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Article

Roofs and Convexity

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Abstract: Convex roof extensions are widely used to create entanglement measures in quantum information theory. The aim of the article is to present some tools which could be helpful for their treatment. Sections 2 and 3 introduce into the subject. It follows descriptions of the Wootters' method, of the "subtraction procedure", and examples on how to use symmetries.

Keywords: roofs; convex roof extensions; entanglement measures

1. Introduction

One often is in the position to know a quantity for pure states of a quantum system, say g, without a definite meaning in classical physics. Then one looks for a method to extend g to all mixed states, see [1–4]. Let G denote such a possible extension.

A reasonable approach is certainly to extend g "as linearly as possible" or, more correctly, "as affine as possible". The mathematical model for such a demand is a "roof" as presented in Section 2.

As it is difficult, to say the least, to imagine higher dimensional geometry, let us look at an elementary example, the real qubits. They fill a disk bounded by a circle. The circle represents the pure states. Considering $g(\pi)$, with π pure, as the height of a wall at the point π. An extension G of g to the disk provides a covering of the ground floor. Let $G(\omega)$ be a point of that covering. To be a roof in the sense of Section 2, we like to have: There is either a straight line or a plane coincident with the roof point $\omega, G(\omega)$ and resting on the wall at two or at three points $\pi_j, g(pi_j)$. If the line or plane is parallel to the ground floor, it is called *flat*. An uncomfortable feature is the rather large arbitrariness: There are plenty of roof extensions allowing, however, as a bonus, much room for playing. Under rather weak assumptions, there is a minimal as well as a maximal roof extension (Proposition 2.1).

Physically stronger motivated seem extensions G of g which are either convex or concave. Heuristically, the convex ones try to suppress the "classical noise" or else the "classical information" by the tendency to attach lower values to the states "far" from the pure ones. The concave extension stress the "classical part", possessing lower values in the vicinity of the pure states.

It is a well known fact that there are maximal convex and minimal concave extensions. If it exists, the minimal roof extension is equal to the maximal convex extension and this facilitate calculations sometimes.

The maximal convex extension $g^\cup$ of g can be gained by

$$g^\cup(\omega) = \inf \sum p_j g(\pi_j) \tag{1}$$

where the inf is running through all convex decompositions

$$\omega = \sum p_j \pi_j, \quad p_j \geq 0. \quad \sum p_j = 1 \tag{2}$$

with pure states π_j, [5]. In quantum information theory this is nowadays a common procedure to define entanglement measures. Its first appearance is in the important paper [6] by C. H. Bennett, D. DiVincenzo, J. Smolin, and W. Wootters, and has been called *entanglement of formation* and is denoted by $E(\omega)$. These authors considered states ω of a bipartite quantum system. The role of g plays $S(\text{Tr}_b \pi)$, the entropy S of the partial trace Tr_b, as a function of a pure bipartite states π.

In the present paper a trace preserving positive map T from the states of a quantum system into another one is called a *stochastic map*. A *channel* is a completely positive stochastic map. If in the definition of entanglement of formation, E, a stochastic channel T is used in place of the partial trace Tr_b, we call the resulting quantity *the entanglement of T* and denote it by E_T. For a channel, E_T is equivalent (in many ways) to the restriction of E onto a face of a bipartite state space of sufficiently high dimension, [7]. In this way, T is seen as a sub-channel of the partial trace: The tensor product is partitioned into subspaces on which the sub-channels are defined. A 1-qubit channel, for example, can be represented by a $2 \times m$ bipartite quantum systems as the restriction of the partial trace over the larger dimensional part onto the density operators supported by a suitable 2-dimensional subspace.

Clearly, E_T is of interest in its own as part of the χ^*-function $\chi^* = S_T - E_T$ with $(S_T)(\omega) = S(T(\omega))$ the maximum of which is the Holevo capacity [8] of T.

Since the importance of E has been realized in [6], several other measures of similar structure have been introduced and discussed, replacing the von Neumann entropy S by another function on the state space of the output system. The perhaps mostly discussed examples are the "tangle" τ_T and the "concurrence" C_T. The connection between them is $C_T(\pi)^2 = \tau_T(\pi)$ for all pure states π. Sometimes one also needs a minimal concave extension ("entanglement of assistance"). All these quantities have been defined by global variational problems of type (1), (2).

A further, even earlier source for the said procedure roots in the problem of defining a "quantum dynamic entropy", generalizing the Kolmogorov–Sinai one. In the approach [9] of A. Connes, H. Narnhofer, and W. Thirring several similar global variational problems wait to be solved. One of them is the search for the convex roof defined by $g(\omega) = S(D_n(\omega))$, S again von Neumann's entropy and D_n the diagonal map, setting all off-diagonal entries of a matrix to zero. The problem initiated the paper [10] of F. Benatti, H. Narnhofer, and A. Uhlmann and further ones.

It is true that complete solutions for these extensions are only known in the lowest non-trivial dimensions. In the present paper general tools are presented to facilitate the treatment of convex or concave roofs. The general aspects are mainly in the Sections 2 and 3. It includes the foliation of the input state space into "convex leaves" onto which the roof becomes affine and, in particular nice situations, even constant, [10,11].

Section 4 is devoted to the Wootters' way [12–14] of presenting the entanglement of formation explicitly, see also [15].

Section 5 shows a more recent way to compute the concurrence of a 1-qubit stochastic map by a substraction procedure. For the concurrence of $2 \times m$ quantum systems it allows to compute the concurrence of any rank two quantum state. An elegant way to do so was opened by Hildebrand, [16,17], using the so-called "S-lemma"of Yakobovich, see [18]. Another one has been chosen by Hellmund and Uhlmann, [19], who use the description of general 1-qubit maps given by Gorini and Sudershan, [20].

For the tangles the pioneering work goes back to Coffman, Kundu, and Wootters, [21], who already remarked that optimal decompositions of length two should be sufficient in the 1-qubit case. That the "substraction procedure" works can be read off from a paper of Osborne and Verstraete, [22]. Here we describe analytical results for axial symmetric channels. There are also results for the 3-tangle roof problem, [25].

Most results, if not numerically, are found by the help of symmetries. Besides the already quoted ones, an essential step has been done by K. G. Vollbrecht and R. F. Werner, [26], and B. M .Terhal and K. G. Vollbrecht [27]. Meanwhile it became a very large domain of research, exceeding the frame of the present paper. Hence, in Section 6, only some aspects, connected with maximal symmetric states, are touched.

Some notations: We use $\mathcal{H}$ for Hilbert spaces, $\mathcal{B}(\mathcal{H})$ for its algebra of operators, $\Omega(\mathcal{H})$ for the set of density operators supported by $\mathcal{H}$. We also say "state" for "density operator" and "state space" for $\Omega(\mathcal{H})$. As a convex set, $\Omega(\mathcal{H})$ is embedded in $\mathrm{Herm}(\mathcal{H})$, the real linear space of Hermitian operators. The symbol Ω is also used for a general compact convex sets in a real linear space. Following [3], the extremal points of a convex set will be called "pure" ones mostly. They are usually symbolized by the letter π. We follow [28] in using $\eta(x) = -x \log x$ and $S(\omega) = \mathrm{Tr}\, \eta(\omega)$, the von Neumann entropy.

2. Roofs, Roof Extensions

We are now going to give an exact meaning to the word "roof". For this purpose we assume G to be a real valued function on a compact convex set Ω, contained in a finite dimensional real linear space.

Definition 2.1a: Roof points

$\omega \in \Omega$ is called a *roof point of G*, if there is at least one extremal convex decomposition

$$\omega = \sum p_j \pi_j, \quad \pi_j \in \Omega^{\mathrm{pure}} \tag{3}$$

such that

$$G(\omega) = \sum p_j G(\pi_j) \tag{4}$$

If this takes place, we call the decomposition (3) *optimal* with respect to G or, equivalently, *G-optimal.* The number of terms in (3) with $p_j \neq 0$ is the *length* of the decomposition.

Definition 2.1b: Flat roof points

A roof point ω of G is called *flat,* if there is a G-optimal decomposition (3) fulfilling

$$G(\omega) = G(\pi_1) = G(\pi_2) = \ldots \tag{5}$$

i.e. all the values $G(\pi_j)$ are equal one to another [29].

Let $f(x)$ be a real function defined on the range of G. The main merit of a flat roof point ω of G is the simple fact, that it remains a flat roof point for $f(G)$: $f(G(\pi_j)) = f(G(\omega))$ for all j and (4) remains true for $f(G)$. In other words, the flat points of $\rho \to G(\rho)$ are also flat roof points of $\rho \to f(G(\rho))$.

Definition 2.2: Roofs, flat roofs

A real function G on Ω is a *roof* if every $\omega \in \Omega$ is a roof point of G.

G is called a *flat roof* if all roof points are flat ones.

In important applications the point of view is a bit different: A function $\pi \to g(\pi)$ is given on the set Ω^{pure} of pure states, or, more generally, on the set of extremal states of an arbitrary compact convex set. Then one asks for meaningful extensions G which coincides with g on Ω^{pure}. In such a generality the problem is too arbitrarily posed and one asks for restrictions to such an extension. Remarkable ones are the roof extensions. They interpolate the values of g "as linearly (or as affine) as possible".

Definition 2.3: Roof extensions

Let $\pi \to g(\pi)$ be a real function on Ω^{pure}. A roof G is called a *roof extension of g,* if $G(\pi) = g(\pi)$ for pure states.

Now observe the following simple fact: The maximum (the minimum)

$$\max\{G_1, \ldots, G_n\} \text{ respectively } \min\{G_1, \ldots, G_n\}$$

of finitely many roof extensions of g is a roof again.

