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Explicit formulae for the Bures metric

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Abstract. The aim of this paper is to derive explicit formulae for the computation of the Riemannian Bures metric g on the manifold $\mathcal{D}$ of (finite-dimensional) nonsingular density matrices ϱ. This Riemannian metric introduced by Uhlmann generalizes the Fubini–Study metric to mixed states and is the infinitesimal version of the Bures distance. Several formulae are known for computing the Bures metric in low dimensions. The formulae presented in this paper allow for computing in finite dimensions without any diagonalization procedures. The first equations we give are, essentially, of the form $g_\varrho = \sum a_{ij} \operatorname{Tr} \mathrm{d}\varrho\, \varrho^{i-1}\, \mathrm{d}\varrho\, \varrho^{j-1}$, where a_{ij} is a matrix of invariants of ϱ. A further formula, $g_\varrho = \sum c_{ij}\, \mathrm{d}p_i \otimes \mathrm{d}p_j + \sum b_{ij} \operatorname{Tr} \mathrm{d}\varrho\, \varrho^{i-1}\, \mathrm{d}\varrho\, \varrho^{j-1}$, is adapted to the local orthogonal decomposition $\mathcal{D} \approx \mathbb{R}^n \times \mathrm{U}(n)/\mathrm{T}^n$ at generic points.

1. Introduction

In recent years many authors considered the Bures metric and the Bures distance because of their importance in quantum statistics and for the understanding of the geometry of quantum state spaces. Explicit computations in this area meet some technical difficulties, since, for example, the Bures metric is defined rather implicitly. The aim of this paper is to provide several equations for computing the Bures metric in any finite dimension using only matrix products, determinants and traces.

Let $\mathcal{D}$ be the manifold of all positive, Hermitian $n\times n$-matrices. The submanifold of trace-one matrices is the space of so-called completely entangled mixed states of a finite-dimensional quantum system. The tangent space $\mathrm{T}_\varrho\mathcal{D}$ consists of all Hermitian $n\times n$-matrices and the Riemannian Bures metric on $\mathcal{D}$ is given by [1],

$$g_\varrho(X', X) = \tfrac{1}{2} \operatorname{Tr} X'G \qquad X, X' \in \mathrm{T}_\varrho\mathcal{D} \tag{1}$$

where G is the (unique) solution of

$$\varrho G + G\varrho = X. \tag{2}$$

It should be mentioned, that (1) also defines a metric on the manifolds $\mathcal{D}_k$ of rank k densities, $k < n$. In this case equation (2) has solutions G for $X \in \mathrm{T}_\varrho\mathcal{D}_k$. This solution is not unique, but the right-hand side of (1) is still well defined for $X' \in \mathrm{T}_\varrho\mathcal{D}_k$. However, we will deal here with the maximal rank $k = n$, only. This metric appears quite naturally on the background of purifications of mixed states and is used in quantum statistics to describe the statistical distance of mixed states [13]. It is an extremal monotone metric, [12], and seems to be quite distinguished for physical and mathematical reasons, see e.g. [3].

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Several formulae and approaches for computing the Bures metric have been given, e.g. [1, 4–8]. Based on the integral representation (cf [9]) of the solution of (2) the metric takes the form [1],

$$g(X', X) = \frac{1}{2}\,\mathrm{Tr}\int_0^\infty X' \mathrm{e}^{-t\varrho} X \mathrm{e}^{-t\varrho}\,\mathrm{d}t.$$

Moreover, if $|\alpha\rangle$, $\alpha = 1, 2, \ldots$, are eigenvectors of ϱ with eigenvalues λ_α, then a simple calculation shows that (1) yields [4],

$$g_\varrho(X, X) = \frac{1}{2}\sum_{\alpha,\beta}\frac{|\langle\alpha|X|\beta\rangle|^2}{\lambda_\alpha + \lambda_\beta}.$$

