Symmetries, group actions, and entanglement

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**Abstract.** We address several problems concerning the geometry of the space of Hermitian operators on a finite-dimensional Hilbert space, in particular the geometry of the space of density states and canonical group actions on it. For quantum composite systems we discuss and give examples of measures of entanglement.

1. Introduction

In his book [1], Dirac uses the description of the interference phenomena, via the superposition rule, to justify the requirement of linearity on the carrier space of states to deal with quantum evolution. However, the probabilistic interpretation of state vectors forces us the identification of physical (pure) states with points of the complex projective space associated with the starting vector space of "states". With this identification a (global) linear structure is no more available, now interference phenomena will be described with the help of a connection (Pancharatnam connection) [2]. The Hermitian structure available on the starting Hilbert space of "states" induces a Kählerian structure on the complex projective space. The induced action of the unitary group, projected from the one on the Hilbert space, allows for the imbedding of the complex projective space into the dual of the Lie algebra of the unitary group itself by means of the momentum map associated with the symplectic action of the group. Within this ambient space, by means of the available linear structure, it is possible to construct convex combinations of pure states (rank-one projectors) and build the totality of density states.
The space so constructed is not linear and gives rise to interesting geometrical structures. To deal with these various non-linearities, recently [3], elaborating on previous geometrical approaches to quantum mechanics [4], we have considered the differential geometry of density states. This approach seems to be quite appropriate to deal with composite systems and the set of separable and entangled states which do not carry a linear structure. In this note we would like to further elaborate on some subtle points which we have encountered in our previous paper [3]. To make the paper self-contained we briefly recall the main results from our previous treatment. The paper is organized as follows: after introducing notations and conventions, in Section 3 we describe the basic geometric structures useful in description of the density states, in particular the invariant Kähler structures on the orbits of unitary representations as well as an action of the general linear group on the dual of the Lie algebra of the unitary group. The description of this action in terms of the Kraus operators along with some of their properties is further elaborated in Sections 5 and 6, where a general linear group action on density states is discovered. In Section 7 we describe the geometry of the set of density states as a convex body, in particular we discuss the smoothness of its boundary. The rest of the paper is devoted to description of the composite systems: in Section 8 we describe the pure and mixed states of such systems in terms of the Segre imbedding and give a general prescription for the construction of entanglement measures. Examples of such constructions are given in Sections 9 and 10 for bipartite and multipartite systems.

2. Notations and conventions

Let $\mathcal{H}$ be an $n$-dimensional Hilbert space with the Hermitian product $\langle x, y \rangle_{\mathcal{H}}$ being, by convention, $\mathbb{C}$-linear with respect to $y$ and anti-linear with respect to $x$. The unitary group $U(\mathcal{H})$ acts on $\mathcal{H}$ preserving the Hermitian product and it consists of those complex linear operators $A \in \text{gl}(\mathcal{H})$ on $\mathcal{H}$ which satisfy $AA^\dagger = I$, where $A^\dagger$ is the Hermitian conjugate of $A$, i.e., $\langle Ax, y \rangle_{\mathcal{H}} = \langle x, A^\dagger y \rangle_{\mathcal{H}}$. The geometric approach to Quantum Mechanics is based on the realification $\mathcal{H}_{\mathbb{R}}$ of $\mathcal{H}$ considered as a Kähler manifold $(\mathcal{H}_{\mathbb{R}}, J, g, \omega)$ with canonical structures: a complex structure $J$, a Riemannian metric $g$, and a symplectic form $\omega$. The latter come from the real and the imaginary parts of the Hermitian product, respectively. After the obvious identification of the vectors tangent to $\mathcal{H}_{\mathbb{R}}$ with $\mathcal{H}_{\mathbb{R}}$, all these structures are constant (do not depend on the actual point of $\mathcal{H}_{\mathbb{R}}$) and read

$$J(x) = i \cdot x, \quad g(x, y) + i \cdot \omega(x, y) = \langle x, y \rangle_{\mathcal{H}}.$$

We have obvious identities

$$J^2 = -I, \quad \omega(x, Jy) = g(x, y), \quad g(Jx, Jy) = g(x, y), \quad \omega(Jx, Jy) = \omega(x, y).$$
Fixing an orthonormal basis \((e_k)\) of \(\mathcal{H}\) allows us to identify the Hermitian product \(\langle x, y \rangle_\mathcal{H}\) on \(\mathcal{H}\) with the canonical Hermitian product on \(\mathbb{C}^n\) of the form \(\langle a, b \rangle_{\mathbb{C}^n} = \sum_{k=1}^{n} a_k b_k\), the group \(U(\mathcal{H})\) of unitary transformations of \(\mathcal{H}\) with \(U(n)\), its Lie algebra \(u(\mathcal{H})\) with \(u(n)\), etc. In this picture \((a_{jk})^\dagger = (\alpha_{kj})\) and \((T^\dagger T)_{jk} = \langle \alpha_j, \alpha_k \rangle\), where \(\alpha_k = (t_{jk}) \in \mathbb{C}^n\) are columns of the matrix \(T = (t_{jk})\). The choice of the basis induces (global) coordinates \((q_k, p_k), k = 1, \ldots, n,\) on \(\mathcal{H}_\mathbb{R}\) by

\[ \langle e_k, x \rangle_\mathcal{H} = (q_k + i \cdot p_k)(x), \]

in which \(\partial_{q_k}\) is represented by \(e_k\) and \(\partial_{p_k}\) by \(i \cdot e_k\). Hence the complex structure reads

\[ J = \sum_k \left( \partial_{p_k} \otimes dq_k - \partial_{q_k} \otimes dp_k \right), \]

the Riemannian tensor

\[ g = \sum_k \left( dq_k \otimes dq_k + dp_k \otimes dp_k \right) = \frac{1}{2} \sum_k \left( dq_k \wedge dp_k + dp_k \wedge dq_k \right) \]

and the symplectic form

\[ \omega = \sum_k dq_k \wedge dp_k, \]

where \(x \wedge y = x \otimes y + y \otimes x\) is the symmetric, and \(x \wedge y = x \otimes y - y \otimes x\) is the wedge product. In complex coordinates \(z_k = q_k + i \cdot p_k\) one can write the Hermitian product as the complex tensor \(\langle \cdot, \cdot \rangle_\mathcal{H} = \sum_k \langle z_k \otimes d\bar{z}_k \rangle\).

One important convention we want to introduce is that we will identify the space of Hermitian operators \(A = A^\dagger\) with the dual \(u^*(\mathcal{H})\) of the (real) Lie algebra \(u(\mathcal{H})\), according to the pairing between Hermitian \(A \in u^*(\mathcal{H})\) and anti-Hermitian \(T \in u(\mathcal{H})\) operators \(\langle A, T \rangle = \frac{i}{2} \cdot \text{Tr}(AT)\). The multiplication by \(i\) establishes further a vector space isomorphism \(u(\mathcal{H}) \ni T \mapsto iT \in u^*(\mathcal{H})\) which identifies the adjoint and the coadjoint action of the group \(U(\mathcal{H})\), \(\text{Ad}_U(T) = U T U^\dagger\). Under this isomorphism \(u^*(\mathcal{H})\) becomes a Lie algebra with the Lie bracket \([A, B] = \frac{1}{2} [A, B]_\cdot\) (where \([A, B]_- = AB - BA\) is the commutator bracket), equipped additionally with the scalar product

\[ \langle [A, B], [A, B] \rangle_{u^*(\mathcal{H})} = \frac{1}{2} \text{Tr}(AB) \]

and an additional algebraic operation, the Jordan product (or bracket) \([A, B]_+ = AB + BA\). The scalar product is invariant with respect to both: the Lie bracket and the Jordan product

\[ \langle [A, \xi], [B] \rangle_{u^*(\mathcal{H})} = \langle A, [\xi, B] \rangle_{u^*(\mathcal{H})}, \]

\[ \langle [A, \xi]_+, [B] \rangle_{u^*(\mathcal{H})} = \langle A, [\xi, B]_+ \rangle_{u^*(\mathcal{H})}. \]
and it identifies once more $u^*(\mathcal{H})$ with its dual, $u^*(\mathcal{H}) \ni A \mapsto \hat{A} = \frac{1}{i}A \in u(\mathcal{H})$, so vectors with covectors. Under this identification the metric \( \langle \cdot , \cdot \rangle \) corresponds to the invariant metric
\[
\langle \hat{A}, \hat{B} \rangle_u = \frac{1}{2} \text{Tr}(AB) \tag{4}
\]
on $u(\mathcal{H})$ which can be viewed also as a contravariant metric on $u^*(\mathcal{H})$.