Indeed, assume for roof extensions $G_1, \ldots, G_n$ of g and $\omega \in \Omega$ the value $G_1(\omega)$ is not less than the other values $G_j(\omega)$. Then one selects a G_1-optimal decomposition for $\max\{G_1, \ldots, G_n\}$.

The reasoning above fails for infinitely many roof extensions. The proof of the following is postponed to that of proposition 3.5.

Proposition 2.1

Let g be a real continuous function on $\Omega^{\mathrm{pure}}(\mathcal{H})$ and G a roof extension of g. For all $\omega \in \Omega(\mathcal{H})$ there exist optimal decompositions (3), (4) the length of which does not exceed $(\dim \mathcal{H})^2 + 1$.

There is a minimal and a maximal roof extension of g.

2.1. Examples

Roof extensions exist in abundance. To see this and also the difficulties, which we may get into, let us consider a few examples showing some typical constructions. We remain within the state space $\Omega(\mathcal{H})$, $\dim \mathcal{H} = d$ and we start with $d = 2$.

Example 2.1: A Bloch ball construction

Seen from convex analysis, the space Ω of all 1-qubit density operators is a 3-dimensional ball, the *Bloch ball*. Ω^{pure} is the *Bloch sphere,* the surface of the Bloch ball.

Now assume there is a function g on the Bloch sphere and we like to find roof extensions G of g. Particular nice ones are gained as following: We take a bundle of straight lines such that every point ω of the Bloch ball is coincident with exactly one line, say L_ω, of the bundle. If ω is not pure, then L_ω hits the Bloch sphere at exactly two points, say π_1 and π_2. Hence, ω is a convex combination of them. Now we define

$$G(\omega) = pg(\pi_1) + (1 - p)g(\pi_2) \text{ if } \omega = p\pi_1 + (1 - p)\pi_2 \tag{6}$$

Because there is just one line from our bundle going through ω, we get a well-defined roof.

Let us now specify our example by choosing a bundle of parallel lines. It belongs exactly one main axis of the Bloch ball to the bundle. We may assume that it is the x_3-axis with respect to the Bloch coordinates x_1, x_2, x_3 of a general Pauli representation

$$\omega = \frac{1}{2}(\mathbf{1} + x_1\sigma_1 + x_2\sigma_2 + x_3\sigma_3) \tag{7}$$

The line L_ω is now fixed by the values x_1 and x_2, letting the third Bloch coordinate arbitrary. L_ω crosses the Bloch Sphere at the pure states $\pi_\pm$ with the Bloch coordinates $x_1, x_2, y_3 = \pm(1 - x_1^2 - x_2^2)^{1/2}$. Hence

$$\pi_\pm = \frac{1}{2}(\mathbf{1} + x_1\sigma_1 + x_2\sigma_2 \pm [1 - x_1^2 - x_2^2]^{1/2}\sigma_3), \quad \omega = p\pi_+ + (1 - p)\pi_- \tag{8}$$

with $0 \leq p \leq 1$. Expressing now g in terms of Bloch coordinates, we obtain the roof

$$G(\omega) = G(x_1, x_2) = pg(x_1, x_2, +\sqrt{1 - x_1^2 - x_2^2}) + (1 - p)g(x_1, x_2, -\sqrt{1 - x_1^2 - x_2^2}) \tag{9}$$

The example is further specified by choosing for g the Shannon entropy of the diagonal elements of ω. Then G becomes the roof

$$E_T(\omega) = H\left(\frac{1 + \sqrt{1 - x_1^2 - x_2^2}}{2}, \frac{1 - \sqrt{1 - x_1^2 - x_2^2}}{2}\right) \tag{10}$$

$T(\omega)$ denotes the diagonal part of ω and H the Shannon entropy of the diagonal elements. That this is the solution for the entanglement of the diagonal channel, has been suggested by Levitin, [30] and Thirring [31]. (10) provides a roof extension as described above. Indeed, it is a flat roof depending on $1 - x_1^2 - x_2^2$, hence a function of the Euclidean distance $\sqrt{x_1^2 + x_2^2}$ of ω from the x_3-axis. It is

$$\langle 0|\omega|1\rangle = \frac{x_1 - ix_2}{2}, \quad x_1^2 + x_2^2 = 4|\langle 0, \omega|1\rangle|^2 \tag{11}$$

Therefore, the concurrence of the diagonal map for qubits can be written

$$C_T(\omega) = |\langle 0|\omega|1\rangle| \tag{12}$$

It is easily to be seen that C is a flat convex roof. It possesses quite large domains where it is just affine: Cut the Bloch ball with a plane containing the x_3-axis. We get a disk, cut by the x_3-axis into two half-disks. The concurrence is affine on every such half-disk.

Indeed, if T is a 1-qubit channel with two different pure fix points, one can observe a similar phenomenon. (The disks will be cut by the axis through the fix points.)

Example 2.2

There is a constructions, similar to the previous one: Given any function $f(x_3)$ on the x_3-axis. We construct a roof by

$$A(\omega) = f(x_3), \quad x_3 = \langle 0|\omega|0\rangle - \langle 1|\omega|1\rangle \tag{13}$$

More generally, given a bundle of planes so that every point of the Bloch ball is coincident with one and only one of these planes. A function, constant on planes, is a roof. This can be achieved by choosing a function f on the x_3-axis and attaching to every plane the value of f at its crossing with this axis.

Similar constructions are possible with higher dimensional balls (ellipsoids). However, on higher dimensional state spaces things are essential more complicated due to the subtle structure of the set of their pure states.

Example 2.3: Affine functions on the state space

An affine function on $\mathrm{Herm}(\mathcal{H})$ is of the form

$$X \to l(X) := a + \mathrm{Tr}\, XA \tag{14}$$

with an Hermitian operator A and a real number a. It is sometimes useful to write (14) in the form

$$l(X) = \mathrm{Tr}\, XB, \quad B = A + \frac{a}{d}\mathbf{1}$$

The function (14) is trivially a roof: If we have any extremal decomposition (3) one immediately gets $l(\rho) = \sum p_j l(\pi_j)$. Thus, every extremal decomposition is optimal.

We easily conclude that with G also $G + l$ is a roof.

A bit more tricky is the assertion that every function (14) is a *flat roof* on the state space $\Omega(\mathcal{H})$.

We prove this by induction to the dimension of the Hilbert space. We start with the qubit case. We can choose a basis in $\mathcal{H}$ such that $A = a + a'\sigma_3$ and

$$\omega = \frac{1}{2}(\mathbf{1} + x_1\sigma_1 + x_3\sigma_3)$$

It suffices to prove the assertion for $A = \sigma_3$, resulting in $l(X) = \mathrm{Tr}\, \sigma_3 X = x_3$. With an unimodular number ϵ we consider the pure states

$$\omega_\pm = \frac{1}{2}(\mathbf{1} + x_1\sigma_1 \pm \epsilon\sqrt{1 - x_1^2 - x_3^2}\sigma_2 + x_3\sigma_3)$$

so that our affine function is constant at the segment $p\omega_+ + (1 - p)\omega_-$. The segment contains ω for $p = 1/2$.

Varying ϵ we see the following: To every affine function l as in (14) there is an axis through the Bloch ball such that l is constant on every plane perpendicular to that axis. We can say something more: Given $\omega \in \Omega$ and two affine functions, l_j, $j = 1, 2$, we use the constants $l_j(\omega) = c_j$ to define two planes by $l_j(X) = c_j$. Because the two planes contain ω, they intersect along a line, say L_ω, containing ω. The intersection of L_ω with the Bloch sphere provides two pure states which define a flat optimal decomposition of ω.

Proposition 2.2

Affine functions on $\Omega(\mathcal{H})$, $\dim \mathcal{H} < \infty$, are flat roofs. Given two affine functions and a density operator ω, there is a common flat optimal decomposition of ω.

Proof. The 2-dimensional case has already been proved. Let $l_j(X) = a_j + \operatorname{Tr} A_j X$, $j = 1, 2$, denote two affine functionals and choose $\omega \in \Omega(\mathcal{H}_d)$. Assume the assertion is true for $\dim \mathcal{H} < d$. If ω is from the boundary of $\Omega(\mathcal{H}_d)$ we are done by our induction hypothesis. Otherwise we consider the linear subspace $\mathcal{L}$ of $\operatorname{Herm}(\mathcal{H}_d)$ orthogonal to A_1 and A_2, *i.e.*, of all Y satisfying $\operatorname{Tr} A_j Y = 0$, $j = 1, 2$. Consider the affine space $\mathcal{L}_\omega = \omega + \mathcal{L}$. It contains ω and it is $l_j(Y) = l_j(\omega)$ for all $Y \in \mathcal{L}_\omega$. The intersection $K = \Omega \cap \mathcal{L}_\omega$ is compact and its extremal points belong to the boundary of $\Omega(\mathcal{H}_d)$. Therefore, we get a decomposition

$$\omega = \sum p_j \omega_j, \quad \operatorname{rank}(\omega_j) < d$$

and, furthermore, $l_j(\omega) = l_j(\omega_j)$ because of $\omega_j \in K$. However, the support of any ω_j is of dimension less than d. Therefore, there are extremal decompositions

$$\omega_j = \sum_k p_{jk} \pi_{jk}, \quad l_j(\omega_j) = l(\pi_{jk})$$

for all j and all k with pure states π_{jk}. Thus

$$\omega = \sum_j p_j \sum_k p_{jk} \pi_{jk}$$

is a flat optimal decomposition of ω for l_1 as well for l_2. Thus the proposition is proved. $\qquad \square$

The following is a corollary.

Proposition 2.3

Let $f(x_1, x_2)$ be a function defined on the range of two affine functions, l_1 and l_2. Then

$$F(\omega) := f(l_1(\omega), l_2(\omega)) \tag{15}$$

is a flat roof.

