Entropy and optimal decompositions of states relative to a maximal commutative subalgebra

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Abstract

To calculate the entropy of a subalgebra or of a channel with respect to a state, one has to solve an intriguing optimalization problem. The latter is also the key part in the entanglement of formation concept, in which case the subalgebra is a subfactor.

I consider some general properties, valid for these definitions in finite dimensions, and apply them to a maximal commutative subalgebra of a full matrix algebra. The main method is an interplay between convexity and symmetry. A collection of helpful tools from convex analysis is collected in an appendix.

INTRODUCTION

This paper considers the entropy of a subalgebra or of a completely positive map with respect to a state, an entropy-like quantity introduced by A. Connes, H. Narnhofer, and W. Thirring. I remain, however, within a rather narrow setting: A pair of algebras, *-isomorphic to the algebra of all \( d \times d \)-matrices, and to its subalgebra of diagonal matrices. I depart from this restriction within this introduction and in discussing some tools from convex analysis (lemmata 1, 2, 3, and appendix).

While the von Neumann entropy is of undoubted relevance for type I algebras (with discrete center), the relative entropy can be meaningfully defined even on the state

\footnote{Dedicated to Walter Thirring at his 70th birthday}
space of an arbitrary \( * \)-algebra. There are, depending on the category of algebras and states, several quite different ways to do so, \[8\].

In \[5\] Narnhofer and Thirring proposed a von Neumann entropy definition by the aid of relative entropy. At the end of their paper they mentioned a quantity now denoted by \( H_\omega(A) \) or \( H_\omega(B|A) \) where \( A \) is a unital subalgebra of \( B \), and \( \omega \) a state of \( B \). Abbreviating the restriction of \( \omega \) onto \( A \) by \( \tilde{\omega} \),

\[
\omega \mapsto \tilde{\omega} := \omega|_A,
\]

their definition reads

\[
H_\omega(B|A) = H_\omega(A) := \sup \sum p_j S(\tilde{\omega}_j, \tilde{\omega}), \quad A \subset B
\]

\[\text{(*)}\]

In this expression \( S(\ldots) \) is the relative entropy for the states of \( A \) and the supremum has to run through all convex decompositions

\[
\omega = \sum p_j \omega_j
\]

of the state \( \omega \) on \( B \). \( \text{(*)} \) was later called “entropy of a subalgebra with respect to a state”.

It depends concavely on the state, is always non-negative, and it inherits from relative entropy its monotonicity:

\[
A_1 \subset A_2 \subset B \longrightarrow H_\omega(A_1) \leq H_\omega(A_2) \leq S(\omega)
\]

According to \[3\] \( S(\omega) = H_\omega(B|B) \) is the von Neumann entropy of \( \omega \).

\( \text{(*)} \) amounts to calculate a number. Seeing the ease and elegance of the definition one might perhaps not believe what a formidable task this is. The calculational difficulties are mainly encoded in \( R \), a functional defined by

\[
H_\omega(B|A) + R(B|A, \omega) = H_\omega(A|A) \equiv S(\tilde{\omega})
\]

where \( \omega \) is a state of \( B \).

All terms are non-negative. If \( S(\tilde{\omega}) < \infty \) they are finite. \( R \) is the convex hull of the function \( \omega \rightarrow S(\tilde{\omega}) \), as explained below. In the finite dimensional case one may write

\[
R(B|A, \omega) = \inf \sum p_j S(\tilde{\varrho}_j),
\]

the infimum being taken over all extremal convex combinations

\[
\omega = \sum p_j \varrho_j, \quad \varrho_k \text{ pure}
\]

Therefore, \( R \) is already determined by its values at pure states.
In the present paper $\mathcal{A}$ is a maximal commutative subalgebra. The case of a general subalgebra has been considered by Benatti, Narnhofer, and Uhlmann, \[10\]. But their main examples concern maximal commutative subalgebras. The same is with the paper of Benatti, \[11\], who shows a relation of (*) to accessible entropy. An example with another subalgebra is in \[14\].

Results and completely independent definitions for the subfactor problem are due to Bennett, DiVincenzo, Smolin, and Wootters, \[13\], who aimed at the $R$-function on the states of a direct product of two finite dimensional factors. They defined the entanglement of formation by

$$\mathcal{A} \textit{ a subfactor } \to E(\omega) \equiv R(\omega) = \textit{ entanglement of } \omega \textit{ with respect to } \mathcal{A}$$

in order to measure entanglement as a resource for quantum information transfer. They obtained estimates and solved interesting examples. Because the reductions of a pure state to a factor and to its commutant have the same entropy, there is a nice symmetry

$$R(\mathcal{B}_1 \otimes \mathcal{B}_2|\mathcal{B}_1, \omega) = R(\mathcal{B}_1 \otimes \mathcal{B}_2|\mathcal{B}_2, \omega)$$

Hill and Wootters, \[15\], solved the problem for rank two states on the direct product of two 2-dimensional matrix algebras.

The definition (*) can be extended to a completely positive unital map, $\alpha$, from one algebra to another one,

$$\alpha : \mathcal{A} \mapsto \mathcal{B}$$

Its transpose, a stochastic mapping,

$$\omega \mapsto \omega \circ \alpha, \quad (\omega \circ \alpha)(A) = \omega(\alpha(A)), \quad A \in \mathcal{A}$$

maps states of $\mathcal{B}$ to those of $\mathcal{A}$.

To get the definition one has only to set $\tilde{\omega} := \omega \circ \alpha$ within (*) to obtain the desired quantity $H_\omega(\alpha)$. This is an invention of Connes, Narnhofer, and Thirring in \[4\].

Ohio and Petz called $\alpha$ a \textit{channel map} acting from the \textit{output algebra} $\mathcal{A}$ to the \textit{input algebra} $\mathcal{B}$, so that its transpose, a stochastic mapping, acts from the states of the input algebra into the state space of the output one. In their monograph \[5\], in which they consider the problem within the $C^*$- and the $W^*$-category, $H_\omega(\alpha)$ is called entropy of the channel $\alpha$ with respect to the state $\omega$. Now the monotonicity property reads

$$H_\omega(\alpha_1 \circ \alpha_2) \leq H_\omega(\alpha_1) \leq S(\omega)$$

whenever $\alpha_1 \circ \alpha_2$ is well defined, unital, and completely positive. As known, the latter requirement can be weakened to Schwarz positivity

$$\alpha(A^*A) \geq |\alpha(A)|^2 \quad \forall \ A \in \mathcal{A}$$

\[2\text{Meanwhile, B.W.Wootters has solved the 2-qubit case completely, quant-ph/9709029 v2.}\]
GENERAL PROPERTIES