For a (real) smooth function $f$ on $\mathcal{H}_\mathbb{R}$ let us denote by $\text{grad}_f$ and $\text{Ham}_f$ the gradient and the Hamiltonian vector field associated with $f$ and the Riemannian and the symplectic tensor, respectively. In other words, $g(\cdot , \text{grad}_f) = df$ and $\omega(\cdot , \text{Ham}_f) = df$. We can define also the corresponding Poisson and Riemann-Jordan brackets of smooth functions on $\mathcal{H}$ by
\[
\{ f, f' \}_\omega = \omega(\text{Ham}_f, \text{Ham}_{f'}), \quad \{ f, f' \}_g = g(\text{grad}_f, \text{grad}_{f'})
\]
and the total bracket by $\{ f, f' \}_{\mathcal{H}} = \{ f, f' \}_g + i \{ f, f' \}_\omega$. Note that any complex linear operator $A \in \text{gl}(\mathcal{H})$ induces a linear vector field $\tilde{A}$ on $\mathcal{H}$ by $\tilde{A}(x) = Ax$ and a quadratic function $f_A(x) = \frac{1}{2} \langle x, Ax \rangle_\mathcal{H}$. The function $f_A$ is real if and only if $A$ is Hermitian, $A = A^\dagger$. It is easy to see the following.

**THEOREM 1.**

(a) For Hermitian $A$ we have
\[
\text{grad}_{f_A} = \hat{A} \quad \text{and} \quad \text{Ham}_{f_A} = i\hat{A}.
\]

(b) For all $A, B \in \text{gl}(\mathcal{H})$ we have $\{ f_A, f_B \}_{\mathcal{H}} = f_{2AB}$. In particular,
\[
\{ f_A, f_B \}_g = f_{AB+BA}, \tag{5}
\]
\[
\{ f_A, f_B \}_\omega = f_{-i(AB-BA)}. \tag{6}
\]

The unitary action of $U(\mathcal{H})$ on $\mathcal{H}$ is in particular Hamiltonian and induces a momentum map $\mu : \mathcal{H}_\mathbb{R} \to u^*(\mathcal{H})$. The fundamental vector field associated with $\frac{1}{i}A \in u(\mathcal{H})$, where $A \in u^*(\mathcal{H})$ is Hermitian, reads $\hat{A}$, since
\[
\frac{d}{dt} \big|_{t=0} \exp(-\frac{t}{i}A)(x) = iA(x).
\]
The Hamiltonian of the vector field $\hat{A}$ is $f_A$, so the momentum map is defined by
\[
\langle \mu(x), \frac{1}{i}A \rangle = f_A(x) = \frac{1}{2} \langle x, Ax \rangle_\mathcal{H}.
\]

But by our convention
\[
\langle \mu(x), \frac{1}{i}A \rangle = \frac{i}{2} \text{Tr}(\mu(x)\frac{1}{i}A) = \frac{1}{2} \text{Tr}(\mu(x)A),
\]
so that $\text{Tr}(\mu(x)A) = \langle x, Ax \rangle_{\mathcal{H}}$ and finally, in the Dirac notation,

$$\mu(x) = |x\rangle\langle x|.$$  \hspace{1cm} (7)

Hence, the image of this momentum map consists of all non-negative Hermitian operators of rank $\leq 1$. The space of all non-negatively defined operators, i.e. of those $\rho \in \mathfrak{gl}(\mathcal{H})$ which can be written in the form $\rho = T^\dagger T$ for a certain $T \in \mathfrak{gl}(\mathcal{H})$, we denote by $\mathcal{P}(\mathcal{H})$. It is a convex cone in $u^*(\mathcal{H})$. The set of density states $\mathcal{D}(\mathcal{H})$ is distinguished in the cone $\mathcal{P}(\mathcal{H})$ by the equation $\text{Tr}(\rho) = 1$, so it is a convex body in $u^*(\mathcal{H})$. Denote by $\mathcal{P}^k(\mathcal{H})$ (resp., $\mathcal{D}^k(\mathcal{H})$) the set of all non-negative hermitian operators (resp., density states) of rank $k$. In the standard terminology, $\mathcal{D}^1(\mathcal{H})$ is the space of pure states, i.e. the set of one-dimensional orthogonal projectors $|x\rangle\langle x|$, $\|x\| = 1$.

It is known that the set of extreme points of $\mathcal{D}(\mathcal{H})$ coincides with the set $\mathcal{D}^1(\mathcal{H})$ of pure states (see Corollary 2). Hence every element of $\mathcal{D}(\mathcal{H})$ is a convex combination of points from $\mathcal{D}^1(\mathcal{H})$. The space $\mathcal{D}^1(\mathcal{H})$ of pure states can be identified with the complex projective space $\mathbb{C}P^{n-1}$ via the projection

$$\mathcal{H} \setminus \{0\} \ni x \mapsto \frac{|x\rangle\langle x|}{\|x\|^2} \in \mathcal{D}^1(\mathcal{H})$$

which identifies the points of the orbits of the $\mathbb{C} \setminus \{0\}$-group action by complex homoteties. It is well known that $\mathcal{D}^1(\mathcal{H})$ is canonically a Kähler manifold. This will be the starting point for the study of geometry of $u^*(\mathcal{H})$ and the set $\mathcal{D}(\mathcal{H})$ of all density states.

### 3. Geometry of $u^*(\mathcal{H})$

Recall that $u^*(\mathcal{H})$ is canonically an Euclidean space with the scalar product $\langle A, B \rangle_{u^*} = \frac{1}{2} \text{Tr}(AB)$. We have also seen that $u^*(\mathcal{H})$ is canonically a Lie and a Jordan algebra with the brackets $[A, B] = \frac{i}{2} (AB - BA)$ and $[A, B]_+ = AB + BA$, respectively. Note also that, for $A$ being Hermitian, $f_A$ is the pullback $f_A = \mu^*(\hat{A}) = \hat{A} \circ \mu$, where $\hat{A} = \langle A, \cdot \rangle_{u^*} = \frac{1}{i} A \in u(\mathcal{H})$. The linear functions $\hat{A}$ generate the cotangent bundle $T^*u^*(\mathcal{H})$, so that (5) and (6) mean that the momentum map $\mu$ relates the contravariant analogs of $g$ and $\omega$, respectively, with the linear contravariant tensors $R$ and $\Lambda$ on $u^*(\mathcal{H})$ corresponding to the Jordan and Lie bracket, respectively. The Riemann-Jordan tensor $R$, defined in the obvious way,

$$R(\xi)(\hat{A}, \hat{B}) = \langle \xi, [A, B]_+ \rangle_{u^*} = \frac{1}{2} \text{Tr}(\xi(AB + BA)),$$

is symmetric and the tensor

$$\Lambda(\xi)(\hat{A}, \hat{B}) = \langle \xi, [A, B] \rangle_{u^*} = \frac{1}{2i} \text{Tr}(\xi(AB - BA)),$$

(8)
is the canonical Kostant-Kirillov-Souriau Poisson tensor on $u^*(\mathcal{H})$. They form together the complex tensor

$$ (R + i \cdot \Lambda)(\xi)(\hat{A}, \hat{B}) = 2\langle \xi, AB \rangle_{u^*} = \text{Tr}(\xi AB) \quad (10) $$

and the momentum map relates this tensor with the Hermitian product.