Example 2.4: An application to the diagonal map

We like to apply the proposition above to the diagonal map

$$X \to D_n(X) = \mathrm{diag}(X) \tag{16}$$

which which is a channel on $\Omega(\mathcal{H})$. $\mathrm{diag}(X)$ denotes the diagonal part of X obtained by replacing all off-diagonal elements of X by zeros. Proposition 2.3 proves that the von Neumann entropy

$$\omega \to S(D_n(\omega)) = \sum \eta(\langle j|\omega|j\rangle) \tag{17}$$

is a flat roof for $n = 2, 3$. For $n = 3$ one replaces the third diagonal element, x_{33}, by $1 - x_{11} - x_{22}$ to see that proposition 2.3 suffices to verify the assertion.

We like to prove the flatness of (17) for all dimensions. This will be done in example 3.2 later on.

Example 3

A general way to obtain roof extensions in state spaces is presented next. It allows for further modifications, but it is difficult to be controlled explicitly.

Let g be a continuous real function on Ω^{pure} and $\omega \in \Omega$. Every basis $|\psi_1\rangle, \ldots, |\psi_d\rangle$ gives rise to a decomposition

$$\omega = \sum \sqrt{\omega}|\psi_j\rangle\langle\psi_j|\sqrt{\omega} \tag{18}$$

of positive rank one operators. After normalization of the rank one operators we get extremal convex decomposition of ω,

$$\omega = \sum_{p_j \neq 0} p_j \frac{\sqrt{\omega}|\psi_j\rangle\langle\psi_j|\sqrt{\omega}}{\langle\psi_j|\omega|\psi_j\rangle}, \quad p_j = \langle\psi_j|\omega|\psi_j\rangle \tag{19}$$

In the following definitions we vary over all bases.

$$G_1(\omega) = \min_{\mathrm{bases}} \sum_{p_j \neq 0} p_j g(\frac{\sqrt{\omega}|\psi_j\rangle\langle\psi_j|\sqrt{\omega}}{\langle\psi_j|\omega|\psi_j\rangle}) \tag{20}$$

where p_j is as in (19). Because continuity of g is assumed, and the set of bases is compact, the minimum in (20) will be attained. Thus, G_1 is a roof extension of g.

One gets another roof extension by

$$G_2(\omega) = \max_{\mathrm{bases}} \sum_{p_j \neq 0} p_j g(\frac{\sqrt{\omega}|\psi_j\rangle\langle\psi_j|\sqrt{\omega}}{\langle\psi_j|\omega|\psi_j\rangle}) \tag{21}$$

One cannot guaranty the roof property without continuity of g.

(21) and (20) are global optimization problems for which there are no explicit expressions known in most cases. There are, however, algorithms to approximate them numerically.

3.   Roofs and Convexity

We start with some definitions and elementary, mostly well-known statements around maximal convex and minimal concave extensions. The second subsection is concerned with sufficient conditions for the existence of convex and concave roofs and their main properties.

3.1.   Convex and Concave Extensions

Let Ω be a compact convex set and g a real function defined on the set Ω^{pure} of its extremal points.

Definition 3.1: Convex (concave) extensions

A convex function G is called a *convex (respectively concave) extension of g* if G is convex (respectively concave) and coincides on Ω^{pure} with g.

Between any convex, concave or roof extension of a function g the inequalities

$$G^{\text{convex}} \leq G^{\text{roof}} \leq G^{\text{concave}} \tag{22}$$

are valid. Indeed, with an optimal decomposition (3) for G^{roof} we get

$$G^{\text{roof}}(\omega) = \sum p_j G^{\text{roof}}(\pi_j) = \sum p_j G^{\text{convex}}(\pi_j)$$

because the extensions coincide on Ω^{pure}. The right sum cannot be smaller than $G^{\text{convex}}(\omega)$ by convexity. Similarly one argues in the concave case.

The proof of (22) is valid pointwise, leading to

Proposition 3.1

Let G^{convex} be a convex, G^{concave} a concave, and G any extension of g. If ω is a roof point of G, then

$$G^{\text{convex}}(\omega) \leq G(\omega) \leq G^{\text{concave}}(\omega) \tag{23}$$

Let G^{convex} and G^{concave} be as in the above proposition and assume in addition equality in (23), $G^{\text{convex}}(\omega) = G^{\text{concave}}(\omega)$. For all convex combination

$$\omega = \sum p_j \omega_j, \quad \omega_j \in \Omega, \quad p_j > 0,$$

we conclude

$$\sum p_j G^{\text{convex}}(\omega_j) \geq G^{\text{convex}}(\omega) = G^{\text{concave}}(\omega) \geq \sum p_j G^{\text{concave}}(\omega_j) \tag{24}$$

because of (22) the conclusion is $G^{\text{convex}}(\omega_j) = G^{\text{concave}}(\omega_j)$ for all j.

To express this finding we need some standard terminology. A subset $K \subset \Omega$ is called a *face* of Ω if $\omega \in K$ and (24) necessarily implies $\omega_j \in K$ for all j. Faces are convex subsets of Ω. If not only Ω but also Ω^{pure} is compact then faces are compact and any face K is convexly generated by $\Omega^{\text{pure}} \cap K$. The intersection of faces is either empty or a face again. The smallest face containing ω will be called ω-*face* of Ω and denoted by $\text{face}_\omega[\Omega]$. If K is a face and ω not a point of the boundary of K, then K is the ω-*face* of Ω.

Now we express the finding above by

Proposition 3.2

Coincide a convex and a concave extension of g at $\omega \in \Omega$, then they coincide on the ω-face of Ω.

The least upper bound of a set of convex functions is convex again. Hence, given g on Ω^{pure}, there is a unique largest convex extension of g from Ω^{pure} to Ω. Similarly there exists a smallest concave extension of g. It is convenient to introduce an extra notation for these extensions:

Definition 3.2: $g^{\cap}$ and $g^{\cup}$

Let g be a real function on Ω^{pure}. We denote by $g^{\cup}$ the largest convex and by $g^{\cap}$ the smallest concave extension of g to Ω,

$$
\begin{aligned}
g^{\cup} &= \quad \text{largest convex extension of } g \text{ from } \Omega^{\mathrm{pure}} \text{ to } \Omega \ , \\
g^{\cap} &= \quad \text{smallest concave extension of } g \text{ from } \Omega^{\mathrm{pure}} \text{ to } \Omega \ .
\end{aligned}
$$

We also write $G = G^{\cup}$ (or $G = G^{\cap}$) if G is the largest convex (or the smallest concave) extension of the restriction of G onto Ω^{pure}.

Proposition 3.3

Let G be an extension of g and ω one of its roof points. If G is convex, then $G(\omega) = g^{\cup}(\omega)$. If G is concave, then $G(\omega) = g^{\cup}(\omega)$.

If a convex (resp. concave) roof extension of g exists, then it is unique. Because G is convex, $G \le g^{\cup}$. Because ω is a roof point, (23) asserts $G(\omega) \ge g^{\cup}(\omega)$.

Is there a convex extension at all for a given g ? If there is one then there is also a largest one, *i.e.* $g^{\cup}$ exists. The answer to the question is affirmative and has been given in [5] by a variational characterization which is well known in quantum information theory as a recipe to construct entanglement measures:

$$
\begin{aligned}
g^{\cup}(\omega) &= \quad \inf \sum p_j g(\pi_j) & (25) \\
g^{\cap}(\omega) &= \quad \sup \sum p_j g(\pi_j) & (26)
\end{aligned}
$$

where the "inf", respectively "sup", is running over all extremal convex decompositions

$$
\omega = \sum p_j \pi_j, \quad \pi_j \in \Omega^{\mathrm{pure}} \tag{27}
$$

of ω.

Indeed, if G is an extension of g which is convex, the right side of (25) must be always larger than $G(\omega)$. On the other hand, given ω_1 and ω_2, one can find decompositions (27) for them differing an arbitrary small amount $\epsilon > o$ from $g^{\cup}(\omega_1)$ respectively $g^{\cup}(\omega_2)$. They may be composed from the pure states $\pi_{i,j}$ and probabilities $p_{i,j}$, $i = 1, 2$. Then

$$
2\epsilon + p g^{\cup}(\omega_1) + (1 - p) g^{\cup}(\omega_2) \ge \sum p p_{1,j} g(\pi_{1,j}) + \sum (1 - p) g(\pi_{2,k})
$$

and this is not smaller than $g^{\cup}(p\omega_1 + (1 - p)\omega_2)$. Because ϵ can be arbitrary near to zero, $g^{\cup}$ is convex. The concave case can be settled by a similar reasoning or by

$$
- g^{\cup} = (-g)^{\cap}, \quad -g^{\cap} = (-g)^{\cup} \tag{28}
$$

Remark: Hulls of functions

The *convex hull* of G is the largest convex function which is smaller than G. The *concave hull* of G is the smallest concave function which is larger than G. In (25) and (26) one uses the values of G at the pure states only. Because the hull construction must respect values on the whole of Ω, there are more constraints to be fulfilled.

The expressions (25) and (26) are similarly structured as those of the convex and the concave hulls of a function G on Ω. One mimics the proofs and gets

$$\text{conv}[G](\omega) = \inf \sum p_j G(\omega_j) \tag{29}$$

$$\text{conc}[G](\omega) = \sup \sum p_j G(\omega_j) \tag{30}$$

where, as in (24), one has to run through all convex combinations

$$\omega = \sum p_j \omega_j, \quad \omega_j \in \Omega, \quad p_j > 0$$

Obviously, $\text{conv}[G]$ is smaller than $G^{\cup}$ and $\text{conc}[G]$ is larger than $G^{\cap}$. This quite simple reasoning provides also

Proposition 3.4

If G is a concave or a roof extension of g then $g^{\cup} = \text{conv}[G]$.