Both formulae are not explicit in the sense that they need the knowledge of eigenvalues of ϱ. Instead we are looking for equations in a finite dimension similar to

$$g = \frac{1}{4\det\varrho}\,\mathrm{d}(\det\varrho)\otimes\mathrm{d}(\det\varrho) + \frac{1}{2}\,\mathrm{Tr}\;\mathrm{d}\varrho\,\mathrm{d}\varrho \qquad \text{(see [1])} \tag{3}$$

$$= \frac{1}{4}\,\mathrm{Tr}\left\{\mathrm{d}\varrho\,\mathrm{d}\varrho + \frac{1}{\det\varrho}(\mathrm{d}\varrho - \varrho\,\mathrm{d}\varrho)(\mathrm{d}\varrho - \varrho\,\mathrm{d}\varrho)\right\} \tag{4}$$

which hold for normalized ($\mathrm{Tr}\,\varrho = 1$), nonsingular 2×2-density matrices (see also [5] for $n = 3$). They do not require any diagonalization procedure. In section 2 we provide such expressions which generalize (4) to arbitrary $n < \infty$ using a method of the theory of matrix equations. In section 3 we give an equation similar to (3), but adapted to the local isometric decomposition of the manifold $\mathcal{D}$. We will not suppose the normalization $\mathrm{Tr}\,\varrho = 1$, this case is included in our expressions by setting $p_1 := \mathrm{Tr}\,\varrho = 1$ and $\mathrm{d}p_1 = 0$.

Notations. *The following quantities depend on a positive (resp. non-negative), Hermitian $n\times n$-matrix ϱ. In order to simplify the notation the dependence on ϱ will be suppressed. By $\lambda_1 \leqslant \cdots \leqslant \lambda_n$, $0 \leqslant \lambda_i$, we denote the eigenvalues of ϱ and by Λ the corresponding diagonal matrix. ϱ is called a generic point of $\mathcal{D}$ if $\varrho > 0$ and all eigenvalues are different. Moreover, V will be the Vandermonde matrix (λ_i^{j-1}) [11]. Operators acting on matrices are denoted by bold italic letters, in particular, if not indicated otherwise, $\boldsymbol{L}$ and $\boldsymbol{R}$ denote the left and right multiplication by ϱ. The Bures metric now takes the form*

$$g = \frac{1}{2}\,\mathrm{Tr}\;\mathrm{d}\varrho\,\frac{1}{\boldsymbol{L}+\boldsymbol{R}}\,\mathrm{d}\varrho. \tag{5}$$

We set

$$\chi(t) := \det(t\mathbf{1} - \varrho) = t^n + k_1 t^{n-1} + \cdots + k_n$$

$k_0 := 1$ and $k_i := 0$ for $k > n$ or $k < 0$. Hence, $e_i := (-1)^i k_i$ is the elementary invariant of degree i and $(-1)^n\chi(t)$ the characteristic polynomial of ϱ. We set $p_i := \mathrm{Tr}\,\varrho^i = \lambda_1^i + \cdots + \lambda_n^i$, then the differential $\mathrm{d}p_i$ applied to a tangent vector X yields $\mathrm{d}p_i(X) = i\;\mathrm{Tr}\,X\varrho^{i-1}$. Finally, we will make use of the following matrix several times:

$$P := \begin{bmatrix} p_1 & p_2 & \cdots & p_n \\ p_2 & p_3 & \cdots & p_{n+1} \\ \vdots & \vdots & \vdots & \vdots \\ p_n & p_{n+1} & \cdots & p_{2n-1} \end{bmatrix}. \tag{6}$$

For instance, we have the following.

Criterion. *A Hermitian $n\times n$-matrix $\varrho \geqslant 0$ is a generic point of $\mathcal{D}$ if* $\det P \neq 0$.

Indeed, $P = V^{\mathrm{T}}\Lambda V$. Therefore, $\det P = \det(\Lambda)\det(V)^2 = \det(\varrho)\prod_{i<j}(\lambda_i - \lambda_j)^2$.