On $u^*(\mathcal{H})$ consider the (generalized) distributions $D_\Lambda$ and $D_R$ induced by the tensor fields $\Lambda$ and $R$, respectively. To be more precise, Denote by $\tilde{\mathcal{J}}$ and $\tilde{\mathcal{R}}$ the $(1,1)$-tensors on $u^*(\mathcal{H})$, viewed as vector bundle morphism induced by the contravariant tensors $\Lambda$ and $R$, respectively,

$$ \tilde{\mathcal{J}} \xi (A) = [A, \xi] = \Lambda_\xi (A), $$

$$ \tilde{\mathcal{R}} \xi (A) = [A, \xi ]_+ = R_\xi (A), $$

for $A \in u^*(\mathcal{H}) \cong T_\xi u^*(\mathcal{H})$. The image of $\tilde{\mathcal{J}}$ is $D_\Lambda$ and the image of $\tilde{\mathcal{R}}$ is $D_R$. It is easy to see that the tensors $\tilde{\mathcal{J}}$ and $\tilde{\mathcal{R}}$ commute and

$$ \tilde{\mathcal{J}}_\xi \circ \tilde{\mathcal{R}} \xi (A) = \tilde{\mathcal{R}}_\xi \circ \tilde{\mathcal{J}}_\xi (A) = [A, \xi_2^2]. \quad (11) $$

We will consider also the generalized distributions $D_1 = D_R + D_\Lambda$ and $D_0 = D_R \cap D_\Lambda$.

1. Distribution $D_\Lambda$.

It is well known that the distribution $D_\Lambda$ can be integrated to a generalized foliation $\mathcal{F}_\Lambda$ whose leaves are orbits of the canonical $U(\mathcal{H})$-action on $u^*(\mathcal{H})$ given by $U(\mathcal{H}) \times u^*(\mathcal{H}) \ni (U, \xi) \mapsto U \xi U^\dagger \in u^*(\mathcal{H})$. They are represented by the spectrum of the operator, i.e. $\rho$ and $\rho'$ belong to the same $U(\mathcal{H})$-orbit if and only if they have the same set of eigenvalues (counted with multiplicities). Moreover, the orbits are symplectic leaves of the Poisson structure $\Lambda$ with the corresponding $U(\mathcal{H})$-invariant symplectic form $\eta^O$. These symplectic structures can be extended to canonical Kähler structures as shows the following.

**THEOREM 2.**

(a) $\tilde{\mathcal{J}}^2_\xi \gamma$ is a self-adjoint with respect to $\langle \cdot, \cdot \rangle_{u^*}$ and non-positively defined operator on $u^*(\mathcal{H})$ with the kernel $D_\Lambda(\xi)^\perp$.

(b) The $(1,1)$-tensor $\mathcal{J}$ on $u^*(\mathcal{H})$ defined by

$$ \mathcal{J}_\xi (A) = \begin{cases} 
0 & \text{if } A \in D_\Lambda(\xi)^\perp \\
\tilde{\mathcal{J}}_\xi \circ (-(\tilde{\mathcal{J}}_\xi^2)_{D_\Lambda(\xi)}^{-\frac{1}{2}} (A) & \text{if } A \in D_\Lambda(\xi)
\end{cases} \quad (12) $$

satisfies $J^3 = -J$ and induces an $U(\mathcal{H})$-invariant complex structure $\mathcal{J}$ on every $U(\mathcal{H})$-orbit $O$. 
(c) For every $U(\mathcal{H})$-orbit $O$ the tensor
\[ \gamma^O_\xi(A, B) = \eta^O_\xi(A, J_\xi(B)) \] (13)
is an $U(\mathcal{H})$-invariant Riemannian metric on $O$ and
\[ \gamma^O_\xi(J_\xi(A), B) = \eta^O_\xi(A, B), \quad A, B \in D_\Lambda(\xi). \] (14)
In particular, $(O, J, \eta^O, \gamma^O)$ is a homogeneous Kähler manifold. Moreover, if $\xi \in u^*(\mathcal{H})$ is a projector, $\xi^2 = \xi$, and $\xi \in O$, then $J_\xi = J_\xi$ and $\gamma^O(A, B) = \langle A, B \rangle_{u^*}$.

Remark. The tensor $J$ is canonically and globally defined. It is however not smooth as a tensor field on $u^*(\mathcal{H})$. It is smooth on the open-dense subset of regular elements and, of course, on every $U(\mathcal{H})$-orbit separately.

2. Distribution $D_R$.
We have some similar results for the tensor $\tilde{R}$ which however are not completely analogous, since the distribution $D_R$ is not integrable.

THEOREM 3.

(a) $\tilde{R}^2_\xi$ is a self-adjoint with respect to $\langle \cdot, \cdot \rangle_{u^*}$ and non-negatively defined operator on $u^*(\mathcal{H})$ with the kernel $D_\Lambda(\xi)^\perp$.

(b) The $(1, 1)$-tensor $R$ on $u^*(\mathcal{H})$ defined by
\[ R_\xi(A) = \begin{cases} 0 & \text{if } A \in D_R(\xi)^\perp, \\ \tilde{R}_\xi \circ |\tilde{R}_\xi|_{D_R(\xi)}^{-1}(A) & \text{if } A \in D_R(\xi) \end{cases} \] (15)
satisfies $R^3 = R$.

3. Distribution $D_0$.
The distribution $D_0 = D_\Lambda \cap D_R$ can be described also as the image of $J_\xi \circ R_\xi = R_\xi \circ J_\xi$. In other words, $D_0(\xi) = \{[A, \xi^2] : A \in u^*(\mathcal{H})\}$.

THEOREM 4. The distribution $D_0$ is integrable and the corresponding foliation $\mathcal{F}_0$ is $U(\mathcal{H})$-invariant, $J$-invariant and $R$-invariant, so that $J$ and $R$ induce on leaves of $\mathcal{F}_0$ a complex and a product structure, respectively. The leaves of the foliation $\mathcal{F}_0$ are also canonically symplectic manifolds with symplectic structures being restrictions of symplectic structures on the leaves of $\mathcal{F}_\Lambda$, so the leaves of $\mathcal{F}_0$ are Kähler submanifolds of the $U(\mathcal{H})$-orbits in $u^*(\mathcal{H})$. 
Note however, that $D_0$ coincides with $D_\Lambda$ on $P(\mathcal{H})$, so that on density states the leaves of $\mathcal{F}_0$ are just the orbits of the unitary group action.

4. Distribution $D_1$.

The distribution $D_1 = D_\Lambda + DR$ is the largest one carrying the most qualitative information. It turns out to be related to a $GL(\mathcal{H})$-action as shows the following.

THEOREM 5.

(a) The generalized distributions $D_1$ is involutive and can be integrated to generalized foliations $\mathcal{F}_1$ whose leaves are the orbits of the $GL(\mathcal{H})$-action $GL(\mathcal{H}) \times u^* (\mathcal{H}) \ni (T, \xi) \mapsto T\xi T^\dagger \in u^* (\mathcal{H})$.