If G is a convex or a roof extension of g then $g^{\cap} = \text{conc}[G]$.

As a matter of fact one can do similar hull constructions with any subset of Ω which convexly generates Ω. This has been emphasized in [26].

3.2. Convex and Concave Roofs

If there is a convex roof extension of g, then it equal to $g^{\cup}$. There is a sufficient condition to guaranty the roof property of $g^{\cup}$ and of $g^{\cap}$.

Proposition 3.5

Let Ω be a convex set. Assume both, Ω and Ω^{pure}, are compact and g continuous on Ω^{pure}. Then $g^{\cup}$ and $g^{\cap}$ are roofs. According to proposition 3.3 they are the minimal respectively maximal roof extensions of g.

Remember that Ω^{pure} is compact if $\Omega = \Omega(\mathcal{H})$ and $\mathcal{H}$ is finite dimensional. The requirement of continuity of g is often satisfied in physically motivated applications, though not always. A counter example is the Schmidt number in bipartite quantum systems. In this case it is not known whether $g^{\cup}$ and $g^{\cap}$ are roofs. Nevertheless. the assumptions needed are rather weak ones. We met them already in proposition 2.1.

The proof will be "constructive" in a certain sense. It is arranged to sharpen "theorem 1" in [10]: If we know an optimal decomposition with pure states $\pi_1, \pi_2, \ldots$, then every convex combination of them

is optimal. In particular, the (convex or concave) roof is affine on the convex set generated by the pure states $\pi_1, \pi_2, \ldots$. Restricted to this this set, the graph of G is a piece of an affine space. The whole graph of G appears as composed of flat pieces [32]. If one would know a covering of Ω by those "convex leaves", one could compute $g^{\cup}$ from the values of g at Ω^{pure}. Things are similar for $g^{\cap}$.

To start proving propositions 3.5 and 2.1 let us repeat the assumptions. Ω is a compact convex set in a real linear space $\mathcal{L}$ of finite dimension, the set Ω^{pure} of all pure (*i.e.*, extremal) points of Ω is compact. g is a real continuous function on Ω^{pure}. The dimension of Ω as a set in $\mathcal{L}$ is denoted by n. It is the dimension of the affine space generated by Ω.

Remark: The space $\Omega(\mathcal{H})$ of density operators is embedded in $\mathrm{Herm}(\mathcal{H})$. The latter is of dimension d^2 if $\dim \mathcal{H} = d$. The affine space generated by $\Omega(\mathcal{H})$ is the hyperplane of Hermitian operators of trace one. The dimension of $\Omega(\mathcal{H})$ is $n = d^2 - 1$.

We enlarge $\mathcal{L}$ to the linear space $\mathcal{L}' = \mathcal{L} \oplus \mathbb{R}$. Its elements, $X \oplus \lambda$, will be written in vector form $\{X, \lambda\}$ with two components, $X \in \mathcal{L}$ and $\lambda \in \mathbb{R}$. We need the set

$$E = \{\pi, g(\pi)\}, \quad \pi \in \Omega^{\mathrm{pure}} \tag{31}$$

E is a compact set by our assumption. Hence its convex hull, denoted by $\Omega[g]$, is a compact convex set. The set of extremal points of $\Omega[g]$ is E. (If one of the elements of E would be a convex combination of the others, the same would be true for the corresponding pure states, contradicting our assumptions.)

Choose $\omega \in \Omega$ and consider in $\mathcal{L} \oplus \mathbb{R}$ the straight line consisting of the points $\{\omega, \lambda\}$, $\lambda \in \mathbb{R}$. The line intersects with $\Omega[g]$ along a compact segment

$$\{\omega, \lambda\} \in \Omega[g] \Leftrightarrow \lambda_0(\omega) \leq \lambda \leq \lambda_1(\omega) \tag{32}$$

λ satisfies (32) if and only if there is an extremal decomposition

$$\{\omega, \lambda\} = \sum p_j \{\pi_j, g(\pi_j)\} = \{\omega, \sum p_j g(\pi_j)\}, \quad \pi_j \in \Omega^{\mathrm{pure}} \tag{33}$$

Therefore,

$$g^{\cup}(\omega) = \lambda_0(\omega) \leq \lambda \leq \lambda_1(\omega) = g^{\cap}(\omega) \tag{34}$$

and there exist extremal decompositions of ω with equality in (25) respectively (26). Therefore, $g^{\cup}$ and $g^{\cap}$ are roofs and proposition 3.5 has been proved.

If G is a roof extension of g, the point $\{\omega, G(\omega)\}$ is contained in $\Omega[g]$. Hence it can be represented by a convex combination of elements from E. As the dimension of $\Omega[g]$ is $n + 1$, there are, by a theorem of Carathèodory, pure convex decomposition of length $n + 2$. This proves proposition 2.1: For $\Omega = \Omega(\mathcal{H})$ it follows $n + 2 = (d^2 - 1) + 2$.

On the other hand, a point $\{\omega, g^{\cup}(\omega)\}$ belongs to a face of the boundary of $\Omega[g]$. Its dimension cannot exceed n. Thus there are, again by Carathèodory, pure decompositions of length $n + 1$. For $\Omega(\mathcal{H})$ this gives an achievable length d^2, an often used fact [33].

Definition 3.2: convex leaves

Let G be a real function on Ω. A subset $K \subset \Omega$ is called a *convex leaf* of G if

(a) K is compact and convex,

(b) K is the convex hull of $K \cap \Omega^{\text{pure}}$,

(c) G is convexly linear on K, *i.e.*

$$G(\sum p_j \rho_j) = \sum p_j G(\rho_j) \text{ if all } \rho_j \in K$$

K is called *complete,* if all pure states which can appear in an optimal decomposition of any $\rho \in K$ are contained in K.

Proposition 3.6

With the assumptions of proposition 3.5 it holds: For $g^{\cup}$ (respectively $g^{\cap}$) and any $\omega \in \Omega$ there are complete convex leaves containing ω.

It makes sense to call the set of all complete convex leaves of G the *convex foliation* of G or, shortly, the G-foliation.

Proof. The proposition will be proved for $g^{\cup}$. The case of $g^{\cap}$ is similar. There is an affine functions l such that

$$l \le g^{\cup}, \quad l(\omega) = g^{\cup}(\omega) \tag{35}$$

We define a subset K of Ω by

$$K = \{\rho \,|\, l(\rho) = g^{\cup}(\rho)\,\} \tag{36}$$

$\square$

Proposition 3.6.a: (36) is a complete $g^{\cup}$-leaf.

Clearly, $\omega \in K$. Let us choose $\rho \in K$. For an optimal pure decomposition, $\rho = \sum p_j \pi_j$, one obtains

$$\sum p_j g^{\cup}(\pi_j) = g^{\cup}(\rho) = l(\rho) = \sum p_j l(\pi_j)$$

However, $l(\pi_j) \le g^{\cup}(\pi_j)$ by assumption. By the equation above, all these inequalities must be equalities. Hence, *the pure composers π_j of every optimal decomposition of any $\rho \in K$ are contained in K, i.e.*, K is complete. Now choose another $\rho' \in K$ and let $\rho' = \sum p_k' \pi_k'$ be an optimal decomposition. For $0 < p < 1$ we get, applying first our assumption and then convexity of $g^{\cup}$,

$$l(p\rho + (1-p)\rho') \le g^{\cup}(p\rho + (1-p)\rho') \le pg^{\cup}(\rho) + (1-p)g^{\cup}(\rho')$$

By the assumption the right hand side can be written

$$pl(\rho) + (1-p)l(\rho') = l(p\rho + (1-p)\rho')$$

and is equal to the left expression. Hence, equality must hold and K must be a convex set. We have seen already that every $\rho \in K$ can be represented by a convex combination of elements from $K \cap \Omega^{\text{pure}}$. Because g is continuous, the set of all π satisfying $g(\pi) = l(\pi)$ is compact. Hence, K is compact. Indeed, it is convexly generated by a compact set.

We repeat a further standard notation. An element ρ of a convex set K is called K-*inner* or "convexly inner" if for any $\nu \in K$ follows $(1 + s)\rho - s\nu \in K$ and small enough positive s. Geometrically, the line segment from ν to ρ can be prolonged a bit without leaving K. There is also a topological

characterization: A K-inner point is an inner point of K with respect to the affine space generated by K. (Example: The invertible density operators are the convexly inner points of $\Omega(\mathcal{H})$.)

The intersection of complete convex leaves is either empty or it is a complete convex leaf. Hence there is a minimal complete convex leaf containing a given $\omega \in \Omega$, the ω-*leaf* of $g^{\cup}$. It is convexly generated by all those $\pi \in \Omega^{\text{pure}}$ which can appear in an optimal decomposition of ω.

The ω-leaf is the largest convex leaf containing ω as convexly inner point.

Now let K_1 be the ω_1-leaf and K_2 that of ω_2. If ω_1 is a convexly inner point of K_2, then $K_1 \subset K_2$. In particular, $K_1 = K_2$ if and only if they contain a point which is commonly inner. Let us draw a corollary:

If K_2 is properly larger than K_1, the convex dimension of K_2 must be strictly larger than that of K_1.

A chain $K_1 \subset K_2 \subset \dots$, consisting of different complete $g^{\cup}$-leaves, cannot contain more than $n + 1$ members. As above, n denotes the convex dimension of Ω. The maximal number of different leaves in any chain is called the *depth* of the $g^{\cup}$-foliation. As said above, the $g^{\cup}$-foliation consists of all complete $g^{\cup}$-leaves.

In the case $\Omega = \Omega(\mathcal{H})$, the depth if bounded by d^2. If the roof is an affine function, see example 2.3, exactly the faces of Ω are its leaves and the bound is reached.