Let $\mathcal{H}$ be a Hilbert space of finite dimension $\dim \mathcal{H} = d$, and $\mathcal{C}$ a maximal commuting subalgebra of $\mathcal{B} := \mathcal{B}(\mathcal{H})$. Let us denote by $P_j = |j\rangle\langle j|$, $j = 1, 2, \ldots, d$, the minimal projection operators of $\mathcal{C}$. They support the distinguished pure states $\varrho_j^C$, i.e.

$$P_j \rho P_j = \varrho_j^C(B) P_j, \quad \forall \, B \in \mathcal{B}$$  \hspace{1cm} (1)

The density matrix of a state of $\mathcal{B}$ is contained in $\mathcal{C}$ iff the latter is a convex combination of the pure states $\varrho_k^C$. The restriction $\tilde{\omega}$ of a state $\omega$ onto $\mathcal{C}$ can hence be described by the reduction map

$$\omega \rightarrow \tilde{\omega} := \sum \omega(P_j) \varrho_j^C$$  \hspace{1cm} (2)

Now we consider entropies. All what is needed is nicely reviewed in [3]. The entropy of the restriction $\tilde{\omega}$ of $\omega$ onto $\mathcal{C}$ reads

$$\bar{S}(\omega) := S(\bar{\omega}) = - \sum \omega(P_j) \ln(\omega(P_j))$$  \hspace{1cm} (3)

It is now possible to write down the entropy of $\mathcal{C}$ with respect of a state $\omega$ of $\mathcal{B}$ as defined by Narnhofer and Thirring [4], Connes [6], and [7]. In the case at hand the general definition is equivalent to

$$H_\omega(\mathcal{C}) := \bar{S}(\omega) - R(\omega), \quad R(\omega) = \inf \sum p_j \bar{S}(\omega_j)$$  \hspace{1cm} (4)

where the infimum runs through all convex decompositions

$$\omega = \sum p_j \omega_j$$  \hspace{1cm} (5)

in the state space $\Omega$ of $\mathcal{B}$. Rockafellar [11] calls the construction used in defining $R$ the convex hull of $\bar{S}$. The convex hull of any function on any convex set is always convex. Thus $H_\omega$ is the sum of two concave functions, $\bar{S}$ and $-R$, and hence concave.

For the following it is essential that $R$ is the convex hull of a concave function, and that $\Omega$ as well as $\Omega^{ex}$, the set of its extremal points, are compact. Being the state space of $\mathcal{B}$, a state is extremal iff it is pure. A state $\varrho$ is pure iff there is a projection operator $P \in \mathcal{B}$, the support of $\varrho$, such that $PBP = \varrho(B) P$ for all $B$ in that algebra. Notice: lemmata 1, 2, and 3 below are valid for every unital subalgebra, the restriction to a maximal commutative subalgebra is not essential for their validity.

The first conclusion is due to the concavity of $\bar{S}$: It is possible to restrict (3) to extremal convex decompositions,
\[ R(\omega) = \inf \sum p_j \tilde{S}(\varrho_j), \quad \varrho_k \in \Omega^\text{ex}, \quad \sum p_j \varrho_j = \omega \]  

(6)

Let us call *optimal* every extremal convex decomposition of \( \omega \) with which the infimum (6) is attained, and for which \( p_k > 0 \) for all its coefficients \([10]\). Thus optimality is expressed by

\[ R(\omega) = \sum p_j \tilde{S}(\varrho_j), \quad \varrho_k \in \Omega^\text{ex}, \quad \forall p_k > 0 \]  

(7)

The graph of \( R \) is a closed subset of the boundary of a compact convex set, \([4]\), see appendix. It implies, by standard arguments, that there are optimal decompositions for every state. Then, according to Carathéodory, there exist simplicial ones. This is the content of

**Lemma 1**

Every \( \omega \) admits an optimal decomposition with at least \( \text{rank}(\omega) \) and at most \( \text{rank}(\omega)^2 \) different pure states. \( \Box \)

I need some further, almost obvious conclusions from the definition of \( R \). For the time being a convex subset \( \Omega_0 \) of \( \Omega \) will be called an \( R \)-set if every \( \omega \in \Omega_0 \) admits an optimal decomposition into pure states of \( \Omega_0 \). It is clear that

a) every \( R \)-set \( \Omega_0 \) of the state space is the convex hull of its pure states. (Therefore, the pure states contained in \( \Omega_0 \) are just the extremal elements of \( \Omega_0 \).)

b) that \( R \), restricted to \( \Omega_0 \), can be computed by optimal decompositions (7) into pure states which are all contained in \( \Omega_0 \),

c) and that every face of \( \Omega \) is an \( R \)-set.

**Lemma 2**

Let \( \Omega_0 \) be an \( R \)-set and \( \Omega_0^\text{ex} \) the set of its pure states. Let \( F \) be a convex function on \( \Omega_0 \) which is not greater than \( R \) on \( \Omega_0^\text{ex} \). Then \( F \leq R \) on \( \Omega_0 \). \( \Box \)

With other words, on any \( R \)-set \( \Omega_0 \) of the state space, \( R \) is the largest convex function which attains at every of its pure states, \( \varrho \), the value \( \tilde{S}(\varrho) \). Indeed, for an optimal decomposition, based on \( \Omega_0 \), convexity of \( F \) implies

\[ R(\omega) = \sum p_j \tilde{S}(\varrho_j) \geq \sum p_j F(\varrho_j) \geq F(\omega) \]

My next task is to apply this simple lemma to affine functions in order to obtain a slight modification of theorem 1 of \([10]\): \( \Omega \) can be covered by convex sets on which \( R \) is affine. This fact I like to call the *roof property* of \( R \). The covering consists of “facets” with pure states as corners. The covering is not a disjunct one. The intersection of two “facets” is either empty or belongs itself to the covering.
To obtain the covering, we use the well known possibility to represent a convex function on a compact convex domain by an upper bound of affine functions, together with the existence of optimal decompositions.

An affine function, \( l, \omega \to l(\omega) \) is said to support \( R \) iff \( l \leq R \) on \( \Omega \), and \( l \) equals \( R \) at least at one state. By virtue of lemma 2 one needs to check the inequality \( l \leq R \) for pure states only.