(b) The Hermitian operators $\rho$ and $\rho'$ belong to the same $GL(\mathcal{H})$-orbit if and only if they have the same number $k_+$ of positive and the same number $k_-$ of negative eigenvalues (counted with multiplicities). Such an orbit, denoted by $u_{k_+,k_-}^*(\mathcal{H})$, is of (real) dimension $2nk - k^2$, where $k = k_+ + k_-$, and its tangent spaces are described by the formula

$$B \in T_\xi u_{k_+,k_-}^*(\mathcal{H}) \iff \forall x,y \in \text{Ker}(\xi) \quad \langle Bx,y \rangle_{\mathcal{H}} = 0.$$  \hfill (16)

(c) Any $GL(\mathcal{H})$-orbit intersecting $P(\mathcal{H})$ lies entirely in $P(\mathcal{H})$, so that $P(\mathcal{H})$ is stratified by the $GL(\mathcal{H})$-orbits. The $GL(\mathcal{H})$-orbits in $P(\mathcal{H})$ are determined by the rank of an operator, i.e. they are exactly $P_k(\mathcal{H})$, $k = 0, 1, \ldots, n$.

The proofs of all results in this section can be found in [3].

4. Explicit coordinates on $GL(\mathcal{H})$-orbits

A choice of an orthonormal basis in $\mathcal{H}$ gives an identification $u^* (\mathcal{H}) \simeq u^* (n)$.

Let $J = \{j_1, \ldots, j_k\} \subset \{1, \ldots, n\}$. Denote $u_{J}^*(n)$ – the open subset in the set $u_{k}^*(n)$ of rank-$k$ Hermitian matrices consisting of matrices $(a_{ij}) \in u_{k}^*(n)$ for which the submatrix $(a_{rs})_{r,s \in J}$ is invertible with the inverse $(a_{rs})_{r,s \in J}$.

LEMMA 6. Let $\xi \in u_{J}^*(n)$. Then the matrix $\xi$ is uniquely determined by its rows indexed by $J$, according to the formula

$$a_{ij} = \sum_{r,s \in J} a_{ir}a_{rs}^{-1}a_{js}.$$ 

THEOREM 7. The maps

$$\Phi_J : u_{J}^*(n) \to \mathbb{R}^k \times \mathbb{C}^{(2nk - k^2 - k)/2} \simeq \mathbb{R}^{2nk - k^2},$$

$$\Phi_J((a_{ij})_{i,j=1}^n) = ((a_{ii})_{i \in J}, (a_{rs})_{r<s,s \in J})$$

form a coordinate system in the manifold $u_{k}^*(n)$. 

THEOREM 8. If a Kraus operator is completely positive, the linear operations which are operations for certain $A$ assume any normalization condition for $K$ ically a Hilbert space with the Hermitian product $\langle K, d \rangle$. Determine the Hermitian matrix of rank 2 whose principal minor is non-vanishing. Which, by definition, are operations and that in this case $A$ implies that one can speak of the semigroup of Kraus operators. Indeed, $K = \Phi_J \rho$ for certain $\rho A B C = 0$. Moreover $K = \Phi_J \rho$ for certain $\rho A B C = 0$. Let us note that the space $gl(\mathcal{H})$ of all complex linear operators on $\mathcal{H}$ is canonically a Hilbert space with the Hermitian product $\langle A, B \rangle_{gl} = \frac{1}{2} \text{Tr}(A^\dagger B)$. Using the Jamiołkowski isomorphism one can identify the Kraus operator $K_A$ with a Hermitian operator on the Hilbert space $gl(\mathcal{H})$, defined as $P_A = \sum_i p_{A_i}$, where $p_{A_i} = |A_i \rangle \langle A_i |$. Using the spectral decomposition one can easily see that any Kraus operator $K_A$ can be written in a canonical form $K_A(\rho) = K_C(\rho) = \sum_k C \rho C^\dagger$, where the operators $C_k \in gl(\mathcal{H})$ are pairwise orthogonal, $\langle C_k, C_{k'} \rangle_{gl} = 0$ for $k \neq k'$, and that in this case $A_i = \alpha_{i,k} C_k$ with $\sum_i \alpha_{i,k} \alpha_{i,k'} = \delta_{k,k'}$.

It is interesting that the operators of the $GL(\mathcal{H})$-action form exactly the largest subgroup in the semigroup of Kraus operators. Since in the literature we could find the analogous fact only for the unitary group and the semigroup of normalized Kraus operators, we will give a short proof of this general result.

THEOREM 8. If a Kraus operator $K_A$ is invertible inside Kraus operators, then $K_A(\rho) = A \rho A^\dagger$ for certain $A \in GL(\mathcal{H})$.

Proof. Assume $K_A^{-1} = K_B$, so that $\sum_{i,j} (A_i B_j) \rho (A_i B_j)^\dagger = \rho$. According to the last observation, $A_i B_j = \alpha_{ij} I$ for certain $\alpha_{ij} \in \mathbb{C}$ with $\sum_{ij} |\alpha_{ij}|^2 = 1$. There is $\alpha_{i_0 j_0} \neq 0$, so $A_{i_0}$ and $B_{j_0}$ are invertible. Moreover $A_{i_0}$ is proportional to $B_{j_0}^{-1}$, namely $A_{i_0} = \alpha_{i_0 j_0} B_{j_0}^{-1}$. Since we can clearly assume that all $A_i$ and all $B_j$ are non-zero, we get that all $A_i$ and all $B_j$ are invertible. Indeed, $A_i$ is not invertible implies that $A_i B_{j_0} = \alpha_{i j_0} I$ is not invertible thus zero, so $A_i = 0$, because $B_{j_0}$ is.
invertible, and similarly for $B_j$. Moreover, every $A_i$ is proportional to $B_{j_0}^{-1}$, whence to $A_{i_0}$, $A_i = \gamma_i A_{i_0}$, $\gamma_i \neq 0$. We get therefore

$$K_A(\rho) = \sum_i A_i \rho A_i^\dagger = (\sqrt{\gamma} A_{i_0}) \rho (\sqrt{\gamma} A_{i_0})^\dagger,$$

where $\gamma = \sum_i |\gamma_i|^2$. $\blacksquare$

6. **Kraus and $GL(\mathcal{H})$-action on density states**

We know already that $P^k(\mathcal{H})$ are $GL(\mathcal{H})$-orbits in $u^*(\mathcal{H})$, so smooth submanifolds. We used this fact in [3] to show that their intersections with the hyperplane $\text{Tr}(\rho) = 1$, i.e. $D^k(\mathcal{H})$ are smooth submanifolds too. Here we want to stress that, in fact, $D^k(\mathcal{H})$ can be regarded again as $GL(\mathcal{H})$-orbits with respect to an action of $GL(\mathcal{H})$ on $D(\mathcal{H})$. Of course, we cannot apply directly the action on $u^*(\mathcal{H})$, as $D(\mathcal{H})$ is not an invariant set under this action. We can, however, modify the $GL(\mathcal{H})$-action (in fact, even the Kraus action) on $P(\mathcal{H})$ in such a way that we get an action on density states whose orbits are $D^k(\mathcal{H})$.

For, suppose $K_A(\rho) = \sum_i A_i \rho A_i^\dagger$ is a non-degenerate Kraus operation, i.e. $\sum_i A_i^\dagger A_i \in GL(\mathcal{H})$. Now, let us define an operation $\tilde{K}_A$ on $D(\mathcal{H})$ by

$$\tilde{K}_A(\rho) = \frac{K_A(\rho)}{\text{Tr}(K_A(\rho))}.$$

The definition makes sense, since $\text{Tr}(K_A(\rho)) > 0$ for any density state $\rho$. Indeed, since

$$\text{Tr}(K_A(\rho)) = \text{Tr}\left(\sum_i A_i \rho A_i^\dagger\right) = \text{Tr}\left((\sum_i A_i^\dagger A_i) \rho\right)$$

and $T = \sum_i A_i^\dagger A_i$ is invertible Hermitian and non-negative, so strictly positive, and since $\rho$ in Hermitian non-negative, $\text{Tr}(T \rho) \leq 0$ only if $\rho = 0$.