2. General formulae

From now on we suppose that ϱ is positive. In order to calculate $g_\varrho(X', X)$ one has to solve the matrix equation (2). The matrix (resp. operator) equation $EG - GF = X$ was intensively studied (for a review, see [9]). Basically, it has a unique solution G if E and F have disjoint spectra (Sylvester–Rosenblum theorem [9]). In our matrix case, $E = \varrho = -F$, this is fulfilled because ϱ is positive. The uniqueness is also clear, not appealing to this theorem, since we may suppose w.l.o.g. that ϱ is diagonal. Then equation (2) reads $(\lambda_i + \lambda_j)G_{ij} = X_{ij}; i, j = 1, \ldots n$. A further, simple but nice, tool in this theory is the use of similarities of block matrices, in our case e.g.

$$\begin{bmatrix} \mathbf{1} & -G \\ 0 & \mathbf{1} \end{bmatrix} \begin{bmatrix} -\varrho & X \\ 0 & \varrho \end{bmatrix} \begin{bmatrix} \mathbf{1} & G \\ 0 & \mathbf{1} \end{bmatrix} = \begin{bmatrix} -\varrho & 0 \\ 0 & \varrho \end{bmatrix}.$$

If we apply the polynomial χ as an operator function to both sides we get in the upper-right box the identity

$$\chi(-\varrho)G + M = 0$$

where M is the upper-right box of χ applied to the above inner matrix containing X;

$$M = \sum_{i=1}^{n} k_{n-i} \sum_{j=0}^{i-1} (-\varrho)^j X \varrho^{i-j-1}. \tag{7}$$

But $\chi(-\varrho)$ is invertible. This can be seen as follows. The characteristic polynomial of $-\varrho$ equals $(-1)^n \chi(-t)$ and the positivity of ϱ implies that $\chi(t)$ and $\chi(-t)$ have no common divisors. Hence, by the Euclidean algorithm there exists two polynomials p, q such that $p(t)\chi(t) + q(t)\chi(-t) = 1$, and inserting ϱ gives $q(\varrho)\chi(-\varrho) = \mathbf{1}$. Therefore, the solution G of (2) is given by

$$G = -\chi(-\varrho)^{-1} \sum_{i=1}^{n} k_{n-i} \sum_{j=0}^{i-1} (-\varrho)^j X \varrho^{i-j-1} \tag{8a}$$

or, in a more compact form,

$$\begin{bmatrix} -\mathbf{1} & G \\ 0 & 0 \end{bmatrix} = -\begin{bmatrix} \chi(-\varrho)^{-1} & 0 \\ 0 & 0 \end{bmatrix} \chi\left(\begin{bmatrix} -\varrho & X \\ 0 & \varrho \end{bmatrix} \right). \tag{8b}$$

The first explicit formula we get for the Bures metric is the following.

Proposition 1.

$$g(X', X) := -\frac{1}{2} \operatorname{Tr} \begin{bmatrix} 0 & 0 \\ X' & 0 \end{bmatrix} \begin{bmatrix} \chi(-\varrho)^{-1} & 0 \\ 0 & 0 \end{bmatrix} \chi\left(\begin{bmatrix} -\varrho & X \\ 0 & \varrho \end{bmatrix} \right). \tag{9}$$

The inverse of $\chi(-\varrho)$ is again a polynomial expression in ϱ. Therefore, we can rewrite (8a) using the Cayley–Hamilton theorem and G will have the form $\sum_{1 \leqslant i,j \leqslant n} a_{ij} \varrho^{i-1} X \varrho^{j-1}$, where the coefficients a_{ij} are invariants of ϱ. That means,

$$\frac{1}{\boldsymbol{L} + \boldsymbol{R}} = \sum_{1 \leqslant i,j \leqslant n} a_{ij} \boldsymbol{L}^{i-1} \boldsymbol{R}^{j-1} \tag{10a}$$

$$= (\boldsymbol{Id}, \boldsymbol{L}, \ldots, \boldsymbol{L}^{n-1}) A (\boldsymbol{Id}, \boldsymbol{R}, \ldots, \boldsymbol{R}^{n-1})^{\mathrm{T}} \qquad A := (a_{ij}). \tag{10b}$$