\( \Omega \) is compact and \( R \) convex. Hence there exists for every \( \omega' \in \Omega \) at least one affine function \( l \) supporting \( R \) at \( \omega' \), i.e. with \( l(\omega') = R(\omega') \). Thus

\[
R(\omega) = \sup_l l(\omega), \quad l \text{ supports } R
\]

Now, if \( l \) is supporting \( R \), let us consider the set

\[
\Omega(l) := \{ \omega' \in \Omega \mid R(\omega') = l(\omega') \}
\]  \hfill (8)

on which \( l \) coincides with \( R \), and let us assume, \( \omega \) belongs to that set. Choosing an optimal decomposition (7) one obtains

\[
\sum p_j R(\varrho_j) = R(\omega) = l(\omega) = \sum p_j l(\varrho_j)
\]

But \( l(\varrho_j) \leq R(\varrho_j) \) as \( l \) is \( R \)-supporting. The positivity of the coefficients \( p_j \) enforces equal values of \( R \) and \( l \) for all involved pure states. This is not the end: \( l \) is affine and equal to \( R \) on some extremal elements \( \varrho_j \). Therefore, by convexity, \( R \leq l \) on the convex hull of the pure states \( \varrho_j \). But \( l \leq R \) by assumption. Hence \( l \) is equal to \( R \) on the convex hull of all the pure states \( \varrho \) which can appear in any optimal decomposition of \( \omega \). This is already the essence of

**Lemma 3**

Let \( \Omega(l) \) be defined by (8) with an affine function \( l \) supporting \( R \). Then \( \Omega(l) \) is a compact, convex \( R \)-set on which \( R \) is affine.

The family of all \( \Omega(l) \), where \( l \) is \( R \)-supporting, is a covering of \( \Omega \). \( \square \)

**Proof:**

Up to the compactness assertion the proof is already done by the chain of arguments above, which can be repeated with every \( \omega \in \Omega(l) \). In particular, \( \Omega(l) \) is an \( R \)-set. Now \( R \) equals \( \hat{S} \) on the compact set \( \Omega^{ex} \). Hence both, \( R \) and \( l_\omega \) are continuous on this compact set. Hence, the subset of \( \Omega^{ex} \), on which both functions take equal values, is compact. This compact set of extremal points generates a compact convex set (Carathéodory) which must be \( \Omega(l) \) as it is an \( R \)-set. \( \square \)

**Remark:**

\( \mathcal{B} \) being finite-dimensional, the Hermitian linear functionals span a real linear space. An affine function on it is of the form \( l(\nu) = \nu(A_1) + a \) with a real constant \( a \) and

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with an Hermitian operator $A_l$. For every state, $\omega$, the constant $a$ can be represented by $a$-times the evaluation of $\omega$ at the identity. Hence, for every affine $l$ supporting $R$, there is exactly one Hermitian operator $A$ such that the expectation value $\omega(A)$ equals $l(\omega)$,

$$l(\omega) = \omega(A_l), \quad A_l = A_l^* \in \mathcal{B}$$ \hfill (9)

With an Hermitian operator $A$, satisfying $\tilde{S}(\rho) \geq \rho(A)$ for all pure states $\rho$, the expectation functional $A \rightarrow \omega(A)$ satisfies $R(\omega) \geq \omega(A)$ on the whole state space by virtue of lemma 2. If, in addition, equality takes place on at least one pure state, then the expectation value of $A$ is supporting $R$. I shall consider this aspect elsewhere. \hfill \Box

There may be many linear functionals $l$ supporting $R$ at a given state $\omega$. For every pure state $\rho$, appearing in any extremal optimal decomposition of $\omega$, we get $l(\rho) = R(\rho)$ and $\rho \in \Omega_l$. Hence

**Corollary**

Let $\omega$ be a state. The intersection

$$\Omega_\omega := \bigcap \Omega(l), \quad l(\omega) = R(\omega)$$ \hfill (10)

enjoys the following properties: It is convex, compact, and it contains every pure state which can appear in an optimal decomposition of $\omega$. $R$, restricted to $\Omega_\omega$, is affine. \hfill \Box

$\Omega_\omega$ is a simplex iff $\omega$ allows for one and only one extremal optimal decomposition (up to the order of its summands).

**Remark:** In [14] I have called $\Phi_\omega$ the convex set generated by those pure states in $\Omega_\omega$ which can appear in an extremal optimal decomposition of $\omega$. Clearly, $\Phi_\omega$ is contained in $\Omega_\omega$. Presently the believe, both sets are equal, remains a conjecture. \hfill \Box

**Lemma 4**

Let $H_\omega = 0$. Then $\omega$ is pure. \hfill \Box

**Proof**

Let us consider an arbitrary convex decomposition (5). Then, by definition of $R$ and by concavity of $S$

$$R(\omega) \leq \sum p_j S(\tilde{\omega}_j) \leq S(\tilde{\omega})$$

The assumption of the lemma implies equality. But $S$ is strictly concave. Hence $\tilde{\omega}$ must be equal to $\tilde{\omega}_j$ for all $j$. Because every state of the face of $\omega$ can occur in a convex decomposition of $\omega$, the whole face is reduced to a single state on $\mathcal{C}$ by (4). For a maximal commuting subalgebra such a face cannot contain more than one state.

3 Thanks to the referee, who pointed at the gap.
Remark that the inverse statement is evident: If \( \rho \) is pure then \( H(\rho) = 0 \). \( \square \)

In the following \( \omega \rightarrow \bar{\omega} \) denotes a complex conjugation such that \( P_j(\bar{\omega} - \omega)P_j = 0 \) for all \( j \). In a suitable base for the density operators the complex conjugation changes the off-diagonal entries to its complex conjugates but does not change the diagonal. If \( \omega = \bar{\omega} \), the state is called real.

**Lemma 5**

If \( \rho \) and \( \bar{\rho} \) both appear in an optimal extremal decomposition then \( \rho = \bar{\rho} \).

Let \( U \in \mathcal{C} \) be a unitary. If \( \rho \) and its transform \( \rho^U \) both appear in a proper optimal decomposition, then they are equal. \( \square \)

**Corollary**

The set of real states is an \( R \)-set. Every pure state occurring in an optimal decomposition of a real state is real. \( \square \)

**Proof:** Let \( \rho \) be a pure state and \( \tau = (\rho + \bar{\rho})/2 \). Then \( \rho, \bar{\rho}, \) and \( \tau \) have the same reduction to \( \mathcal{C} \) and the same \( \bar{S} \)-value. Assume the two extremal elements would appear in an optimal decomposition. Then \( R \) is affine on their convex hull. (lemma 3). Hence \( R(\tau) = \bar{S}(\tau) \). By lemma 4 \( \tau \) has to be pure implying \( \rho = \bar{\rho} \). The same chain of arguments is valid in the other case of the lemma. \( \square \)

**USING SYMMETRIES**

If only \( U^* \mathcal{C} U = \mathcal{C} \) is required, things are not covered by lemma 5. These unitaries form the normalizer of \( \mathcal{C} \) in \( \mathcal{B} \). They permute the minimal projection operators \( P_j \) of \( \mathcal{C} \). Let \( U \) a unitary from the normalizer. Then there is a permutation \( i \rightarrow j(i) \) with \( UP_jU^* = P_{j(i)} \). This way we obtain the well known homomorphism from the normalizer onto the permutation group of \( d = \text{dim} \mathcal{H} \) elements. Let us call \( U \) a transposition iff it interchanges two minimal projections while the other ones remain unchanged.