Now, it is a fundamental observation that we get in this way really an action of the semigroup of Kraus operations, i.e. that $\tilde{K}_A \circ \tilde{K}_B = \tilde{K}_{A \cdot B}$. But it is straightforward, since

$$\tilde{K}_A \circ \tilde{K}_B(\rho) = \frac{K_A\left(\frac{K_B(\rho)}{\text{Tr}(K_B(\rho))}\right)}{\text{Tr}\left(K_A\left(\frac{K_B(\rho)}{\text{Tr}(K_B(\rho))}\right)\right)} = \frac{K_A \circ K_B(\rho)}{\text{Tr}(K_A \circ K_B(\rho))} = \tilde{K}_{A \cdot B}(\rho).$$

Note that, though this action is not affine, convex sets are mapped into convex sets, as

$$\tilde{K}_A(\lambda \rho + (1 - \lambda) \rho') = \lambda \tilde{K}_A(\rho) + (1 - \lambda) \tilde{K}_A(\rho'),$$

(17)
where
\[ \tilde{\lambda} = \frac{\lambda \text{Tr}(\tilde{K}_A(\rho))}{\lambda \text{Tr}(\tilde{K}_A(\rho)) + (1 - \lambda) \text{Tr}(\tilde{K}_A(\rho'))} . \]

Of course, we can reduce this action of the semigroup of non-degenerate Kraus operations to its largest subgroup, i.e. to $GL(H)$, obtaining the action
\[ GL(H) \times D(H) \ni (A, \rho) \mapsto \tilde{A}(\rho) = \frac{A \rho A^\dagger}{\text{Tr}(A \rho A^\dagger)} \in D(H). \] (18)

This action preserves the rank and one can easily derive from Theorem 3 the following.

**THEOREM 9.** The decomposition of the convex body of density states $D(H)$ into orbits of the $GL(H)$-action (18) is exactly the stratification $D(H) = \bigcup_{k=1}^n D^k(H)$ into states of a given rank.

### 7. The geometry of density states

The boundary $\partial D(H)$ of the convex body of density states consists of the states of rank $< n$, $\partial D(H) = \bigcup_{k=1}^{n-1} D^k(H)$. Each stratum $D^k(H)$ is a smooth submanifold in $u^*(H)$. However, the boundary $\partial D(H)$ is not smooth (except for the case $n = 2$), since its maximal stratum $D^{n-1}(H)$ is sewed up along $\bigcup_{k=1}^{n-2} D^k(H)$ with edges there, as shows the following ([3], Theorem 2).

**THEOREM 10.** Every smooth curve $\gamma : \mathbb{R} \rightarrow u^*(H)$ through the convex body of density states is at every point tangent to the stratum to which it actually belongs, i.e. $\gamma(t) \in D^k(H)$ implies $T\gamma(t) \in T_{\gamma(t)} D^k(H)$.

The above theorem means that inside $D(H)$ we cannot smoothly cross the stratum $D^k(H)$ of the boundary transversally to it, like living on a cube we cannot smoothly cross an edge of the cube transversally to it.

**Corollary 1.** The boundary of the convex body $D(H)$ of density states is a smooth submanifold of $u^*(H)$ if and only if $\text{dim}(H) \leq 2$.

**Remark.** It is well known that for $n = 2$ the convex set of density states is the three-dimensional ball and its boundary – the two-dimensional sphere (so called Bloch sphere), so it is a smooth manifold.

The next problem concerning the geometry of density states we will consider is the question of the faces of $D(H)$, i.e. the intersections of $D(H)$ with supporting affine hyperplanes. In other words, a non-empty closed convex subset $K_0$ of a closed convex set $K$ is called a face (or extremal subset) of $K$ if any closed segment in $K$ with an interior point in $K_0$ lies entirely in $K_0$; a point $x$ is called an extremal
point of $K$ if the set $\{x\}$ is a face of $K$. For $\rho \in \mathcal{D}(\mathcal{H})$ consider the decomposition

$$\mathcal{H} = \mathcal{H}_+^\rho \oplus \mathcal{H}_0^\rho = \text{Im}(\rho) \oplus \text{Ker}(\rho), \quad x = x_+^\rho + x_0^\rho, \quad (19)$$

into the kernel and the image of $\rho$.

**THEOREM 11.** The face of $\mathcal{D}(\mathcal{H})$ through $\rho \in \mathcal{D}^k(\mathcal{H})$ consists of operators $A \in \mathcal{D}(\mathcal{H})$ which, according to the decomposition (19), have the form $A(x_+^\rho + x_0^\rho) = A_+^\rho(x_+^\rho)$ for certain $A_+^\rho \in \mathcal{D}(\text{Im}(\rho))$, so it is affinely equivalent to the convex body of density states in dimension $k$.

**Corollary 2** Extremal points of $\mathcal{D}(\mathcal{H})$ are exactly pure states.

**Corollary 3** All non-trivial faces of $\mathcal{D}(\mathcal{H})$ of maximal dimension, i.e. faces through $\mathcal{D}^{n-1}(\mathcal{H})$, are tangent to the sphere $S(I/n; r)$, centered at $I/n$ with the radius $r = \frac{1}{\sqrt{n(n-1)}}$, at points which are collinear with the center and one of the pure states.

### 8. Composite systems and separability

Suppose now that our Hilbert space has a fixed decomposition into the tensor product of two Hilbert spaces $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ (of dimensions $n_1$ and $n_2$, respectively). This additional input is crucial in studying composite quantum systems and it has a great impact on the geometrical structures we have considered. The rest of this paper will be devoted to related problems.

Observe first that the tensor product map

$$\bigotimes : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \quad (20)$$

associates the product of rays with a ray, so it induces a canonical imbedding on the level of complex projective spaces

$$\text{Seg} : \mathcal{P}\mathcal{H}_1 \times \mathcal{P}\mathcal{H}_2 \to \mathcal{P}\mathcal{H} = \mathcal{P}(\mathcal{H}_1 \otimes \mathcal{H}_2),$$

$$(|x^1\rangle\langle x^1|, |x^2\rangle\langle x^2|) \mapsto |x^1 \otimes x^2\rangle|x^1 \otimes x^2\rangle. \quad (22)$$

This imbedding of product of complex projective spaces into the projective space of the tensor product is called in the literature the *Segre imbedding* [6]. The elements of the image $\text{Seg}(\mathcal{P}\mathcal{H}_1 \times \mathcal{P}\mathcal{H}_2)$ in $\mathcal{P}\mathcal{H} = \mathcal{P}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ are called *separable* pure states (with respect to the decomposition $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$).

The Segre imbedding is related to the (external) tensor product of the basic representations of the unitary groups $U(\mathcal{H}_1)$ and $U(\mathcal{H}_2)$, i.e. with the representation of the direct product group in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$,

$$U(\mathcal{H}_1) \times U(\mathcal{H}_2) \ni (\rho^1, \rho^2) \mapsto \rho^1 \otimes \rho^2 \in U(\mathcal{H}) = U(\mathcal{H}_1 \otimes \mathcal{H}_2),$$

$$(\rho^1 \otimes \rho^2)(x^1 \otimes x^2) = \rho^1(x^1) \otimes \rho^2(x^2).$$
Note that $\rho_1 \otimes \rho_2$ is unitary, since the Hermitian product in $\mathcal{H}$ is related to the Hermitian products in $\mathcal{H}^1$ and $\mathcal{H}^2$ by

$$\langle x^1 \otimes x^2, y^1 \otimes y^2 \rangle_{\mathcal{H}} = \langle x^1, y^1 \rangle_{\mathcal{H}^1} \cdot \langle x^2, y^2 \rangle_{\mathcal{H}^2}. \quad (23)$$

The above group imbedding gives rise to the corresponding imbedding of Lie algebras or, by our identification, of their duals, which, with some abuse of notation, we will denote by

$$\text{Seg} : u^*(\mathcal{H}^1) \times u^*(\mathcal{H}^2) \to u^*(\mathcal{H}), \quad (\xi_1, \xi_2) \mapsto \xi_1 \otimes \xi_2. \quad (24)$$

The original Segre imbedding is just the latter map reduced to pure states. In fact, a more general result holds true.

