R} \right) \circ \Delta. \]  

(9)

The evaluation of this trace yields:

Proposition 3: The scalar curvature on \( D \) resp. \( D^1 \) equals

\[ S_{(1)}^\varrho = 6 \text{Tr} \varrho \frac{\chi\varrho(-\varrho)^2}{\chi\varrho(-\varrho)} - \frac{3}{2} \text{Tr} \varrho^{-1} + \left( n^2 - 1 \right) \left( n^2 - 2 \right), \]

(10a)

\[ = \text{Tr} h\varrho(\varrho) + \left( n^2 - 1 \right) \left( n^2 - 2 \right), \]  

(10b)

where \( \chi\varrho \) is the characteristic polynomial of \( \varrho \), \( \chi\varrho' \) its derivative and \( h\varrho \) the function given by

\[ h\varrho(t) := 6 t \left( \text{Tr} \frac{1}{\varrho + t} \right)^2 - \frac{3}{2} t. \]

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. \( \square \)

Proof: It is sufficient to prove the assertion for diagonal \( \varrho \). For such \( \varrho \) it is easy to calculate the trace (8) and we obtain
This is in accordance with formulae (10). The additional term in the normalized case is obvious by (8b).

The scalar curvature depends only on the invariants of $\mathcal{K}$. In order to express it in terms of invariants we introduce the following matrix depending on $\mathcal{K}$:

$$E := \begin{bmatrix} E_{ij} \end{bmatrix}_{n}$$

$$E_{ij} := \begin{cases} 1 & \text{for } i + 1 = j \\ (-1)^{i-j}e_{n+1-j} & \text{for } i = n \\ 0 & \text{otherwise} \end{cases}$$

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

Corollary 2:

$$S^{(1)} = 6 \text{ Tr } \mathcal{E} \frac{\chi'(-\mathcal{E})^2}{\chi(-\mathcal{E})^2} - \frac{3}{2} \text{ Tr } \mathcal{E}^{-1} + \left( (n^2 - 1)(n^2 - 2) \right),$$

$$= \text{ Tr } h_{\mathcal{E}}(\mathcal{E}) + \left( (n^2 - 1)(n^2 - 2) \right),$$

where

$$h_{\mathcal{E}}(t) := 6t \left( \text{ Tr } \frac{1}{\mathcal{E} + t1} \right)^2 - \frac{3}{2t}.$$  

Since the set of $\mathcal{K}$ 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 3:

$$S_\mathcal{K}^1 \geq \frac{(5n^2 - 4)(n^2 - 1)}{2}.$$  

For $n > 3$ equality holds iff $\mathcal{K} = \frac{1}{n}1$. For $n = 2$ the scalar curvature equals 24 for all $\mathcal{K}$.

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

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

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, equations (\(\Pi\)) and (\(\Pi\)) imply

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

Moreover, the bound is achieved for \(\varrho = \frac{1}{n} 1\). Finally we note that for \(n = 2\) the above estimations are, in fact, equations (\(S^1 = 24\)). 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, \(\varrho = \frac{1}{n} 1\) is the only minimal point. \(\square\)

There is no upper bound for \(n > 2\). Indeed, by (\(\Pi\)) 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, \(S^1\) tends to infinity iff \(e_{n-1}\) tends to zero, because \(e_{n-1}\) is the sum of all \(\lambda_{i_1} \ldots \lambda_{i_{n-1}}\), \(i_1 < i_2 < \ldots < i_{n-1}\). Roughly speaking \(S^1\) 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 \(D^1\) for \(n = 3\) using Corollary 2: We have to set \(e_1 = 1\). Then

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

\[
\chi(-\mathcal{E}) = 2 \begin{pmatrix} e_3 \\ e_3 \\ e_3 \end{pmatrix} - e_2 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \chi'(-\mathcal{E}) = \begin{pmatrix} -e_2 \\ -3e_3 \\ -5e_3 \end{pmatrix} - 2 \begin{pmatrix} -2 \\ 5e_2 - 3e_3 \\ 2e_2 - 5 \end{pmatrix},
\]

and we obtain

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

Similarly we get for \(n = 4\):

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

**ACKNOWLEDGMENTS**

I would like to thank A. Uhlmann for valuable remarks.
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