My aim is to consider optimal decompositions of states which are generated by symmetries. If \( U \) is a unitary, \( \omega^U \) is defined by \( \omega^U(A) = \omega(UAU^*) \) for all \( A \) in the algebra. The computations are conveniently done by the help of density operators. Using the trace of \( \mathcal{B} \), the latter is defined by

\[
\omega(A) = \text{Tr} \, D \, A, \quad D = D_\omega, \quad \forall A \tag{11}
\]

If \( \omega \) is transformed to \( \omega^U \), the density operator becomes \( U^*DU \).

The rank of a state is by definition equal to the rank of the smallest projection operator, say \( Q \), satisfying \( \omega(Q) = \omega(1) \). \( Q \) is called support of \( \omega \) and of the operator
\( D = D_\omega \). We mention the equality of the rank of \( \omega \) with the dimension of the supporting subspace \( Q\mathcal{H} \). We shall need further

\[
\mathcal{H}_\omega := Q\mathcal{H}, \quad \mathcal{B}_\omega := QBQ = B(\mathcal{H}_\omega) \cong \mathcal{M}_k
\]  

where \( k = \text{rank} \omega \). \( Q \) is the unit element of \( \mathcal{B}_\omega \). If \( A \in \mathcal{B}_\omega \) is of rank \( k \), then \( A \) is invertible in that algebra, i.e. there is a unique \( B \in \mathcal{B}_\omega \) with \( AB = Q \). In particular, every positive power \( D^s \) is invertible in \( \mathcal{B}_\omega \). Below this will be used with \( k = 2 \), in which case things can be controlled explicitly by the help of Pauli operators. Before going to that issue, let us rewrite (3) with the projection operator \( s \), \( P_j \), of our maximal commutative subalgebra \( \mathcal{C} \)

\[
\tilde{S}(\omega) = \sum s(\text{Tr} P_j D)
\]

Consider now a rank two state \( \omega \) with density operator \( D \) and support \( Q \). Then

\[
\frac{1}{2} Q = (1 - \text{Tr} D^2)^{-1}(D - D^2),
\]

Lemma 6

Let \( \omega \) be a state of rank two and \( U \) be a transposition such that \( \omega^U = \omega \), so that its density operator \( D = D_\omega \) commutes with \( U \). Then the following properties are equivalent:

(a) There is no other \( U \)-invariant state in \( \Omega_\omega \) than \( \omega \).

(b) \( \omega \) allows for an optimal decomposition of \( \omega \) of length two, and at least one element of \( \Omega_\omega \) does not commute with \( U \).

(c) \( \Omega_{\omega}^{ex} \) consists of two elements which are interchanged by \( U \). \( \Box \)

Proof. To be definite we choose a transposition \( U \) fulfilling

\[
UP_1 = P_2 U, \quad UP_j = P_j U, \quad \forall j \geq 2 \quad (14)
\]

There is a 180°-rotation in \( \mathcal{B}_\omega \) through the action of \( U \). (If not, all elements of that algebra had to be \( U \)-invariant, contradicting every of the three properties, a, b, c.) We choose matrices, \( \sigma_j \), in this algebra satisfying the algebraic properties of the Pauli matrices, with \( \sigma_3 \) defining the rotational axis of \( U \). We are allowed to require

\[
\sigma_3 := U Q, \quad \sigma_j U + U \sigma_j = 0, \quad j = 1, 2 \quad (15)
\]

because \( U \) commutes with \( U \) by virtue of (13), and, being a transposition, \( U = U^* \). Therefore, \( \sigma_3 \) of (13) is Hermitian and its square equals \( Q \). But \( Q \neq U Q \) because \( U \) induces a non-trivial rotation of the supporting subspace. As we now can see, every \( U \)-invariant operator in \( \mathcal{B}_\omega \) is a linear combination of \( Q \) and \( \sigma_3 \). In particular,
\[ D = \frac{1}{2}(Q + x_3 \sigma_3), \quad \frac{1}{2}(1 + x_3^2) = \text{Tr} \, D^2 \]  \quad (16)

With any pure \( \rho \) also \( \rho^U \) is contained in \( \Omega_\omega \). Assuming property (a) of lemma 6 we obtain the optimal decomposition

\[ \frac{1}{2}(\rho + \rho^U) = \omega \]  \quad (17)

Thus (a) \( \to \) (b).

The density operator \( D_\rho \) of any pure \( \rho \) satisfying (17) must be of the form

\[ D_\rho = \frac{1}{2}(Q + \sum x_j \sigma_j), \quad x_1^2 + x_2^2 = 1 - x_3^2 = 2(1 - \text{Tr} \, D^2) \]  \quad (18)

For \( j > 2 \) the projections \( P_j \) commute with \( U \). But \( P_j \sigma_k, \, k = 1, 2 \), change sign if transformed with \( U \). Their traces must be zero. This implies

\[ \text{Tr} \, P_j D = \text{Tr} \, P_j D_\rho, \quad j > 2 \]  \quad (19)

\[ \frac{1}{2} \text{Tr} \, (P_1 + P_2)D_\rho = \text{Tr} \, P_1 D = \text{Tr} \, P_2 D \]  \quad (20)

In order that (c) follows from (b) there should be only two choices for \( \rho \) if optimality is required. By (13) and (20) the remaining possibility to get \( \tilde{S}(\rho) \) as small as possible is in making the modulus of the difference \( \text{Tr}(P_1 - P_2)D_\rho \) as large as possible. To do this is the next aim.

If the above mentioned difference is zero, then \( \text{Tr}P_j D_\rho = \text{Tr}P_j D \) for all \( j \). But then the entropy of \( \tilde{\rho} \) and \( \tilde{\omega} \) would be equal, and, consequently, \( H_\omega = 0 \). By lemma 4 this contradicts the rank two assumption for \( \omega \). Therefore, the first of the operators

\[ D_\rho(P_1 - P_2)D_\rho, \quad Q(P_1 - P_2)Q, \quad \sqrt{D}(P_1 - P_2)\sqrt{D} \]

is not zero. (Remark \( D_\rho = \sqrt{D_\rho} \), for \( \rho \) is pure.) But the first operator results from multiplying the second one from the right and the left by \( D_\rho \). Thus the second operator is again not the zero of \( B_\omega \). And, lastly, the root of \( D \) is invertible in \( B_\omega \). This means the third operator is not the zero. All the operators of our list are Hermitian. All change sign if transformed with \( U \). Hence they are real linear combinations of \( \sigma_1 \) and \( \sigma_2 \). We use the remaining freedom in the choice of the Pauli operators by requiring

\[ Q(P_1 - P_2)Q = y \sigma_1, \quad y > 0 \]  \quad (21)

Multiplication with \( D_\rho \) and taking the trace gives
\[ \text{Tr} (P_1 - P_2) D_\varrho = x_1 y \] (22)

according to (18). The left hand side is maximal (minimal) iff \( |x_1| \) is as large as possible. This takes place if and only if \( x_2 = 0 \), see (18).