**Proposition 1** The imbedding (24) maps $D^k(\mathcal{H}^1) \times D^l(\mathcal{H}^2)$ into $D^{kl}(\mathcal{H})$.

Let us denote the image $\text{Seg}(D^1(\mathcal{H}^1) \times D^1(\mathcal{H}^2))$ – the set of *separable pure states* – by $S^1(\mathcal{H})$, and its convex hull $\text{conv}(S^1(\mathcal{H}))$ – the set of all *separable states* in $u^*(\mathcal{H})$ – by $S(\mathcal{H})$. The states from

$$E(\mathcal{H}) = D(\mathcal{H}) \setminus S(\mathcal{H}),$$

i.e. those which are not separable, are called *entangled states*. It is well known (see e.g. [3]) that $S^1(\mathcal{H})$ is exactly the set of extremal points of $S(\mathcal{H})$.

Of course, by means of the tensor product of representations the group product $GL(\mathcal{H}^1) \times GL(\mathcal{H}^2)$ is canonically embedded in $GL(\mathcal{H})$ like in the case of the unitary groups. The canonical actions (18) on $D(\mathcal{H}^1)$ and $D(\mathcal{H}^2)$ give rise to the action to the corresponding action of $GL(\mathcal{H}^1) \times GL(\mathcal{H}^2)$ on $D(\mathcal{H}^1) \times D(\mathcal{H}^2)$:

$$(\tilde{A}_1, \tilde{A}_2)(\rho_1, \rho_2) = (\tilde{A}_1(\rho_1), \tilde{A}_2(\rho_2)).$$

On the other hand, $GL(\mathcal{H}^1) \times GL(\mathcal{H}^2)$ as being embedded in $GL(\mathcal{H})$ acts on $D(\mathcal{H})$.

**THEOREM 12.** The aforementioned actions of $GL(\mathcal{H}^1) \times GL(\mathcal{H}^2)$ are equivariant with respect to the Segre map

$$\text{Seg} : D(\mathcal{H}^1) \times D(\mathcal{H}^2) \to D(\mathcal{H}).$$

Moreover, the set $S^1(\mathcal{H})$ of pure separable states and the set $S(\mathcal{H})$ of all separable states are invariant with respect to the canonical $GL(\mathcal{H}^1) \times GL(\mathcal{H}^2)$-action on $D(\mathcal{H})$:

$$(\tilde{A}_1, \tilde{A}_2)(\rho) = \frac{(A_1 \otimes A_2)\rho(A_1 \otimes A_2)^\dagger}{\text{Tr}((A_1 \otimes A_2)\rho(A_1 \otimes A_2)^\dagger)}.$$
Proof. We get easily

\[
(\tilde{A}_1, \tilde{A}_2)(\rho_1 \otimes \rho_2) = \frac{(A_1 \rho_1 A_1^\dagger) \otimes (A_2 \rho_2 A_2^\dagger)}{\text{Tr}((A_1 \rho_1 A_1^\dagger) \otimes (A_2 \rho_2 A_2^\dagger))} = \frac{(A_1 \rho_1 A_1^\dagger) \otimes (A_2 \rho_2 A_2^\dagger)}{\text{Tr}(A_1 \rho_1 A_1^\dagger) \text{Tr}(A_2 \rho_2 A_2^\dagger)} = \tilde{A}_1(\rho_1) \otimes \tilde{A}_2(\rho_2)
\]

that proves equivariance and the invariance of \(S^1(\mathcal{H})\). The invariance of \(S(\mathcal{H})\) is not automatic, like in the case of the group \(U(\mathcal{H}^1) \times U(\mathcal{H}^2)\), since the \(GL(\mathcal{H}^1) \times GL(\mathcal{H}^2)\)-action is not affine. On the other hand, (17) implies that the convex hull thus separability is respected:

\[
(\tilde{A}_1, \tilde{A}_2)(\lambda \rho_1 \otimes \rho_2 + \lambda' \rho'_1 \otimes \rho'_2) = \tilde{\lambda}(\tilde{A}_1, \tilde{A}_2)(\rho_1 \otimes \rho_2) + \tilde{\lambda}'(\tilde{A}_1, \tilde{A}_2)(\rho'_1 \otimes \rho'_2) = \tilde{\lambda}A_1(\rho_1) \otimes \tilde{A}_2(\rho_2) + \tilde{\lambda}'A_1(\rho'_1) \otimes \tilde{A}_2(\rho'_2),
\]

where \(\lambda' = 1 - \lambda\) and \(\tilde{\lambda}' = 1 - \tilde{\lambda}\). □

It is a common opinion that the \(U(\mathcal{H}^1) \times U(\mathcal{H}^2)\)-action, as preserving separability, is crucial for understanding the entanglement. We see, however, that the \(GL(\mathcal{H}^1) \times GL(\mathcal{H}^2)\)-action preserves the separability as well and, since the orbits are larger, it carries more qualitative information, thus information which is easier to handle. As an example, consider the corresponding \(U(\mathcal{H}^1) \times U(\mathcal{H}^2)\) and \(GL(\mathcal{H}^1) \times GL(\mathcal{H}^2)\) orbits inside pure states.

**Proposition 2** With respect to the Schmidt decomposition

\[
|\Psi\rangle = \sum_{k=1}^m \lambda_k |\varphi_k^1\rangle \otimes |\varphi_k^2\rangle
\]  

(25)

of the unit vector \(|\Psi\rangle \in \mathcal{H}\) representing a pure state, the \(U(\mathcal{H}^1) \times U(\mathcal{H}^2)\)-orbits in \(D^1(\mathcal{H})\) are distinguished by the sequence \(\lambda_1 \geq \ldots \lambda_m > 0\), while the \(GL(\mathcal{H}^1) \times GL(\mathcal{H}^2)\)-orbits are distinguished only by the Schmidt number \(m\).

**Proof.** It is clear that the form of the Schmidt decomposition is preserved by the \(U(\mathcal{H}^1) \times U(\mathcal{H}^2)\)-action. On the other hand, if we have two such decompositions \(\sum_{k=1}^m \lambda_k |\varphi_k^1\rangle \otimes |\varphi_k^2\rangle\) and \(\sum_{k=1}^m \lambda_k |\eta_k^1\rangle \otimes |\eta_k^2\rangle\), then, since \(\varphi_k^1\) are pairwise orthonormal, since \(\varphi_k^2\) are pairwise orthonormal, etc., there are \(U^i \in U(\mathcal{H}^i), i=1,2\), such that \(U^1(\varphi_k^1) = \eta_k^1\) and \(U^2(\varphi_k^2) = \eta_k^2\), \(k = 1, \ldots, m\), so

\[
(U^1 \otimes U^2)(\sum_{k=1}^m \lambda_k |\varphi_k^1\rangle \otimes |\varphi_k^2\rangle) = \sum_{k=1}^m \lambda_k |\eta_k^1\rangle \otimes |\eta_k^2\rangle.
\]

A similar reasoning gives the description of \(GL(\mathcal{H}^1) \times GL(\mathcal{H}^2)\)-orbits, if we only take into account that the exact values of the coefficients \(\lambda_k\) are irrelevant for this
action, as the group does not respect the length of the vector.

The entangled states play an important role in quantum computing and one of main problems is to decide effectively whether a given composite state is entangled or not. An abstract measurement of entanglement can be based on the following observation (see also Ref. [7]).