Let us look again to the setting above in more geometric terms. We shall see that the ω-leaves of $g^{\cup}$ and $g^{\cap}$ correspond uniquely to the faces of $\Omega[g]$.

The triple $\{\Omega[g], \Omega, \Pi\}$ is a *fiber bundle* with bundle space $\Omega[g]$, base space Ω, and projection

$$\Pi : \quad \{\omega, \lambda\} \to \omega \tag{37}$$

In this scheme a roof G becomes a *cross section*, say s_G, by setting

$$\omega \to s_G(\omega) = \{\omega, G(\omega)\} \in \Omega[g] \tag{38}$$

we get $\Pi(s_G(\omega)) = \omega$, which is necessary for a bundle structure.

The boundary, $\partial\Omega[g]$, of $\Omega[g]$ is the union of three disjunct sets:

$$\partial^0\Omega[g] = \{\{\omega, g^{\cup}(\omega)\} \mid g^{\cup}(\omega) = g^{\cap}(\omega)\} \tag{39}$$

$$\partial^-\Omega[g] = \{\{\omega, g^{\cup}(\omega)\} \mid g^{\cup}(\omega) \neq g^{\cap}(\omega)\} \tag{40}$$

$$\partial^+\Omega[g] = \{\{\omega, g^{\cap}(\omega)\} \mid g^{\cup}(\omega) \neq g^{\cap}(\omega)\} \tag{41}$$

The cross section (38) with $G = g^{\cup}$ maps Ω onto $\partial^0\Omega[g] \cup \partial^-\Omega[g]$ while the cross section with $G = g^{\cap}$ maps the base space onto $\partial^0\Omega[g] \cup \partial^+\Omega[g]$.

The fibres degenerate to a point at the boundary part (39) and can be identified with a subset of Ω. By proposition 3.2 that subset consists of the pure point and possibly of some faces at which $g^{\cup} = g^{\cap}$, and all roof extensions of g coincide and are affine.

Let us consider a face $\tilde{K}$ contained in the "lower" part $\partial^-\Omega[g]$ of the boundary (40). $\tilde{K}$ is convex by definition and compact because of the compactness of $\Omega[g]^{\text{pure}}$. Therefore, the projection K of $\tilde{K}$ to Ω, $\Pi\,\tilde{K} = K$, is convex and compact, see (37). We use the supposed face property: $\tilde{\omega} \in \tilde{K}$ implies

$$\tilde{\omega} = \sum p_j \tilde{\omega}_j \Rightarrow \tilde{\omega}_j \in \tilde{K} \tag{42}$$

if all $p_j > 0$. Writing this out in the manner $\tilde{\omega} = \{\omega, g^{\cup}(\omega)\}$, and so on, we arrive at

$$\{\omega, g^{\cup}(\omega)\} = \sum p_j\{\omega_j, g^{\cup}(\omega_j)\} = \{\omega, \sum p_j g^{\cup}(\omega_j)\} \tag{43}$$

Now we can state

Proposition 3.7

There is a one-to-one correspondence between the faces of $\Omega[g]$ contained in $\partial^0\Omega[g] \cup \partial^-\Omega[g]$ and the complete convex leaves of $g^\cup$. The cross section s_G, with $G = g^\cup$, maps complete convex leaves of $g^\cup$ onto faces of $\Omega[g]$. The bundle projection Π returns them back to Ω.

For the concave roof things are similar.

3.3. Illustrating Examples

Example 3.1: Minimum and maximum of g

On Ω^{pure} let $g_{\min}$ be the minimum of g and $g_{\max}$ its maximum. The convex hull of the set

$$\{\pi \in \Omega^{\text{pure}} \,|\, g(\pi) = g_{\min}\} \tag{44}$$

is a complete convex leaf of $g^\cup$. The convex hull of the set

$$\{\pi \in \Omega^{\text{pure}} \,|\, g(\pi) = g_{\max}\} \tag{45}$$

is a complete convex leaf of $g^\cap$.

Let us again consider the diagonal map $D(X) = \text{diag}(X)$ as in (16) and its von Neumann entropy $S(D(.))$, see (17). $g(\pi) = S(D(\pi))$ is the output entropy of the pure state π. The Hilbert space dimension is denoted by d. As well known, the minimum output entropy is zero and the maximal one $\log d$.

Things become more refined by restricting the channel onto a face of Ω. As an example we take a short look at the $(d-1)$-dimensional subspace $\mathcal{H}_0$ which is orthogonal to the vector $|\varphi\rangle = d^{-1/2}\sum|j\rangle$. $\mathcal{H}_0$ consists of vectors $\sum a_j|j\rangle$ such that $\sum a_j = 0$. $\mathcal{H}_0$ supports some pure states satisfying $D(\pi) = d^{-1}\mathbf{1}$ and the maximal output entropy is $\log d$ again.

There is a reasonable conjecture, saying that the *minimal output entropy is independent of d and equal to* $\log 2$. There are $d(d-1)/2$ pure states π_{jk}, $j < k$. The matrix elements a_{nm} of π_{jk} are $1/2$ for $n = m = j$ and $n = m = k$. They are $-1/2$ for $n = j, m = k$ and $m = j, n = k$, and all other entries are zeros. Hence it is evident that $S(\text{diag}(\pi_{jk})) = \log 2$ and, therefore,

$$E_D(\rho) \leq \log 2, \quad \rho = \frac{1}{d-1}(\mathbf{1} - |\varphi\rangle\langle\varphi|)$$

because we can represent ρ by a convex combination of the pure states π_{jk}. The conjecture asserts that the decomposition is an optimal one. The conjecture rests on the fact that for no other state than π_{jk}, supported by $\mathcal{H}_0$, the output of the diagonal map is of rank two. Then one applies a theorem of Michelson and Jozsa, see appendix of [34], reducing in the case at hand the minimization of the entropy to that of minimizing the second elementary symmetric function or, equivalently, to the minimization of the concurrence. For $d = 2$ this is trivial, for $d = 3$ it can be done, for $d > 3$ it is yet a conjecture.

Under the assumption, the conjecture is true, the convex set generated by the π_{jk} is a complete leaf. The minimal length of an optimal decomposition of ρ is equal to $d(d-1)/2$.

Example 3.2: Again the diagonal map

We return to the example 2.4 to prove the flatness of the Entropy (17) of the diagonal map (16). Hence, since we know from von Neumann's work the concavity of $\omega \to S(D(\omega))$, flatness of (17) proves the diagonal map a flat concave roof for all dimensions d of $\mathcal{H}$. In other words, for

$$g(\pi) = S(\text{diag}(\pi)), \quad \pi \in \Omega(\mathcal{H}) \tag{46}$$

it follows for any density operator ω

$$g^{\cap}(\omega) = S(\text{diag}(\omega)) \tag{47}$$

Proposition 3.8

Choose $\omega \in \Omega(\mathcal{H})$. The set K_ω of all states ρ with $\text{diag}(\rho) = \text{diag}(\omega)$ is a complete convex leaf of (47). $g^{\cap}$ is a flat concave roof.

The set K_ω is compact, convex, and $S(D(.))$ is constant on it. Transversal to the sets K_ω the function $S(D(.))$ is strictly concave. This excludes that two density operators with different diagonals can belong to a convex leaf. Hence, the sets K_ω are convex leaves.

4. Wootters' Method

We are going to describe the fundamental idea in [13], see also [12], and its generalizations [14]. After a short introduction to anti-linearity, which is on the heart of the method, we present slightly simplified proofs for a class of convex and concave roofs. For reasons of uniqueness we sometimes write $\langle .,. \rangle$ for the scalar product instead of Dirac's $\langle .|. \rangle$.

The use of anti-linearity [35] goes back, at least in physics, to Wigner. He applied it to the time reversal symmetry [36] and he discovered the structure of anti-unitary operators, [37]. A highlight in the further development of this line of thinking is the proof of the CPT-theorem within Wightman's axiomatic quantum field theory.

4.1. Anti-Linearity in Short

We start with some elementary remarks. An anti-linear operator, say ϑ, obeys the rule

$$\vartheta(\, a_1|\phi_1\rangle + a_2|\phi_2\rangle\,) = a_1^* \vartheta|\phi_1\rangle + a_2^* \vartheta|\phi_2\rangle \tag{48}$$

An important fact follows immediately: Because of $c\vartheta = \vartheta c^*$ the eigenvalues of ϑ form a set of circles. Indeed, if $|x\rangle$ is an eigenvector of ϑ with eigenvalue a, then $\epsilon|x\rangle$, $|\epsilon| = 1$, is an eigenvector with eigenvalue $\epsilon^* a$. Consequently, most of the unitary invariants of linear operators are undefined for anti-linear ones. The trace, for example, does not exist for anti-linear operators.

The Hermitian adjoint $\vartheta^\dagger$ of an anti-linear operator ϑ is defined by

$$\langle \phi_1, \vartheta^\dagger \phi_2 \rangle = \langle \phi_2, \vartheta \phi_1 \rangle \tag{49}$$

There is to set a caution mark: Do not apply an anti-linear operator to a bra in the usual Dirac manner! By (49) one may get absurd results.

A useful class of anti-linear operators are the Hermitian ones. By (49) any matrix representation must result in a complex symmetric matrix. About symmetric matrices see [38]. It follows that the Hermitian anti-linear operators constitute a complex linear space of dimension $d(d+1)/2$ if $\dim \mathcal{H} = d$.

An anti-unitary, V, is an anti-linear operator which is unitary, *i.e.*, satisfies $V^\dagger = V^{-1}$. A conjugation, Θ, is an anti-unitary which is Hermitian. It implies $\Theta^2 = \mathbf{1}$. In accordance with what has been said about eigenvalues, one can find an orthogonal basis $|\phi_1\rangle, \ldots$ such that $\Theta|\phi_j\rangle = \epsilon_j |\phi_j\rangle$ with arbitrarily chosen unimodular numbers ϵ_j.