That proves (b) \( \rightarrow \) (c).

Indeed, with \( x_2 = 0 \), just one choice for \( x_1 > 0 \) is allowed,

\[ \Omega^\text{ex}_{\omega} = \{ \varrho, \varrho^U \}, \quad D_\varrho = \frac{1}{2} (Q + x_1 \sigma_1 + x_3 \sigma_3) = D + \frac{1}{2} \sqrt{1 - x_3^2 \sigma_1} \] (23)

Evidently, (a) follows from (c), and the proof is done. \( \square \)

Let us register the following observation:

**Corollary**

Let \( \omega \) satisfy the conditions of Lemma 6. The choice (13), (21) of the Pauli operators \( \sigma_j \) depends only on the support \( Q \) of \( \omega \). \( \square \)

To see it, remind that \( P_j \) are rank one projections and that the traces of \( P_1 Q, P_2 Q \) are equal. We get \( y \) by squaring (21) and taking the trace. Reinserting in (21) yields

\[ (\sqrt{\text{Tr}(P_1 Q) \text{Tr}(P_2 Q) - \text{Tr}(P_1 Q P_2 Q)}) \sigma_1 = Q(P_1 - P_2)Q \] (24)

Similarly we see from (18) and by sandwiching (21) with \( \sqrt{D} \)

\[ \sqrt{D}(P_1 - P_2)\sqrt{D} = \frac{1}{2} x_1 y \sigma_1 \] (25)

Squaring and taking the trace comes down to

\[ \frac{1}{4} x_1^2 y^2 = \text{Tr}(P_1 D) \text{Tr}(P_2 D) - \text{Tr}(P_1 D P_2 D) \] (26)

To be able to calculate \( \tilde{S}(\varrho) = R(\omega) \) we need the traces of \( D_\varrho P_j, j = 1, 2 \). This can be done by combing (20) and (22):

\[ \text{Tr} P_1 D_\varrho = \text{Tr}(P_1 D) + (x_1 y)/2, \quad \text{Tr} P_2 D_\varrho = \text{Tr}(P_1 D) - (x_1 y)/2 \]

Now, because of (26), explicit expressions for \( R \) and \( H_\omega \) are

\[ R(\omega) = s(\text{Tr}(P_1 D) + \frac{1}{2} x_1 y) + s(\text{Tr}(P_1 D) - \frac{1}{2} x_1 y) + \sum_{j>2} s(\text{Tr} P_j D) \] (27)
\[ H_\omega = 2s(\text{Tr}(P_1 D) - s(\text{Tr}(P_1 D) + \frac{1}{2}x_1y) - s(\text{Tr}(P_1 D) - \frac{1}{2}x_1y) \] (28)

provided the assumption of lemma 6 are satisfied. The trace of \( P_j D \) is the expectation value of \( D \) with the vector \(|j\rangle\). Similarly, (28) may be written

\[ \frac{1}{4}x_1^2y^2 = \langle 1|D|1\rangle\langle 2|D|2\rangle - \langle 1|D|2\rangle\langle 2|D|1\rangle \]

Looking at all this, the difficulties in extending lemma 6 to symmetric density operators of higher rank are as follows: (13) becomes an equation of degree rank(\( \omega \)), and the number of parameters goes quadratically with the rank.

There is a remarkable outcome of lemma 6. With an arbitrary pure state \( \rho \) and a given transposition \( U \) there is a twofold alternative. At first, either \( \rho = \rho^U \) or the arithmetic mean (17) of \( \rho \) and \( \rho^U \) is of rank two. In the latter case \( \Omega_\omega \) is \( U \)-invariant. Hence, either the conditions of lemma 6 are satisfied or they are not. In the latter case, \( \rho \) is not optimal. However, because of the symmetry, there is necessarily at least one optimal pure \( \rho_1 \) in \( \Omega_\omega \) such that lemma 6 applies to the arithmetic mean of \( \rho_1 \) and \( \rho_1^U \). Hence \( \Omega_\omega^{ex} \) consists of one or more pairs of pure states, which are pairwise permuted by \( U \), and, possibly, of some \( U \)-invariant pure states.

**Corollary**

If \( \omega \) is \( U \)-invariant but \( \Omega_\omega \) is not elementwise \( U \)-invariant then \( \Omega_\omega \) contains at least one state to which lemma 6 applies.

**Symmetric Real Density Operators**

Let us compare the treatment above with that of some highly symmetric density operators of maximal rank according to [10]. Assuming \( \omega \) real, every optimal decomposition of \( \omega \) is real (lemma 5). Even more essential, \( D = D_\omega \), the density operator of \( \omega \), is supposed to commute with all permutation matrices, \( U \), fulfilling \( UCU^* = \mathcal{C} \). In the following the latter assumption is always required.

To every permutation, \( \pi \), there is a unique permutation matrix, \( U_\pi \), in the normalizer of \( \mathcal{C} \). These matrices are real unitaries with entries 0 or 1, and in every row and every column there is just one 1. If a real density operator is commuting with all real permutation matrices, only one free parameter remains: It is the common value, \( z \), of the off-diagonal elements. The diagonal elements equal \( 1/d \), \( d \) the dimension of our Hilbert space. The common off-diagonal value is bounded from above by \( 1/d \) and from below by \( -1/d(d-1) \).

Now let a pure state \( \rho \) with density operator \( D_\rho \) appear in an optimal decomposition of a real permutation invariant state. Then every transform \( \rho^U \) of \( \rho \) by a permutation
matrix is contained in $\Omega^\text{ex}_\omega$. Therefore, lemma 3 shows optimality of the decomposition (which is not necessarily short)

$$ D = \frac{1}{d!} \sum_{\pi} U_{\pi} D_{\theta} U^*_{\pi} $$

(29)

One of the relations following from (29) reads

$$ \text{Tr} D_{\theta} D = \text{Tr} D^2 = \frac{1}{d} + d(d - 1) z^2 $$

(30)

We may write

$$ D_{\theta} = |\varphi\rangle\langle \varphi| $$

(31)

with a real unit vector $\varphi$. Denoting by $\phi_1, \ldots, \phi_d$ the components of $\varphi$ in a base that diagonalizes the minimal projections $P_j$ of $C$, the relation (30) implies

$$ \sum \phi_k = a, \quad a = \sqrt{1 + zd(d - 1)} \geq 0 $$

(32)

where the sign of the real $a$ is fixed by $a \geq 0$. This seemingly harmless convention has an important effect. Being real, $\varphi$ is defined by (31) up to a sign. If $a \neq 0$, this sign has been fixed by (32). (32) is an affine hyperplane, intersecting the $(d - 1)$-sphere spanned by the real unit vectors $\varphi$. As long $a > 0$ the map $D_{\theta} \to \varphi$ is a section from the real pure states into the Hilbert space. For $a = 0$ we get a double covering because with $\varphi$ also $-\varphi$ belongs to the sphere. That is, in the limit $a \to 0$ the simple covering bifurcates to a double covering.