Let \( E \) be the set of all extreme points of a compact convex set \( K \) in a finite-dimensional real vector space \( V \) and let \( E_0 \) be a compact subset of \( E \) with the convex hull \( K_0 = \text{conv}(E_0) \subset K \). For every non-negative function \( f : E \rightarrow \mathbb{R}_+ \) define its extension \( f_K : K \rightarrow \mathbb{R}_+ \) by

\[
f_K(x) = \inf_{x=\sum_i \alpha_i} \sum_i t_i f(\alpha_i),
\]

where the \( \infimum \) is taken with respect to all expressions of \( x \) in the form of convex combinations of points from \( E \). Recall that, according to Krein-Milman theorem, \( K \) is the convex hull of its extreme points.

THEOREM 13. For every non-negative continuous function \( f : E \rightarrow \mathbb{R}_+ \) which vanishes exactly on \( E_0 \) the function \( f_K \) is convex on \( K \) and vanishes exactly on \( K_0 \).

Corollary 4 Let \( F : D^1(\mathcal{H}^1 \otimes \mathcal{H}^2) \rightarrow \mathbb{R}_+ \) be a continuous function which vanishes exactly on \( S^1(\mathcal{H}^1 \otimes \mathcal{H}^2) \). Then

\[
\mu = F_{D(\mathcal{H}^1 \otimes \mathcal{H}^2)} : D(\mathcal{H}^1 \otimes \mathcal{H}^2) \rightarrow \mathbb{R}_+
\]

is a measure of entanglement, i.e. \( \mu \) is convex and \( \mu(x) = 0 \iff x \in S(\mathcal{H}) \). Moreover, if \( f \) is taken \( U(\mathcal{H}^1) \times U(\mathcal{H}^2) \)-invariant (resp. \( GL(\mathcal{H}^1) \times GL(\mathcal{H}^2) \)-invariant), then \( \mu \) is \( U(\mathcal{H}^1) \times U(\mathcal{H}^2) \)-invariant (resp. \( GL(\mathcal{H}^1) \times GL(\mathcal{H}^2) \)-invariant).

9. Bipartite entanglement

One of measures constructed according to the above described prescription is the concurrence introduced originally as an auxiliary quantity, used to calculate so called entanglement of formation of \( 2 \times 2 \) systems [8]. For pure states [25] it is defined as

\[
c(\Psi) := \sqrt{1 - \text{Tr}_1 \rho_1^2} = \sqrt{||\Psi||^2 - \text{Tr}_1 \left( \text{Tr}_2(|\Psi\rangle \langle \Psi|) \cdot \text{Tr}_2(|\Psi\rangle \langle \Psi|) \right)},
\]

where \( \text{Tr}_i, i = 1, 2 \), denotes tracing over the \( i \)-th subsystem, and \( \rho_1 := \text{Tr}_2 |\Psi\rangle \langle \Psi| \).

It is clear that, indeed, it vanishes for separable states (for which \( \text{Tr}_1 \rho_1^2 = 1 \)). For
further generalizations (see Section 10) it is convenient to rewrite (27) in slightly different form. To this end let us define:

\[ A : \mathcal{H} \otimes \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}, \quad A = 4P_+^{(1)} \otimes P_+^{(2)}, \]  

(28)

where \( P_+^{(i)} \) is the orthogonal projection on the antisymmetric part \( \mathcal{H}_i \wedge \mathcal{H}_i \) of the tensor product \( \mathcal{H}_i \otimes \mathcal{H}_i \), and we identify in an obvious manner \( \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_1 \otimes \mathcal{H}_2 \) and \( \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_2 \). It is now a matter of a straightforward calculation that \( c(\Psi) \) can be expressed as:

\[ c(\Psi) = \sqrt{\left( \langle \Psi | \otimes \langle \Psi | \right) A (|\Psi \rangle \otimes |\Psi \rangle)}. \]

(29)

Extension of the concurrence (27) to mixed states is defined via (26), i.e.

\[ c(\rho) = \inf_{\rho = \sum t_i |\Psi_i \rangle \langle \Psi_i |} \sum t_i c(\Psi_i). \]

(30)

Calculation of \( c(\rho) \) for an arbitrary mixed state \( \rho \) requires a high dimensional optimization procedure, it is however possible to derive a lower bound for it which in general suffices to discriminate between a separable and an entangled state. Our bound is given by a purely algebraic expression easily evaluated for arbitrary states and can be, if needed, tightened numerically by optimizing over a parameter space of much lower dimensionality than it is demanded by the original definition (30) [9, 10]. To this end we first replace the \( |\Psi_i \rangle \) by the subnormalized states \( |\psi_i \rangle = \sqrt{t_i} |\Psi_i \rangle \) in Eq. (30). Given a valid decomposition \( \rho = \sum |\phi_i \rangle \langle \phi_i | \) into \( M \) subnormalized states \( \{|\phi_i \rangle, i = 1, \ldots, M\} \), any other suitable set \( \{|\psi_i \rangle, i = 1, \ldots, N\} \) such that

\[ \rho = \sum |\psi_i \rangle \langle \psi_i |, \]

(31)

is obtained [11] by:

\[ |\psi_i \rangle = \sum_{j=1}^{M} V_{ij} |\phi_j \rangle, \quad V \in \mathbb{C}^{N \times M}, \quad \sum_{i=1}^{N} V_{ik} \overline{V_{ij}} = \delta_{jk}, \]

(32)

where both \( N \) and \( M \) are not smaller than the rank \( r \) of \( \rho \). It can be shown [12] that for the purposes of the present considerations, it is enough to take \( N \leq n_1 n_2 \). We can now choose as the starting point eg. the decomposition \( \{|\phi_i \rangle, i = 1, \ldots, r\} \) of \( \rho \) defined in terms of its (subnormalized) eigenvectors

\[ \rho = \sum_{i=1}^{r} |\phi_i \rangle \langle \phi_i |, \quad \rho |\phi_i \rangle = a_i |\phi_i \rangle, \]

(33)
where $a_i, i = 1, \ldots, r$, are non-vanishing eigenvalues of $\rho$. Now the concurrence can be rewritten as:

$$c(\rho) = \inf_V \sum_i \sqrt{\langle (V \otimes V) A (V^\dagger \otimes V^\dagger) \rangle_{ii}}^i,$$

(34)

where

$$A_{jk}^m = \langle \phi_j | \langle \phi_m | A (|\phi_j \rangle \otimes |\phi_k \rangle),$$

(35)

and the infimum is now taken on over matrices $V$ fulfilling (32). The expression simplifies further if expressed in terms of eigenvectors of $A$, i.e.

$$A = \sum_{\alpha=1}^m |\chi_\alpha\rangle \langle \chi_\alpha|,$$  

$\alpha = 1, \ldots, m = n_1(n_1 - 1)n_2(n_2 - 1)/4$. Namely

$$c(\rho) = \inf_V \sum_i \sqrt{\sum_\alpha |V T^\alpha V^T|_{ii}}^i,$$

(36)

where $T^\alpha_{jk} = (|\alpha\rangle (|\phi_j \rangle \otimes |\phi_k \rangle))$. Obviously any given decomposition (31) provides a straightforward upper bound of the concurrence, $c(\rho) \leq \sum_i \sqrt{\sum_\alpha |T^\alpha_{ii}(\psi)|^2}$. From the point of view of distinguishing separable and entangled states it is much more interesting to find a lower bound for $c$ in an effective way. To this end let us write, using Cauchy-Schwarz inequality,

$$\sum_\alpha |V T^\alpha V^T|_{ii} \geq \sum_\alpha |V z_\alpha T^\alpha V^T|_{ii} \geq \sum_\alpha |V z_\alpha T^\alpha V^T|_{ii}^2,$$

(37)

for arbitrary $z_\alpha$, $\alpha = 1, \ldots, m$. We obtain thus:

$$c(\rho) \geq \inf_V \sum_{i=1}^N \left| V \left( \sum_\alpha z_\alpha T^\alpha \right) V^T \right|_{ii},$$