A conjugation Θ distinguishes a *real* Hilbert subspace $\mathcal{H}_\Theta$ of $\mathcal{H}$ consisting of all Θ-real vectors, $\Theta|\psi\rangle = |\psi\rangle$.

There is a polar decomposition, $\vartheta = V|\vartheta|$, for any anti-linear operator ϑ. $|\vartheta|$ denotes the positive root $(\vartheta^\dagger \vartheta)^{1/2}$ and V is an anti-unitary operator. The proof is similar to the linear case [39].

Now we turn to the case of an anti-linear Hermitian operator $\vartheta = \vartheta^\dagger$. It commutes with the positive (linear!) operator ϑ^2 and, therefore, with $|\vartheta| = (\vartheta^2)^{1/2}$. With a non-singular ϑ we perform $\Theta = \vartheta^{-1}|\vartheta|$ the square of which is $\mathbf{1}$. As it is Hermitian too, it is a conjugation. We conclude

$$\vartheta = \Theta|\vartheta| = |\vartheta|\Theta, \quad \Theta = \Theta^\dagger = \Theta^{-1} \tag{50}$$

By continuity, or by a more detailed analysis, (50) can be verified for all Hermitian and anti-linear ϑ.

4.2. *Building Roofs with an Anti-Linear Hermitian ϑ*

Let ϑ be Hermitian and anti-linear on a Hilbert space $\mathcal{H}$ of dimension d. This setting provides a function

$$g(\pi) = |\langle \psi, \vartheta\, \psi \rangle|, \quad \pi = |\psi\rangle\langle\psi| \tag{51}$$

on the pure states of $\Omega(\mathcal{H})$. Now $g^\cap$ and $g^\cup$ are well defined and we shall prove:

Proposition 4.1

Let g be as in (51). If $\{\lambda_1 \geq \lambda_2 \geq \ldots\}$ denote the eigenvalues of $|\sqrt{\omega}\vartheta\sqrt{\omega}|$, then

$$g^\cup(\omega) = \max\{0, \ \lambda_1 - \sum_{j>1} \lambda_j\}, \tag{52}$$

$$g^\cap(\omega) = \sum \lambda_j \tag{53}$$

$g^\cup$ and $g^\cap$ are flat roofs.

At first we simplify the assertion by starting with

$$\vartheta_\omega := \sqrt{\omega}\vartheta\sqrt{\omega}, \quad |\vartheta_\omega| = (\sqrt{\omega}\,\vartheta\omega\vartheta\,\sqrt{\omega})^{1/2} \tag{54}$$

Up to normalization every pure decomposition of ω can be gained from a decomposition of the unit operator $\mathbf{1}$,

$$\omega = \sum \sqrt{\omega}\pi_j\sqrt{\omega}, \quad \mathbf{1} = \sum \pi_j \tag{55}$$

(51) is 1-homogeneous on the positive rank one operators. Comparing (55) with (25) and (26), it can be seen that

$$g^\cup(\omega) = \inf \sum |\langle \psi_j, \vartheta_\omega \psi_j \rangle| \quad , g^\cap(\omega) = \sup \sum |\langle \psi_j, \vartheta_\omega \psi_j \rangle| \tag{56}$$

where we have to run through all rank one decompositions of **1**,

$$\sum |\psi_j\rangle\langle\psi_j| = \mathbf{1} \tag{57}$$

Now ϑ_ω is Hermitian and anti-linear. Therefore there is to any chosen set of phase factors $\epsilon_1, \epsilon_2, \dots$ a basis $\varphi_1, \varphi_2, \dots$ satisfying

$$|\vartheta_\omega| \, |\varphi_j\rangle = \lambda_j |\varphi_j\rangle, \quad \vartheta_\omega |\varphi_j\rangle = \lambda_j \epsilon_j |\varphi_j\rangle \tag{58}$$

and the conjugation Θ in the polar decomposition multiplies the j-th basis vector by ϵ_j.

For the next step we assume the existence of a real $d \times d$ Hadamard matrix. Then we can choose a basis $\{|\chi_i\rangle\}$ fulfilling

$$|\chi_i\rangle = \frac{1}{\sqrt{d}} \sum_j a_{ij} |\varphi_j\rangle, \quad a_{ij} = \pm 1 \tag{59}$$

because of the orthogonality and $a_{ki}^2 = 1$ we get for all k

$$d \langle \chi_k, \vartheta_\omega \chi_k \rangle = \sum_{ij} a_{ki} a_{kj} \langle \varphi_i, \vartheta_\omega \varphi_j \rangle = \sum \epsilon_j \lambda_j \tag{60}$$

Therefore, by (51), we get

$$g^\cup(\omega) \le | \sum \epsilon_j \lambda_j | \le g^\cap(\omega) \tag{61}$$

By varying the unimodular numbers ϵ_j, which could be chosen arbitrarily, one arrives at

$$g^\cup(\omega) \le \max\{0, \ \lambda_1 - \sum_{j>1} \lambda_j\}, \quad g^\cap(\omega) \ge \sum \lambda_j \tag{62}$$

Assuming equality in (62), we see from (60) that ω is a flat point of $g^\cap$ and of $g^\cup$. If $g^\cup(\omega) > 0$, then we choose $\epsilon_1 = 1$ and $\epsilon_j = -1$ for $j > 1$ to obtain from (58) an optimal basis $\{|\chi_k\}$. In the concave case we set $\epsilon_j = 1$ for all j.

Now we are going to prove equality in (62), starting with $g^\cup$. We clearly get an estimation from below in (56) by

$$\inf | \sum \xi_k | \, , \quad \xi_k = \langle \psi_k, \vartheta_\omega \psi_k \rangle | \tag{63}$$

Sandwiching with the eigenbasis (58) it yields

$$\sum \xi_j = \sum_{jk} \langle \psi_k, \vartheta_\omega \varphi_j \rangle \langle \varphi_j, \psi_k \rangle = \sum_{jk} \epsilon_j \lambda_j \langle \psi_k, \varphi_j \rangle \langle \varphi_j, \psi_k \rangle$$

and this shows, summing first over k,

$$| \sum_k \xi_k | = | \sum_k \epsilon_j \lambda_j |$$

Its minimum is attained by the largest of the two numbers 0 and $\lambda_1 - \lambda_2 - \dots$ and the first equation in (54) is true.

Now we prove equality in (62) for $g^\cap$. the second equation of (56). It is

$$|\langle \psi_k, \vartheta_\omega \psi_k \rangle| = |\langle \psi_k, |\vartheta_\omega| \psi_k' \rangle|, \quad |\psi_k'\rangle = \Theta |\psi_k\rangle$$

We apply Cauchy's inequality. The result is

$$|\langle \psi_k, |\vartheta_\omega|\psi'_k\rangle|^2 \leq \langle \psi_k, |\vartheta_\omega|\psi_k\rangle \langle \psi'_k, |\vartheta_\omega|\psi'_k\rangle$$

and, because Θ is an involution, hence anti-unitary, we arrive at

$$|\langle \psi_k, \vartheta_\omega \psi_k\rangle| \leq \langle \psi_k, |\vartheta_\omega|\psi_k\rangle \tag{64}$$

Summing up we get the trace of $|\vartheta_\omega|$ which upper bounds $g^\cap(\omega)$.

Up to now the proof of proposition 4.1 rests on particular bases $\{|\chi_k\rangle\}$. They exist if there is a real $d \times d$ Hadamard matrix, $d = \dim \mathcal{H}$. To overcome the restriction we go to a larger Hilbert space, $\mathcal{H} \oplus \mathcal{H}_0$, for which the proposition has been proved. Then we restrict to the face of density operators supported by the original Hilbert space $\mathcal{H}$. Because a (flat) roof remains a (flat) roof if restricted to a face, the proof will become complete.

To do so, we choose $d' = \dim \mathcal{H} \oplus \mathcal{H}_0$ sufficiently large and extend ϑ to ϑ' by requiring $\vartheta'|\psi_0\rangle = 0$ for all $|\psi_0\rangle \in \mathcal{H}_0$. We then choose any conjugation Θ_0 on $\mathcal{H}_0$ and use $\Theta' = \Theta \oplus \Theta_0$. Now, if there is a real $d' \times d'$ Hadamard matrix, we are done.

Hadamard matrices exist in dimensions $d' = 2^m$. This suffices for the proof.

Proposition 4.2

Let $g(\pi) = |\langle \psi, \vartheta\psi\rangle|$. Then $g^\cup$ and $g^\cap$ allow for flat optimal decompositions of length d' where $d \leq d' = 2^m$. More generally, if $d \leq d'$ and there is a real $d' \times d'$ Hadamard matrix, then there are flat optimal decompositions of length d'.

4.3. Cases of Application

Indeed, the question is now: How to find a suitable anti-linear Hermitian operator ϑ to calculate concurrence, tangle, and entanglement entropy (as particular cases of entanglement of formation) in $2 \times n$ systems. Clearly, this can be fully successful for flat roofs only.

Let T be a trace preserving positive map from the states

$$\omega \in \Omega^d := \Omega(\mathcal{H}), \quad \dim \mathcal{H} = d$$

into the 1-qubit state space $\Omega(\mathcal{H}_2)$. Because the trace of the output, $\operatorname{Tr} T(\omega)$ is one, $T(\omega)$ is characterized, up to a unitary transformation, by one variable. It is common to use $4 \det T(\omega)$ or its square root to be this variable. Let us abbreviate the convex roofs on Ω^d, playing a role below. By

$$C_T = 2(\sqrt{\det T})^\cup, \quad (\det T)(\omega) = \det T(\omega) \tag{65}$$

$$\tau_T = 4(\det T)^\cup \tag{66}$$

$$E_T = (S_T)^\cup, \quad S_T(\omega) = S(T(\omega)) \tag{67}$$

(65) is the concurrence, (66) the 1-tangle, and (67) the entanglement of T. (67) is the entanglement of formation if T is a partial trace of a bipartite quantum system. By its very definition we need only the values of $\det T$ and of S_T for pure input states.