The point for all this comes from lemma 3, showing that (29) implies $R(\omega) = S(\tilde{\varphi})$ because $R$ is affine on the convex set generated by an optimal set of pure states.

Thus we have to minimize $S(\tilde{\varphi})$ on the intersection of the $(d - 1)$-sphere of real unit vectors with the hyperplane (32), i.e. on a $(d - 2)$-sphere $S_{a}^{d-2}$. Its radius $r$ in Hilbert space turns out to be

$$ r = r(S_{a}^{d-2}) = \sqrt{1 - \frac{a^2}{d}} = \sqrt{\frac{(d-1)(1-zd)}{d}} $$

(33)

From $z = 1/d$, where it degenerates to a point, the radius grows up to one with growing $z$. At the same time $a$ goes from $\sqrt{d}$ to zero.

Let $\varphi \in S_{a}^{d-2}$ and denote by $\varphi^\perp$ its antipode on that sphere. Then their Hilbert distance is twice the radius (33), which amounts to
so that the transition amplitude remains positive as long as the radius does not exceed \( r_0 := \sqrt{0.5} \). Thus, for \( 0 \leq r \leq r_0 \), the Bures distance of the states \(|\varphi\rangle\langle\varphi|\) and \(|\varphi^\perp\rangle\langle\varphi^\perp|\) is equal to the Hilbert distance of \( \varphi \) to its antipode \( \varphi^\perp \). But for \( r_0 < r < 1 \) the transition amplitude becomes negative and the mentioned Bures distance gets the value \( 2\sqrt{1-r^2} \). This can be rephrased as following: Within \( 0 \leq r < 1 \) the sphere \( S^{d-2}_0 \) is one to one mapped into the state space. This mapping is locally isometric. The local isometry is a global one for \( 0 \leq r \leq r_0 \). But it becomes globally deformed if \( r \) is larger than \( r_0 \) in order to “prepare” the bifurcation at \( r = 1 \). Because of the described scenario something should happen with the optimization and its outcome \( R \). What it is, is definitely known \([10]\) in case \( d = 3 \), and will be described below.

For the next considerations I assume \( d = 3 \). With \( d - 2 = 1 \) the optimization takes place on an 1-sphere. There are three permutation matrices which are transpositions. They are denoted by \( U_{12}, U_{23} \), and \( U_{31} \). In particular, the real unitary \( U_{12} \) interchanges the components \( \phi_1 \) and \( \phi_2 \) of \( \varphi \), while \( \phi_3 \) remains unchanged, and so forth. The product of any two of the three transpositions is a cyclic permutation of the components of \( \varphi \).

Now I return to an important result of \([10]\) which clarifies the structure of \( \Omega^\text{ex}_\omega \) in its dependence on \( z \).

There is a special \( z \)-value, the bifurcation value \( z_* \), which is \(-0.14\) approximately. For values \(-1/6 < z < z_* \) the convex set \( \Omega^\text{ex}_\omega \) is an hexagon. But for \( z_* \leq z < 1/3 \) it is a triangle, i.e. a simplex.

In the triangle case there is, up to reordering of its extremal states, exactly one short optimal decomposition of \( \omega \). It is of length three and explicitly known \([10]\). The following representation of their density matrices \( D_j \) is in \([11]\). It is

\[
\omega = \frac{1}{3} (\varrho_1 + \varrho_2 + \varrho_3), \quad D_j := 3 \sqrt{\omega} P_j \sqrt{\omega} \quad (35)
\]

This representation is equivalent to \([23]\). The \( 6 = 3! \) terms in \((29)\) become pairwise equal. Every transposition permutes two of the three pure states in \( \Phi_\omega \), allowing for an application of lemma 6, but let the third one unaffected. On the other hand, a cyclic permutation matrix induces a cyclic reordering of \( \Omega^\text{ex}_\omega \), i.e. of three pure states of \((35)\).

More involved is the hexagon case. After the bifurcation value every of the three optimal pure states of the simplicial decomposition splits into two other ones. That is to say, from every one of the three pure states \( \varrho_j \), \( j = 1, 2, 3 \) of the triangular optimal decomposition originates two new ones, \( \varrho_{ja} \) and \( \varrho_{jb} \). A transposition, say \( U_{12} \), previously interchanging \( 1 \leftrightarrow 2 \) but letting \( 3 \) fixed, now does a more complicated
job: $1a \leftrightarrow 2b$, $1b \leftrightarrow 2a$, and $3a \leftrightarrow 3b$. The pair $\varrho_{3a}$, $\varrho_{3b}$, together with $U_{12}$ allows for the application of lemma 6.

The states labelled by $a$ are interchanged by a cyclic permutations, and the same is with the $b$-states $\varrho_{bj}$. From that one obtains two essentially different simplicial decompositions,

$$\omega = \frac{1}{3}(\varrho_{1a} + \varrho_{2a} + \varrho_{3a}) = \frac{1}{3}(\varrho_{1b} + \varrho_{2b} + \varrho_{3b})$$  (36)

However, no pair with the same index “a” satisfies the assumptions of lemma 6. The same is with respect to the index “b”: Only states on the line segment containing two neighbored extremal points can have a unique extremal decomposition.

We already know: Something appears if $z$ goes down to $-1/6$. The Study-Fubini distance of the pairs of pure states labelled by $(1a, 2b)$, $(2a, 3b)$, or $(3a, 1b)$ respectively, is diminishing. The distance finally becomes zero for $z = -1/6$, resulting in $\varrho_{1a} = \varrho_{2b}$, and so on. The hexagon bifurcates and becomes again a triangle in state space.

In the Hilbert space one gets an equilateral hexagon at $z = -1/6$. As explained above, it becomes our triangle in state space by identifying the vectors $\varphi$ and $-\varphi$ (Hopf bifurcation). From this point of view it really looks as if we had to compensate that Hopf bifurcation by the bifurcation of the optimal decomposition rule at $z^\star$. If this impression is correct, the appearance of $z^\star$ is necessary by general geometric reasons. Only its value should come from the particular properties of the function $s(x)$.