Of course, one can also directly see the existence of such a representation. The operator $\boldsymbol{L} + \boldsymbol{R}$ acts on a finite-dimensional space. Therefore, its inverse is a polynomial in $\boldsymbol{L} + \boldsymbol{R}$, which we can reduce to the above form using $\chi(\boldsymbol{L}) = \boldsymbol{L}_{\chi(\varrho)} = 0$ and similarly for $\boldsymbol{R}$. The solution of (2) given by Smith in [10] is, essentially, of this form. The formulae for the coefficients in terms of the invariants of ϱ that one reads off from [10] will be given at the end of this section.

The representation (10) is unique provided ϱ is generic. Indeed, if there were coefficients such that $\sum_{1\leqslant i,j\leqslant n} a'_{ij}\boldsymbol{L}^{i-1}\boldsymbol{R}^{j-1}=0$ then applying this operator to all vectors of a common eigenbasis of $\boldsymbol{L}$ and $\boldsymbol{R}$ would result in $V^{\mathrm{T}}A'V=0$. But the Vandermonde matrix V is nonsingular for a generic ϱ and we would conclude $a'_{ij}=0$. Moreover, in the generic case the matrix A is necessarily symmetric.

In order to get a compact expression for the coefficient matrix A in (10) we define the $n\times n$-matrix K by

$$K := \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ -k_n & -k_{n-1} & -k_{n-2} & \dots & -k_1 \end{bmatrix}. \tag{11}$$

K carries out the reduction of powers of ϱ by $\chi(\varrho)=0$. Indeed we have

$$\begin{bmatrix} \varrho \\ \varrho^2 \\ \vdots \\ \varrho^n \end{bmatrix} = K \begin{bmatrix} \mathbf{1} \\ \varrho \\ \vdots \\ \varrho^{n-1} \end{bmatrix}$$

and similarly for the reduction of powers of $\boldsymbol{L}$ and $\boldsymbol{R}$. Thus, the multiplication of (10*b*) by $\boldsymbol{L}+\boldsymbol{R}$ leads to

$$K^{\mathrm{T}}A + AK = C$$

where

$$C := \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix}$$

represents the identity operator $\boldsymbol{Id}=\boldsymbol{L}^0\boldsymbol{R}^0$. Note that K has the same characteristic polynomial as ϱ. Now we may proceed as above to find A. For this purpose we apply $\chi(t)$ to

$$\begin{bmatrix} \mathbf{1} & -A \\ 0 & \mathbf{1} \end{bmatrix} \begin{bmatrix} -K^{\mathrm{T}} & C \\ 0 & K \end{bmatrix} \begin{bmatrix} \mathbf{1} & A \\ 0 & \mathbf{1} \end{bmatrix} = \begin{bmatrix} -K^{\mathrm{T}} & 0 \\ 0 & K \end{bmatrix}.$$

Instead of (8) and (7) we obtain

$$A = -\chi(-K^{\mathrm{T}})^{-1}N$$

where

$$N = \chi\left(\begin{bmatrix} -K^{\mathrm{T}} & C \\ 0 & K \end{bmatrix}\right)_{12} = \sum_{i=1}^{n} k_{n-i} \sum_{j=0}^{i-1} (-K^{\mathrm{T}})^j C K^{i-j-1}$$

$$= \begin{bmatrix} k_{n-1} & k_{n-2} & \dots & k_1 & 1 \\ -k_{n-2} & -k_{n-3} & \dots & -1 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ (-1)^{n-1} & 0 & \dots & 0 & 0 \end{bmatrix} = [(-1)^{i+1}k_{n+1-i-j}]_{i,j=1}^{n}. \tag{12}$$

To see the last equation note that $K^{\mathrm{T}i}CK^j$ has only one in the $(i+1,\, j+1)$-position and zero otherwise; K moves the ‘1’ coming from C to the right and K^{T} moves it down. Hence we get the following.