(38)

for arbitrary $z_\alpha$ such that $\sum_\alpha |z_\alpha|^2 = 1$. The infimum over $V$ can be effectively performed and is given by max $\{ \lambda_1 - \sum_{i>1} \lambda_i, 0 \}$, where $\lambda_j$ are the singular values of $T = \sum_\alpha z_\alpha T^\alpha$, i.e. the square roots of the eigenvalues of the positive hermitian matrix $TT^\dagger$ in the decreasing order [13]. The obtained bound still depends on the choice of the $z_\alpha$, what allows to tighten the estimate. Thus, one is left with an optimization problem on an $2m$-dimensional sphere. Note that the constraint $\sum_\alpha |z_\alpha|^2 = 1$ is by far simpler to implement than $V^T V$ (cf. 32). Moreover, the dimension $m$ of optimization space is significantly reduced as compared to the dimension $n_1^2 n_2^2$ of the original optimization problem defined by Eq. (32). Let us, however, point out that any choice of $z_\alpha$ gives some lower bound and taking eg. all but one $z_\alpha$ equal to zero, we can dispose of the optimization entirely if we are only interested whether $c$ is positive, which is enough to establish nonseperability of the state in question [9].
10. Multipartite entanglement

Separability of multipartite systems, where the Hilbert space of the whole system $\mathcal{H}$ has a fixed decomposition into the tensor product of Hilbert spaces $\mathcal{H} = \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_K$ of subsystems of dimensions $n_1, \ldots, n_K$ is defined by a straightforward extension of the two-component case (cf. Section 8), i.e. via a canonical imbedding of the product of projective spaces $P\mathcal{H}_1 \times \ldots \times P\mathcal{H}_K$ into the projectivisation of the tensor product $P(\mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_K)$ and the corresponding imbedding on the level of Lie algebras and their duals. The pure separable states are thus identified with the image under this imbedding of $D(\mathcal{H}_1) \times \ldots \times D(\mathcal{H}_K)$ and its convex hull with the set of all separable states.

In order to investigate the separability of multipartite states we proposed the following generalization of the concurrence considered in the preceding section [14]. Let us, in an analogy with (28) define

$$A_{\{s_j\}} : \mathcal{H} \otimes \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H}, \quad A_{\{s_j\}} = 2^K \bigotimes_{j=1}^K P_{s_j}^{(j)}, \quad (39)$$

where $s_j = \pm$ and $P_{s_j}^{(j)}$ (respectively $P_{s_j}^{(j)}$) are orthogonal projections on the anti-symmetric (resp. symmetric) subspace $\mathcal{H}_j \wedge \mathcal{H}_j$ (resp. $\mathcal{H}_j \vee \mathcal{H}_j$), define concurrence for pure states as

$$c_{\{s_j\}}(\Psi) = \sqrt{\langle \Psi | \otimes \langle \Psi | A_{\{s_j\}} | \Psi \rangle \otimes | \Psi \rangle}, \quad (40)$$

and its extension to mixed states by

$$c_{\{s_j\}}(\rho) = \inf_{\rho = \sum t_i |\Psi_i\rangle \langle \Psi_i|} \sum t_i c_{\{s_j\}}(\Psi_i). \quad (41)$$

Closer examination of the action of $A_{\{s_j\}}$ reveals that if an odd number of projectors on anti-symmetric subspaces appears in its definition, the corresponding $c_{\{s_j\}}(\Psi)$ vanishes identically. Moreover, if $s_i = +$ for all $i$, i.e. when only projections on symmetric subspaces are involved, $A_{\{s_j\}}$ is not helpful in detecting entanglement [14, 15].

The techniques which were devised to ease the task of estimating the concurrence for arbitrary states in the bipartite case in the previous section, can be generalized in a straightforward manner, because the algebraic structure of the above $K$-partite concurrences is strictly identical to the bipartite definition (30). Thus one can invoke the Cauchy-Schwarz and the triangle inequality and bound the concurrence of an arbitrary mixed state from below by

$$c_{\{s_j\}}(\rho) = \inf_{V} \sum_i \sqrt{\sum_\alpha \|VTV^T\|_{ii}^{\alpha_i}} \geq \inf_{V} \sum_i \|VTV^T\|_{ii} \geq \max\left\{\lambda_1 - \sum_{j>1} \lambda_j, 0\right\}, \quad (42)$$
where \( T = \sum_{\alpha} z_{\alpha} T^{\alpha} \), \( T^{\alpha}_j = \langle \chi_{\alpha} | \langle \phi_j \rangle \otimes | \phi_k \rangle \rangle \), \( A_{\{s_j\}} = \sum_{\alpha=1} \langle \chi_{\alpha} | \chi_{\alpha} \rangle \otimes | \phi_k \rangle \rangle \) are the subnormalized eigenvectors of \( \rho \), \( V \) defines the transition between different decompositions of \( \rho \) as in (32), and \( \lambda_j \) are eigenvalues of \( T^{\dagger} T \) in decreasing order. For the proof of the last equality in (42) see [13] or [10]. As in the bipartite case, the inequality (42) holds for an arbitrary set of complex numbers \( z_{\alpha} \), such that \( \sum_{\alpha} |z_{\alpha}|^2 = 1 \), what allows for further optimization.

The above does not only apply to the discrete set of concurrences discussed so far, but also to the following continuous interpolation between them: Instead of a single direct product of projectors onto symmetric and anti-symmetric subspaces, one may equally well consider convex combinations thereof,

\[
A = 2^K \sum_{s_1, \ldots, s_K} p_{s_1, \ldots, s_K} P^{(1)}_{s_1} \otimes \cdots \otimes P^{(K)}_{s_K} \tag{43}
\]

where \( s_i \in \{+, -\}, p_{s_1, \ldots, s_K} \geq 0 \) and the summation is restricted to contributions with an even, non-zero number of projectors onto anti-symmetric subspaces. The corresponding pure-state concurrence \( \text{(10)} \) can be written in terms of the partial traces:

\[
c(\Psi) = \sqrt{\sum_{S \in 2^{\{1, \ldots, K\}}} \alpha_S \text{Tr} \left( \text{Tr}_A (|\Psi\rangle \langle \Psi|)^2 \right)}, \tag{44}
\]

where \( 2^{\{1, \ldots, K\}} \) denotes the set of all subsets of \( \{1, \ldots, K\} \), and

\[
\alpha_S = \sum_{s_1, \ldots, s_K} p_{s_1, \ldots, s_K} \prod_{i \in S} s_i. \tag{45}
\]

Various choices of the coefficients \( p_{s_1, \ldots, s_K} \) allow to distinguish different categories of multipartite entanglement. As an illustration, let us focus on some exemplary tri- and four-partite concurrences.

The so-called biseparable pure states (i.e. states taking the form of tensor product of a state of one subsystem with a, possibly entangled, state of the other two subsystems) in the tri-partite case are easily detected with \( A = P^{(1)}_+ \otimes P^{(2)}_+ \otimes P^{(3)}_- \), \( A = P^{(1)}_- \otimes P^{(2)}_+ \otimes P^{(3)}_- \), and \( A = P^{(1)}_- \otimes P^{(2)}_- \otimes P^{(3)}_+ \). Whereas corresponding concurrences vanish identically for bi-separable states like \( |\psi\rangle = |\varphi_{12}\rangle \otimes |\zeta_3\rangle \) for the first and second choice of \( A \), the last one which reduces to the bi-partite concurrence of \( |\varphi_{12}\rangle \).

Similarly, different kinds of separability are also captured in larger systems. For example, concurrences defined with the help of \( A = 4P^{(1)}_{s_1} \otimes P^{(2)}_{s_2} \otimes P^{(3)}_{s_3} \otimes P^{(4)}_{s_4} \), \( s_i = s_j = + \), and \( s_k = - \) for \( i \neq k \neq j \), determine with respect to which bipartite partition a mixed 4-particle state is separable, and quantify the value of bi-, resp. tri-partite concurrences of the entangled part \( \text{(4)} \).
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