Let us compare this reasoning again with lemma 6. Let $\varrho$ be a real pure state, $U$ a real transposition that does not commute with $\varrho$, and denote by $\omega'$ their arithmetical mean, $\omega' = (\varrho + \varrho^U)/2$. If the latter is not an optimal decomposition, then $\Omega_{\omega'}$ is spanned by more than two extremal states. The assumption, that we then fall into the triangle or hexagon case, is compatible with the symmetry and geometrically tempting. This conjecture reads:

Let $\varrho$ a real pure state, $U$ be a real transposition, and $\varrho \neq \varrho^U$. If the assumptions of lemma 6 do not apply to the state $(\varrho + \varrho^U)/2$, then $\varrho$ belongs to an optimal decomposition of a real and maximally symmetric state. $\square$

The conjecture is supported by numerical studies and the results of [10]. To get a complete proof, one has to exclude further bifurcations. I do not know how to achieve this. $\square$

Remark: For $d = 2$ every pair $\varrho, \varrho^U$ of pure states, $U$ a transposition of the minimal projections of $\mathcal{C}$ is optimal. Indeed, this remains true if $-x \ln x$ is replaced by an arbitrary concave $s(x)$ with $s(0) = s(1) = 0$. $\square$

For $d > 3$ a similar analysis is preliminary only. To obtain a pure state $|\varphi\rangle\langle \varphi|$ belonging to an optimal decomposition $|\varphi\rangle\langle \varphi|$ it suffices to restrict oneself to the following
assumption: The components of \( \varphi \) do not attain more than three different values. This can be shown by straightforward variational analysis.

Moreover, if the components of \( \phi \) attain only two different values, \( \varrho \) is either a local minimum, a maximum, or a turning point of \( R \). Nearby \( z = 1/d \) the vector \( \varphi \) with components

\[
\sum \phi_j \geq 0, \quad \phi_1 > \phi_2 = \phi_3 = \ldots = \phi_d \tag{37}
\]
gives at least a local minimum of \( S(\tilde{\omega}) \) which is presumably a global one. The \( U^\pi \) transforms of \( D\varrho = |\varphi\rangle\langle\varphi| \), where \( \varphi \) satisfies (37), generate a simplex spanned by \( d \) extremal states. For \( z \)-values satisfying (32) and (37), and such that (29) becomes optimal (though not short), the simplex decomposition will be

\[
\omega = \frac{1}{d} \sum \varrho_j, \quad D_j := d \sqrt{\varrho} P_j \sqrt{\varrho} \tag{38}
\]

This is supposed to be the counterpart, for \( d > 3 \), of the \( d = 3 \) triangle case. Of course, much more has to be known to clarify the \( d > 3 \) situation even in the real and maximally symmetric case.

What is to learn about the role of symmetries from all that? Given a state \( \omega \), one is tempted to look at the subgroup

\[
\Gamma(\omega) := \{ U \mid U^\dagger C U = C, \ U^\dagger \Omega \omega U = \Omega \omega \} \tag{39}
\]
of the normalizer of \( C \). As seen in the previous examples, a certain classification can be reached by examining to the detail the action of \( \Gamma(\omega) \) on the pure states contained in \( \Omega^\omega \). Is it always true, as in the examples considered above, that there is exactly one \( \omega' \in \Omega \omega \) which is invariant with respect to \( \Gamma(\omega) \)? And, if yes, is this group large enough to get an optimal decomposition of \( \omega' \), starting with any of its optimal pure states?

**Appendix: Roofs**

A function enjoys some very nice properties if defined according the rule of (3). Some of them have been used by Benatti, Narnhofer, and Uhlmann [10], by Uhlmann [14], by Hill and Wootters [13], and others to examine either the entropy of a channel or of a subalgebra with respect to a state, [7], or the entanglement of formation, [13]. They can also provide computational help to Holevo’s channel capacity [2]. In addition there are connections to the optimization problem of accessible entropy shown by Benatti [11]. They explain certain similarities to results of Davies [4], Levitin [4], Fuchs and Peres [12].
In the following I treat these general properties within an abstract setting. Its first requirement is as follows:

**ASSUMPTION 1**: \( \Omega \) is a compact convex set in a finite dimensional real space \( \mathcal{L} \).

**Remark**: In most physical applications \( \Omega \) is the state space or the space of density operators of an algebra \( \mathcal{B}(\mathcal{H}) \), *-isomorphic to a full matrix algebra. \( \mathcal{H} \) denotes an Hilbert-space of finite dimension \( d \). Fixing \( \Omega \) to be the convex set of all density operators, \( \mathcal{L} \) is the real linear space of Hermitian operators, \( \text{Herm}(\mathcal{H}) \), of \( \mathcal{H} \). Then \( \mathcal{L} \) is of dimension \( d^2 \). The dimension of \( \Omega \) is \( d^2 - 1 \). Only for reference within the appendix I call this the standard setting. It is convenient to require

\[
 n := \dim \mathcal{L} = 1 + \dim \Omega, \quad 0 \notin \Omega \quad (40)
\]

This provides the following: Because the zero of \( \mathcal{L} \) is not contained in \( \Omega \), the linear span of \( \Omega \) coincides with \( \mathcal{L} \). Choose \( \tau \in \Omega \) arbitrarily. To every \( \nu \in \mathcal{L} \) there is one and only one real number \( \lambda \) such that \( \nu - \lambda \tau \in \Omega \). For the remainder \( \tau \) is chosen once for all as a reference state. It is often convenient, though not necessary, to assume invariance of \( \tau \) against all affine automorphisms of \( \Omega \). (\( \tau \) is then called maximally symmetric.)

**ASSUMPTION 2**: The set of extremal elements, \( \Omega^{\text{ex}} \), of \( \Omega \) is compact. A continuous function, \( \varrho \to f(\varrho) \), is given on \( \Omega^{\text{ex}} \). \( \square \)

The next aim is to extend the function given on the extremal boundary of \( \Omega \) to the whole convex set \( \Omega \). Of course, there are many ways to do so. But there exists two distinguished among them, respecting maximally the convex structure of \( \Omega \). For reasons which will become evident soon, I call them the convex and the concave roof based on \( f \). The convex roof, \( f^{\text{inf}} \), is defined by

\[
f^{\text{inf}}(\omega) := \inf \sum p_j f(\varrho_j), \quad \varrho_k \in \Omega^{\text{ex}}, \quad \sum p_j \varrho_j = \omega \quad (41)
\]

where the infimum runs through all extremal convex decompositions of \( \omega \). Completely similar, the concave roof, \( f^{\text{sup}} \), is defined by

\[
f^{\text{sup}}(\omega) := \sup \sum p_j f(\varrho_j), \quad \varrho_k \in \Omega^{\text{ex}}, \quad \sum p_j \varrho_j = \omega \quad (42)
\]

Because \( -f^{\text{sup}} = (-f)^{\text{inf}} \) every property of convex roofs can be translated in one for concave roofs, and vice versa. Evidently \( f^{\text{sup}} \geq f^{\text{inf}} \).