Proposition 2. *The Bures metric equals*

$$g = \tfrac{1}{2} \sum_{i,j=1}^{n} a_{ij} \,\mathrm{Tr}\, \mathrm{d}\varrho\, \varrho^{i-1}\, \mathrm{d}\varrho\, \varrho^{j-1} \tag{13}$$

where $(a_{ij}) = -\chi(-K^{\mathrm{T}})^{-1}N$, *$K$ and N are given by (12) and (11).*

The probably 'most explicit' form of the coefficients a_{ij} is given by the following.

Proposition 3. *(Smith [10]):*

$$a_{ij} = \frac{(-1)^i}{2\det H} \sum_{r=0}^{n-i} \sum_{s=0}^{n-j} (-1)^r k_r k_s \Phi\left(\frac{i+j+r+s}{2}\right) \tag{14}$$

where

$$H = \begin{bmatrix} k_1 & k_3 & \dots & k_{2n-1} \\ k_0 & k_2 & \dots & k_{2n-2} \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & k_n \end{bmatrix} = [k_{2j-i}]_{i,j=1}^{n}$$

and $\Phi(m) = 0$ *if m is not an integer, and otherwise $\Phi(m)$ is the cofactor in* $\det H$ *of the element in the first row and mth column of H.*

Remark. *The determinant of H is not equal to zero, more precisely:*

$$\det H = (-1)^{\frac{n(n+1)}{2}} \prod_i \lambda_i \prod_{i<j} (\lambda_i + \lambda_j) \neq 0.$$

Indeed, changing the order of rows and columns yields $\det H = (-1)^{\frac{n(n+1)}{2}} \det[e_{n+1-2i+j}]$. But the last determinant is just the (symmetric) Schur function of the eigenvalues of ϱ (cf [11], I.3) related to the partition $(n, n-1, \dots, 1) = (1, \dots, 1) + (n-1, \dots, 0)$ leading to the above product.

3. A formula adapted to $\mathcal{D} \approx \mathbb{R}^n \times \mathrm{U}(n)/\mathrm{T}^n$

Every $\varrho \in \mathcal{D}$ can be diagonalized with a suitable unitary u;

$$\varrho = u\mu^2 u^* \qquad \mu = \mathrm{diag}(\mu_1, \dots, \mu_n) \qquad \mu_i \in \mathbb{R}_+$$

and we have $\mathrm{d}\varrho = 2u\mu\, \mathrm{d}\mu\, u^* + u\,[u^*\,\mathrm{d}u, \mu^2]u^*$. By a straightforward calculation we find

$$\frac{1}{\boldsymbol{L}_\varrho + \boldsymbol{R}_\varrho}(\mathrm{d}\varrho) = u\left(\mu^{-1}\,\mathrm{d}\mu + \frac{1}{\boldsymbol{L}_{\mu^2} + \boldsymbol{R}_{\mu^2}}([u^*\,\mathrm{d}u, \mu^2])\right)u^*$$

and

$$g_\varrho = \mathrm{Tr}\, \mathrm{d}\mu\, \mathrm{d}\mu + \frac{1}{2}\mathrm{Tr}[\,u^*\,\mathrm{d}u, \mu^2\,]\frac{1}{\boldsymbol{L}_\mu^2 + \boldsymbol{R}_\mu^2}([u^*\,\mathrm{d}u, \mu^2]). \tag{15}$$

Therefore, in a neighbourhood of a generic point the Riemannian manifold $\mathcal{D}$ locally looks like $\mathbb{R}^n \times {}^{\mathrm{U}(n)}/_{\mathrm{T}^n}$, where $\mathbb{R}^n$ is equipped with the standard metric and the metric on the homogeneous space $\mathrm{U}(n)/\mathrm{T}^n$ depends on the first parameter. The tangent space at ϱ splits into

$$\mathrm{T}_\varrho\mathcal{D} = \mathrm{T}_\varrho^{||} + \mathrm{T}_\varrho^{||\perp} \tag{16}$$

where $\mathrm{T}_\varrho^{||}$ is the subspace of Hermitian matrices commuting with ϱ. Its orthogonal complement (wrt. the Bures metric) is the space of all $[a, \varrho]$, a is anti-Hermitian. If ϱ is diagonal then (16) is the decomposition into diagonal and off-diagonal Hermitian matrices.