There are some general relation between these three roofs. The first is typical also for more general settings: C_T is a positive convex function and so does its square. For pure input states the tangle and the squared concurrence coincide. Hence, because τ_T is maximal within all convex extensions, it is not less than C_T^2. On the other hand, if ω turns out to be a flat point of C_T, than this remains true for its square. Thus,

Proposition 4.3

For stochastic maps with 1-qubit outputs it holds

$$\tau_T(\omega) \geq C_T(\omega)^2 \tag{68}$$

and equality takes place for flat roof points of C_T.

Let us now switch to S_T. With use the abbreviations $\eta(x) = -x \log x$ and

$$\xi(x) = \eta\left(\frac{1-y}{2}\right) + \eta\left(\frac{1+y}{2}\right), \quad 1 = x^2 + y^2 \tag{69}$$

ξ is defined and continuous for $-1 \leq x \leq 1$ and it is strictly convex. Therefore, ξ is the sup of a family of functions $ax + b$. Inserting a convex function C defined on any convex set with values $-1 \leq C \leq 1$, we get $\xi(C)$ by a sup of convex functions $aC + b$. Therefore, $\xi(C)$ is a convex function on the domain of definition of C.

We apply this fact to the concurrence C_T yielding:

$$\omega \to \xi_T(\omega) := \xi(\,C_T(\omega)\,) \tag{70}$$

is a convex function on Ω^d. C_T for pure states π we get $2\sqrt{\det T(\pi)}$. We insert in (70),

$$\xi_T(\pi) = \eta\left(\frac{1 - \sqrt{1 - 4 \det T(\pi)}}{2}\right) + \eta\left(\frac{1 + \sqrt{1 - 4 \det T(\pi)}}{2}\right)$$

and one identifies the arguments in η as the two eigenvalues of $T(\pi)$.

$$\xi_T(\pi) = S(T(\pi)), \quad \pi \in \Omega^{d,\mathrm{pure}} \tag{71}$$

proves ξ_T to be a convex extension of the pure states output entropies. Reasoning as for proposition 4.3 results in

Proposition 4.4

For stochastic maps with 1-qubit outputs it holds

$$E_T(\omega) \geq \xi(\,C_T(\omega)\,) \tag{72}$$

Equality takes place if ω is a flat roof point.

It should be underlined hat there are more and different estimations for concurrence and entanglement of formation in higher dimensions, see [40–44]. In [56] there is an application to states with only two different, but arbitrarily degenerated eigenvalues.

4.4. How to Find ϑ

There is a general recipe to get the wanted anti-linear operator for channels T mapping the states of a quantum system $\mathcal{H}_d$ to 1-qubit states. Assume a Kraus representation

$$T(X) = \sum A_j X A_j^\dagger, \qquad A_j : \quad \mathcal{H}_d \mapsto \mathcal{H}_2 \tag{73}$$

There is an additional condition to be fulfilled: T must be Kraus representable with not more than two Kraus operators. But at first we remain within the more general (73).

The key to the following is the existence of the "time reversal" or "spin flip" anti-unitary operator θ_f on $\mathcal{H}_2$,

$$\theta_f(c_0|0\rangle + c_1|1\rangle) = c_1^*|0\rangle - c_0^*|1\rangle \tag{74}$$

Apart from the obvious

$$\theta_f^\dagger = \theta_f^{-1} = -\theta_f$$

the relation

$$\theta_f Y^\dagger \theta_f Y = -(\det Y)\, \mathbf{1}_2 \tag{75}$$

is valid for all operators $Y \in \mathcal{B}(\mathcal{H}_2)$. Up to a multiplicative constant, only the spin flip commutes with all $U \in \mathrm{SU}(2)$, It is really a very special anti-unitary operator.

The task is in inserting $Y = T(X)$ into (75) and to get something similar for $\det T$. This goes through particulary nice if X is of rank one, $X = |\psi_2\rangle\langle\psi_1|$. Calculations show

$$\det T(|\psi_2\rangle\langle\psi_1|) = \sum_{j<k} \langle\psi_1, \vartheta_{jk}\psi_1\rangle \langle\psi_2, \vartheta_{jk}\psi_2\rangle^*, \quad |\psi_i\rangle \in \mathcal{H}_d \tag{76}$$

The anti-linear Hermitian operators ϑ_{jk} are defined by

$$\vartheta_{jk} = \frac{1}{2}(A_j^* \theta_f A_k - A_k^* \theta_f A_j) \tag{77}$$

using the Kraus operators A_j from any Kraus representation (73) of T. The operators ϑ_{jk} are Hermitian and anti-linear.

In the lucky case of channels (73) with just two Kraus operators, A_1 and A_2, we get only one operator ϑ by (75) and, hence,

$$\sqrt{\det T(|\psi\rangle\langle\psi|)} = |\langle\psi, \vartheta\,\psi\rangle| \tag{78}$$

and, by proposition 4.1, we are done.

Wether and how one can replace the operation $X \to \vartheta X \vartheta$ by an anti-linear stochastic map to obtain a more general roof construction, is unknown. An (implicit) attempt is in [46] by taking $X \to (\mathrm{Tr}\,X)\mathbf{1} - X$ as an higher dimensional substitute for the flip operation.

4.5. Applications

The partial trace of a 2-quibt system can be represented by two Kraus operators: Looking at the operators over $\mathcal{H}_2 \otimes \mathcal{H}_2$ as block matrices, the partial trace over the second part is the map

$$X = \begin{pmatrix} X_{00} & X_{01} \\ X_{10} & X_{11} \end{pmatrix} \longrightarrow X_{00} + X_{11} = Y \tag{79}$$

One immediately sees a possible choice for the Kraus operators,

$$A_1 = \frac{1}{\sqrt{2}}\{\mathbf{1}_2, \mathbf{0}_2\}, \quad A_2 = \frac{1}{\sqrt{2}}\{\mathbf{0}_2, \mathbf{1}_2\} \tag{80}$$

Now we can compute ϑ according to (77). We get, eventually up to a sign, Wootters' conjugation, $\vartheta = \theta_{\mathrm{w}}$,

$$4\vartheta = \theta_{\mathrm{w}} = \begin{pmatrix} \mathbf{0} & \theta_{\mathrm{f}} \\ -\theta_{\mathrm{f}} & \mathbf{0} \end{pmatrix} = \theta_{\mathrm{f}} \otimes \theta_{\mathrm{f}} \tag{81}$$

Remark: The concurrence of a 2-qubit system is a flat convex roof. Generally, complete convex leaves consists of a set of flat ones.

Let us choose two operators, $A_1 = A$, $A_2 = B$, from $\mathcal{B}(\mathcal{H}_2)$ so that (73) becomes a 1-qubit channel. Then there are only two eigenvalues, λ_1, λ_2, of $|\sqrt{\omega}\vartheta\sqrt{\omega}|$ to respect and (52) simplifies to

$$g^{\cup}(\omega) = |\lambda_2 - \lambda_1| \tag{82}$$

One has to solve a quadratic equation to get the general expression

$$\frac{1}{4} C_T(\omega)^2 = \mathrm{Tr}\,(\omega\vartheta\omega\vartheta) - 2(\det X)\,(\det \vartheta^2)^{1/2} \tag{83}$$

There are standard forms for 1-qubit channels, [20,47–49]. For channels with two Kraus operators one can assume

$$A = \begin{pmatrix} a_{00} & 0 \\ 0 & a_{11} \end{pmatrix}, \quad B = \begin{pmatrix} 0 & b_{01} \\ b_{10} & 0 \end{pmatrix} \tag{84}$$

up to unitary equivalence. With this choice ϑ acts as

$$\vartheta(c_0|0\rangle + c_1|1\rangle) = (b_{10}a_{00}c_0)^*|0\rangle - (b_{01}a_{11}c_1)^*|1\rangle \tag{85}$$

After inserting in the relevant expressions one observes that the concurrence is the restriction of a semi-norm to the state space. Indeed, one obtains, [50,51],

$$C_T(X) = |\,|b_{10}a_{00}|x_{00} + |b_{01}a_{11}|x_{11} + zx_{10} - z^*x_{01}\,| \tag{86}$$

z is one of the roots of

$$z^2 = a_{00}^* a_{11} b_{01} b_{10}^* \tag{87}$$

5. A Subtraction Procedure

We start with a simple example not covered by Wootters' method and showing the principle. The idea is to subtract from $\det T(X)$ a suitable multiple of $\det(X)$ to get the squared concurrence or the tangle of a stochastic 1-qubit map T. We choose for T the map

$$\begin{pmatrix} x_{00} & x_{01} \\ x_{10} & x_{11} \end{pmatrix} \longrightarrow \begin{pmatrix} x_{00} + (1-\gamma)x_{11} & 0 \\ 0 & \gamma x_{11} \end{pmatrix} \tag{88}$$

and consider

$$\gamma x_{00}x_{11} + \gamma(1-\gamma)x_{11}^2 - w(x_{00}x_{11} - x_{01}x_{10}) \tag{89}$$

With $w = \gamma$, we arrive at the squared concurrence of T,

$$\frac{1}{4} C_T(X)^2 = \gamma(1 - \gamma)x_{11}^2 + \gamma x_{01}x_{10} \tag{90}$$

At first (90) is a positive semi-definite quadratic form implying that its square root is convex. Secondly, by its very construction it coincides for pure states π with $4 \det T(\pi)$. Finally, on the state space, it is a roof. To indicate a general way to proof the roof property we polarize (90) and get

$$(X, Y)_T := \gamma(1 - \gamma)x_{11}y_{11} + \frac{1}{2}\gamma(x_{01}y_{10} + x_{10}y_{01}) \tag{91}$$

which is a positive semi-definite bilinear form in the space of Hermitian matrices. For the pure state $\pi_0 = |0\rangle\langle 0|$ (90) becomes zero. Applying the Schwarz inequality we get $(X, \pi_0) = 0$ for all X. Hence, with any pure state π,

$$\omega_s = (1 - s)\pi_0 + s\pi \implies (\omega_s, \omega_s) = s^2(\pi, \pi) \tag{92}$$

Taking the root we see that $s \to \omega_s$, $0 \leq s \leq 1$, is a convex leaf of C_T for every π. Now the assertion is proved and, the more, C_T is *not* a flat roof.