The task is now to show how the graphs of \( f^{\text{sup}} \) and \( f^{\text{inf}} \) unite to the boundary of a compact convex set \( \Xi \) of dimension \( n \). It will be done by a construction depending on the reference state \( \tau \). The set

\[
\Xi^{\text{ex}} := \{ f(\varrho) \tau + \varrho \mid \varrho \in \Omega^{\text{ex}} \} \quad (43)
\]
does not contain convex linear combinations of their elements with the exception of the trivial ones. Otherwise $\Omega_{ex}$ could not be a set of extremal points of a convex set. Continuity of $f$ and compactness of $\Omega_{ex}$ imply compactness of $\Xi_{ex}$. Hence (Carathéodory)

**Lemma A-1**
The convex hull $\Xi$ of $\Xi_{ex}$ is compact. $\Xi_{ex}$ is the set of extremal points of $\Xi$. $\square$

$\nu \in \Xi$ iff $\nu$ allows for an extremal decomposition

$$\nu = \left[ \sum p_j f(\omega_j) \right] \tau + \sum p_j \omega_j$$

resulting in

$$\lambda \tau + \omega \in \Xi \iff f^\inf \leq \lambda \leq f^\sup$$

(44)

The compactness of $\Xi$ ensures the compactness of the $\lambda$-interval defined by (44). It follows the existence of optimal decompositions with which the “inf” in (41) or the “sup” in (42) are attained respectively. Moreover, $\lambda \tau + \omega$ belongs to the boundary of $\Xi$ iff $\lambda$ equals either $f^\inf(\omega)$ or $f^\sup(\omega)$. The dimension of its face cannot exceed $n - 1$. Carathéodory’s theorem guaranties optimal decompositions of length $n$.

**Lemma A-2**

$f^\inf$ as well as $f^\sup$ allows for optimal decompositions of length not exceeding $n$. $\square$

There is another construction, [1], valid on every convex set. Let $\omega \rightarrow G(\omega)$ denote an arbitrary function on $\Omega$. Its convex hull is defined by

$$G_{\inf}(\omega) := \inf \sum p_j G(\omega_j), \quad \omega_k \in \Omega, \quad \sum p_j \omega_j = \omega$$

(45)

where the inf runs through all representations of $\omega$ by convex combinations, i.e. not necessarily extremal ones. It is known, see [1], and easily verified, that every convex hull is a convex function.

In the same spirit one may define the concave hull of a function just by replacing the “inf” in (15) by “sup”. With this definition the concave hull of a function is concave.

Now assume in (15) a concave function $G$. Then we may restrict ourselves to extremal decompositions to get the desired infimum: The convex hull of a concave function depends on it values at the extremal points only. Now it is straightforward to see

**Lemma A-3**

$f^\inf$ is the convex hull of $f^\sup$. $f^\inf$ is convex. Let $F$ be a convex function which is not larger than $f$ on $\Omega_{ex}$. Then $F \leq f^\inf$ on $\Omega$.

$f^\sup$ is the concave hull of $f^\inf$. $f^\sup$ is concave. Let $F$ be a concave function which is not smaller than $f$ on $\Omega_{ex}$. Then $F \geq f^\sup$ on $\Omega$. $\square$
Remark A1.2: Let us consider the standard setting where \( \Omega \) is a state space and \( S \) the von Neumann entropy. If \( \omega \to \omega \circ \alpha \) denotes an affine mapping of the state space into itself then

\[
\omega \mapsto \tilde{S}(\omega) := S(\omega \circ \alpha)
\]

is a concave function on \( \Omega \). Its convex hull, \( \tilde{S}_{\text{inf}} \), is denoted by \( R \) in [10] and [14] and by \( E \) for “entanglement” in [13] and [15]. Let \( f \) denote the restriction of \( \tilde{S} \) onto \( \Omega^{\text{ex}} \). We have

\[
\tilde{S} \geq f^{\sup} \geq f^{\inf} = \tilde{S}_{\text{inf}}, \quad H_{\omega} = \tilde{S} - \tilde{S}_{\text{inf}} \geq f^{\sup} - f^{\inf}
\]

Because all the functions are non-negative, they are defined for general state spaces (say in the C*-category) if the von Neumann entropy remains finite on \( \Omega \circ \alpha \).

Now a further notation is introduced. Let \( F \) be a function on \( \Omega \). A set of extremal points of \( \Omega \) is called \( F \)-optimal if and only if \( F \) is affine on its convex hull.

I call \( F \) a roof if every element \( \omega \) is contained in the convex hull of an \( F \)-optimal set.

This is consistent with the notations above: The concave and the convex roof of a function \( f \), which is defined on the extremal points, are roofs. It is the content of theorem 1 in [10]. As already indicated in the main text (lemmata 1-3), one can do a little bit more. What there is called \( \Omega_{\omega} \) will now be denoted by \( \Omega^{\inf}_{\omega} \) to distinguish it from \( \Omega^{\sup}_{\omega} \).

\( \Omega^{\inf}_{\omega} \) is the smallest convex set containing all extremal points of all extremal decompositions of \( \omega \) which are optimal for \( f^{\inf} \).

\( \Omega^{\sup}_{\omega} \) is the smallest convex set containing all extremal points of all extremal decompositions of \( \omega \) which are optimal for \( f^{\sup} \).

**Lemma A-4**

\( f^{\inf} \) and \( f^{\sup} \) are roofs. They are affine on \( \Omega^{\inf}_{\omega} \) and \( \Omega^{\sup}_{\omega} \) respectively.

**Corollary**

The convex hull of a concave function and the concave hull of a convex function are roofs.

Two convex (or two concave) roofs are equal iff they coincide on the extremal points.

The proofs are mere reformulations of those in the main text. They can be done also more explicitly as in [10].

Remark: We may now rephrase the definition of \( H_{\omega} \) as following: \( H_{\omega} \) vanishes on \( \Omega^{\text{ex}} \) and it is the sum of \( \tilde{S} \) and of a concave roof.

What happens if equality holds, \( f^{\sup}(\omega) = f^{\inf}(\omega) \), for a certain \( \omega \). From the very definition

\[
f^{\inf}(\omega) \leq \sum p_j \varrho_j \leq f^{\sup}(\omega)
\]
so that every extremal decomposition is optimal for both roofs. That implies $\Omega^\inf_\omega$ is the face of $\omega$ in $\Omega$. Now the roof property implies:

**Lemma A-5**

Let $f^{\sup}(\omega) = f^{\inf}(\omega)$. Then

$$\Omega^\inf_\omega = \Omega^\sup_\omega = \text{face of } \omega \text{ in } \Omega \quad (46)$$

and $f^{\inf}$ is equal to $f^{\sup}$ on the face of $\omega$.

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