From now on let ϱ be a generic point of $\mathcal{D}$. By $\boldsymbol{P}$ and $\boldsymbol{P}^{\perp} = \boldsymbol{Id} - \boldsymbol{P}$ we denote the (orthogonal) projectors onto the subspaces in (16).

Lemma.

$$\boldsymbol{P}(X) = \sum_{i,j=1}^{n} \varrho^i (P^{-1})_{ij} \operatorname{Tr} X\varrho^{j-1} \tag{17a}$$

$$= \sum_{i,j=1}^{n} (P^{-1})_{ij} \varrho^i X \varrho^{j-1} \tag{17b}$$

where P is the matrix of power invariants given by (6).

Proof. To show (17*a*) we use that for a generic ϱ the powers $\varrho, \varrho^2, \ldots, \varrho^n$ form a basis of the vector space of all Hermitian matrices commuting with ϱ. Moreover, $P_{ij} = \operatorname{Tr} \varrho^{i+j-1} = 4\, g_\varrho(\varrho^i, \varrho^j)$ and $\operatorname{Tr} X\varrho^{j-1} = 4\, g_\varrho(X, \varrho^j)$. Bearing this in mind (17*a*) is just the usual formula for the orthogonal projection onto a subspace with a given basis;

$$\mathrm{P}(v) = \sum_{i,j} b_i (\langle b_\alpha | b_\beta \rangle)^{-1}_{ij} \langle b_j | v \rangle.$$

To see (17*b*) let $X_{\alpha\beta}$, $\alpha, \beta = 1, \ldots, n$ be a common eigenbasis of $\boldsymbol{L}$ and $\boldsymbol{R}$, $\varrho X_{\alpha\beta} = \lambda_\alpha X_{\alpha\beta}$, $X_{\alpha\beta}\,\varrho = \lambda_\beta X_{\alpha\beta}$ ($X_{\alpha\beta}$ may not be Hermitian). Then the complex span of $\mathrm{T}^{||}_\varrho$ resp. $\mathrm{T}^{||\perp}_\varrho$ is generated by all $X_{\alpha\beta}$ with $\alpha = \beta$ resp. $\alpha \neq \beta$. For $X = X_{\alpha\beta}$ the right-hand side of (17*b*) yields $\eta_{\alpha\beta} X_{\alpha\beta}$, where

$$\eta_{\alpha\beta} = \sum_{i,j=1}^{n} (P^{-1})_{ij} \lambda_\alpha^i \lambda_\beta^{j-1} = (\Lambda V P^{-1} V^{\mathrm{T}})_{\alpha\beta}.$$

V is the Vandermonde matrix of eigenvalues of ϱ. But $P = V^{\mathrm{T}} \Lambda V$ implies $\eta_{\alpha\beta} = \delta_{\alpha\beta}$. □

From (17) we now get

$$\frac{1}{\boldsymbol{L}+\boldsymbol{R}} \boldsymbol{P}(X) = \frac{1}{2} \sum_{i,j=1}^{n} \varrho^{i-1} (P^{-1})_{ij} \frac{\mathrm{d}p_j}{j}(X)$$

$$\frac{1}{\boldsymbol{L}+\boldsymbol{R}} \boldsymbol{P}^{\perp}(X) = \sum_{i,j=1}^{n} \left\{ a_{ij} - \frac{1}{2}(P^{-1})_{ij} \right\} \varrho^{i-1} X \varrho^{j-1}$$

where we used $\operatorname{Tr} jX\varrho^{j-1} = \mathrm{d}p_j(X)$ and $\frac{1}{\boldsymbol{L}+\boldsymbol{R}}(X) = \frac{1}{2}\varrho^{-1}X$ for $X \in \mathrm{T}^{||}$. The matrix (a_{ij}) is given by proposition 2 or 3. Inserting these equations into

$$g = \frac{1}{2} \operatorname{Tr} \left(\boldsymbol{P}(\mathrm{d}\varrho) \frac{1}{\boldsymbol{L}+\boldsymbol{R}} \boldsymbol{P}(\mathrm{d}\varrho) + \mathrm{d}\varrho \frac{1}{\boldsymbol{L}+\boldsymbol{R}} \boldsymbol{P}^{\perp}(\mathrm{d}\varrho) \right)$$

yields the following.

Proposition 4. *The decomposition $g = g_{\restriction_{\mathrm{T}^{||}}} + g_{\restriction_{\mathrm{T}^{||\perp}}}$ of the Bures metric is given by*

$$g = \frac{1}{4} \sum_{i,j=1}^{n} \frac{\mathrm{d}p_i}{i} (P^{-1})_{ij} \frac{\mathrm{d}p_j}{j} + \frac{1}{4} \sum_{i,j=1}^{n} (2a_{ij} - (P^{-1})_{ij}) \operatorname{Tr} \mathrm{d}\varrho\, \varrho^{i-1}\, \mathrm{d}\varrho\, \varrho^{j-1}. \tag{18}$$

4. Examples

Propositions 1–4 involve elementary and power invariants, which can be expressed by each other (cf [11]). Rewriting the identity

$$mk_m + \sum_{r=1}^{m} p_r k_{m-r} = 0 \qquad m = 1, 2, \ldots$$

as a system of linear equations for the e_i resp. the p_i one obtains the relations

$$e_i = \frac{1}{i!} \det \begin{bmatrix} p_1 & 1 & 0 & \ldots & 0 \\ p_2 & p_1 & 2 & \ldots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ p_{i-1} & p_{i-2} & p_{i-3} & \ldots & i-1 \\ p_i & p_{i-1} & p_{i-2} & \ldots & p_1 \end{bmatrix}$$

$$p_i = \det \begin{bmatrix} e_1 & 1 & 0 & \ldots & 0 \\ 2e_2 & e_1 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ (i-1)e_{i-1} & e_{i-2} & e_{i-3} & \ldots & 1 \\ ie_i & e_{i-1} & e_{i-2} & \ldots & e_1 \end{bmatrix}.$$

This identity also allows for expressing a power invariant p_m, $m > n$, by invariants of a degree less or equal to n. Especially the $i+1$-row of our matrix P equals $(p_{i+1}, \ldots, p_{n+i}) = (p_1, \ldots, p_n)K^i$.

The number of terms in propositions 1–4 rapidly increases with the dimension n. Thus we give only certain expressions for $n = 2, 3$ in terms of power resp. elementary invariants. Concerning proposition 1 we get

$$g(X', X) := \frac{1}{2} \begin{cases} \operatorname{Tr} X'(\varrho^2 + e_1\varrho + e_2\mathbf{1})^{-1}(\varrho X - X\varrho + e_1 X) & \text{for } n = 2 \\ \operatorname{Tr} X'(\varrho^3 + e_1\varrho^2 + e_2\varrho + e_3\mathbf{1})^{-1} & \\ \qquad \times(\varrho^2 X - \varrho X\varrho + X\varrho^2 + e_1(\varrho X - X\varrho) + e_2 X) & \text{for } n = 3. \end{cases}$$

The following terms appear in propositions 2–4:

$n = 2$:

$$g_{\restriction_{\mathrm{T}^{\|}}} = \frac{1}{4(p_1p_3 - p_2^2)} \left(\frac{\mathrm{d}p_1}{1} \;,\; \frac{\mathrm{d}p_2}{2} \right) \begin{bmatrix} p_3 & -p_2 \\ -p_2 & p_1 \end{bmatrix} \begin{pmatrix} \frac{\mathrm{d}p_1}{1} \\ \frac{\mathrm{d}p_2}{2} \end{pmatrix}$$

$$= \frac{1}{4e_2(e_1^2 - 4e_2)} (\mathrm{d}e_1 \;,\; \mathrm{d}e_2) \begin{bmatrix} e_1e_2 & -2e_2 \\ -2e_2 & e_1 \end{bmatrix} \begin{pmatrix} \mathrm{d}e_1 \\ \mathrm{d}e_2 \end{pmatrix}$$

$$A = \frac{1}{2e_1e_2} \begin{bmatrix} e_1^2 + e_2 & -e_1 \\ -e_1 & 1 \end{bmatrix}$$

$$2A - P^{-1} = \frac{2}{e_1(e_1^2 - 4e_2)} \begin{bmatrix} -2e_2 & e_1 \\ e_1 & -2 \end{bmatrix} = \frac{2}{p_1(2p_2 - p_1^2)} \begin{bmatrix} p_2 - p_1^2 & p_1 \\ p_1 & -2 \end{bmatrix}$$

$n = 3$:

$$\det P = -p_3^3 + 2p_2p_3p_4 - p_1p_4^2 - p_2^2p_5 + p_1p_3p_5$$

$$P^{-1} = \frac{1}{\det P} \begin{bmatrix} p_3p_5 - p_4^2 & p_3p_4 - p_2p_5 & p_2p_4 - p_3^2 \\ * & p_1p_5 - p_3^2 & p_2p_3 - p_1p_4 \\ * & * & p_1p_3 - p_2^2 \end{bmatrix}$$

$$A = \frac{1}{2e_3(e_1e_2 - e_3)} \begin{bmatrix} e_1e_2^2 + e_1^2e_3 - e_2e_3 & -e_1^2e_2 & e_1e_2 - e_3 \\ * & e_1^3 + e_3 & -e_1^2 \\ * & * & e_1 \end{bmatrix}.$$

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References

[1] Uhlmann A 1992 The metric of Bures and the geometric phase *Quantum Groups and Related Topics* ed R Gielerak *et al* (Dordrecht: Kluwer) pp 267–74

[2] Uhlmann A 1986 Parallel transport and 'quantum holonomy' *Rep. Math. Phys.* **24** 229–40

[3] Dittmann J and Uhlmann A 1998 Connections and metrics respecting purification of quantum states *J. Math. Phys.* to appear

[4] Hübner M 1992 Explicit computation of the Bures distance for density matrices *Phys. Lett.* A **163** 239–42

[5] Dittmann J 1993 On the Riemannian geometry of finite dimensional mixed states *Sem. S. Lie* **3** 73–87

[6] Twamley J 1996 Bures and statistical distance for squeezed thermal states *J. Phys. A: Math. Gen.* **29** 3723

[7] Slater P B 1998 Bures metrics for certain high-dimensional quantum systems *Phys. Lett.* A **244** 35–42

[8] Slater P B 1996 Quantum Fisher–Bures information and two-level systems and a tree-level extension *J. Phys. A: Math. Gen.* **29** L271–5

[9] Bhatia R and Rosenthal P 1997 How and why to solve the operator equation $AX - XB = Y$ *Bull. Lond. Math. Soc.* **29** 1–21

[10] Smith R A 1966 Matrix calculations for Lyapunov quadratic forms *J. Diff. Eqns* **2** 208–17

[11] MacDonald I G 1995 *Symmetric Functions and Hall Polynomials* (Oxford: Clarendon)

[12] Petz D 1996 Monotone metrics on matrix spaces *Linear Algebr. Appl.* **244** 81–96

[13] Braunstein S L and Caves C M 1994 Statistical distance and the geometry of quantum states *Phys. Rev. Lett.* **72** 3439–43