One may ask, whether one can diminish w a bit without destroying convexity on Ω. Let us use in (89) the new value $w' = \gamma^2$. Then (89) becomes

$$\gamma x_{00}x_{11} + \gamma(1 - \gamma)x_{11}^2 - \gamma^2(x_{00}x_{11} - x_{01}x_{10})$$

Different to the former case we restrict ourselves to $\Omega(\mathcal{H}_2)$ and respect the condition $x_{00} + x_{11} = 1$. After some manipulations we arrive at a convex roof which coincides with $\det T(\pi)$ for pure states. Up to a factor it must be the tangle of T on Ω.

$$\frac{1}{4}\tau_T(X) = \gamma(1 - \gamma)x_{11} + \gamma^2 x_{01}x_{10} \tag{93}$$

The tangle is affine on the set of density operators with $x_{01} = $ constant. As the square of the concurrence is equal to the tangle for pure states, we have the inequality $\tau_T(\omega) > C_T(\omega)^2$ for mixed states.

That the ansatz (89) is working generally for the concurrence has been shown first in [16,17,52], by means of the "S-lemma of Yakobovich" and, using the explicit expression for general stochastic 1-qubit maps of [20], in [19]. The case of the tangle can be read off from [22].

5.1. Concurrence of Stochastic 1-Qubit Maps

Let T be a stochastic, *i.e.*, a positive trace preserving map. We prove

Proposition 5.1

There is a real number $0 \leq w \leq 1$ such that for all $\rho \in \Omega(\mathcal{H}_2)$

$$\frac{1}{4} C_T(\rho)^2 = \det T(\rho) - w \det \rho \tag{94}$$

At first we show the w-bounds. With $w < 0$, (94) becomes the sum of two concave functions on Ω and C_T could not be convex. To prove $1 \geq w$ we insert $\rho_0 = (1/2)\mathbf{1}$ and get $\det T(\rho_0) \geq w/4$. However, $\det T(\rho_0) \leq 1/4$ is required by stochasticity. $w > 1$ would be a contradiction.

Next, we consider the expression (94) on the Bloch space of all Hermitian operators of trace one,

$$X = \frac{1}{2}(\mathbf{1} + x_1\sigma_1 + x_2\sigma_2 + x_3\sigma_3) \tag{95}$$

The determinant of X is a quadratic function

$$\det X = \frac{1}{4}(1 - x_1^2 - x_2^2 - x_3^2)$$

in the Bloch coordinates. The same is with $\det T(X)$. In the terminology of the S-lemma, the quadratic function $\det T(X)$ is called *co-positive with* $\det X$ because from $\det X \geq 0$ it follows $\det T(X) \geq 0$ under the constraint $\operatorname{Tr} X = 1$.

The S-lemma, [18], states the following: Let q_1 and q_2 be two quadratic functions on $\mathbb{R}^n$, not necessarily homogeneous. If $q_1(x) \geq 0$ implies $q_2(x) \geq 0$ then q_2 is co-positive with q_1.

S-lemma

Let q_1 be strictly positive at least at one point. Then there exists a real number w such that

$$q_2(x) - wq_1(x) \geq 0 \text{ for all } x \in \mathbb{R}^n \tag{96}$$

if and only if q_2 is co-positive with q_1.

Now it is proved: The right expression of (94) can be made non-negative with suitable numbers w for all Hermitian trace one operators. Then, substituting $x_j \to x_j/x_0$ and multiplying by x_0^2, we see that

$$\det \operatorname{Tr}(X) - w\det X \geq 0 \tag{97}$$

becomes a positive semi-definite and homogeneous polynomial in the variables x_0, x_1, x_2, x_3 for some w. Polarizing (97) as in (91) yields a positive semi-definite symmetric form $(X, Y)_w$ satisfying

$$(X, X)_w = \det T(X) - w\det X \tag{98}$$

We now may assume (97) for all values w which are bounded by $1 \geq w_1 \geq w \geq w_2 \geq 0$. We can further assume that $(X, Y)_w$ is degenerated for $w = w_1$ and for $w = w_2$. But wether degenerate or not, (97) implies Cauchy's inequality

$$|(X, Y)_w|^2 \leq (X, X)_w(Y, Y)_w \tag{99}$$

In particular, if $Y = \nu$ is in the null-space, $(\nu, \nu)_w = 0$, then $\det T(\nu) = w\det\nu$ and $\det T(\nu) \geq w'\det\nu$ for all allowed w', *i.e.*,

$$(w - w')\det\nu \geq 0, \quad w_1 \geq w' \geq w_2 \tag{100}$$

Furthermore, $(\nu, X)_w = 0$ for all Hermitian X.

We like to show: If $w = w_2$ every density operator ρ is a roof point.

We have to distinguish several cases. The first one is $\operatorname{Tr}\nu = 0$. Then, with $\rho \in \Omega$, we define

$$\rho_s = \rho + s\nu \tag{101}$$

On this line $(\rho_s, \rho_s)_W$ is independent of s. Therefore, because of (94), its intersection with Ω is a flat convex leaf of C_T.

Being Hermitian and not identical zero, $\text{Tr}\,\nu = 0$ results in $\det\nu < 0$. Because of (100) one concludes $w = w_2$.

For the next cases we suppose $\text{Tr}\,\nu = 1$ and start with

$$\rho_s = (1-s)\nu + s\rho \tag{102}$$

Then $(\rho_s, \rho_s)_W = s^2$. If the sign of s does not change while ρ_s is inside the Bloch ball, we can take the root and get a convex leaf. This takes place if ν is *not* an inner point of Ω, *i.e.*, not a properly mixed state.

The condition is certainly satisfied if $\det\nu = 0$ and ν is a pure state. The condition implies the w-independence of $(\nu, \nu)_w$ which becomes equal to $\det T(\nu)$. As there is only one convex roof C_T it is $w_1 = w_2$ necessarily [23].

ν is outside Ω if $\det\nu \neq 0$. We conclude $w = w_2$ from (100) and we get convex leaves by intersecting the lines (102) with the Bloch ball.

In addition one observes: $\det\nu \neq 0$ is necessary for $w_1 > w_2$. Indeed, by (100) we see $(\nu, \nu)_w = 0$ can be satisfied if either $w = w_1$ and $\det\nu > 0$ or by $w = w_2$ and $\det\nu < 0$.

Now, all relevant cases are discussed and proposition 5.1 is proved.

In the course of the proof one obtains two more general insights:

Proposition 5.2

The concurrence of stochastic 1-qubit maps is the restriction of a Hilbert semi-norm to the state space. Every state allows for an optimal decomposition of length two.

5.2. Axial Symmetric Maps, Concurrence

We shall list the subtraction parameter w for the class of axial symmetric stochastic maps. A standard form for them reads

$$T(X) = \begin{pmatrix} \alpha x_{00} + (1-\gamma)x_{11} & \beta x_{01} \\ \beta x_{10} & \gamma x_{11} + (1-\alpha)x_{00} \end{pmatrix} \tag{103}$$

with real non-negative parameters α, β, γ. The trace preserving is obvious. Positivity requires $0 \leq \alpha \leq 1$, $0 \leq \gamma \leq 1$, and

$$\beta^2 \leq \beta_{\max}^2 := 1 + 2\alpha\gamma - \alpha - \gamma + 2\sqrt{\alpha(1-\alpha)\gamma(1-\gamma)} \tag{104}$$

T is a channel, hence completely positive, if $\beta^2 \leq \alpha\gamma$. To express w one needs the "critical" β_c

$$\beta_c := 1 + 2\alpha\gamma - \alpha - \gamma - 2\sqrt{\alpha(1-\alpha)\gamma(1-\gamma)} \tag{105}$$

Then, see [52],

$$w = \max\{\beta^2, \beta_c^2\} \tag{106}$$

At the bifurcation point $\beta = \beta_c$ the T-concurrence is affine on Ω. For $\beta \geq \beta_c$ the roof is flat. Otherwise it looks similar to the particular one (88). See [52] for more details.

5.3. Axial Symmetric Maps, Tangle

The tangle for stochastic 1-qubit maps can be found in [16,17]. For 1-qubit channels it is already in [22]. These tangles always allow for optimal decompositions of length two.

The axial symmetric maps (103) can be treated explicitly. The following is due to [53].

Case A: If $|\beta| > |\alpha + \gamma - 1|$ one has to use $w = \beta^2$. It results in

$$\frac{1}{4}\tau_T(X) = 1 - \beta^2 - (\alpha - \gamma)^2 - 2(\alpha - \gamma)(\alpha + \gamma - 1)x_3 + [\beta^2 - (\alpha - \gamma - 1)^2]x_3^2 \qquad (107)$$

Case B: Here $|\beta| = |\alpha + \gamma - 1|$, a bifurcation point in the parameter space. $w = \beta^2$ results in

$$\frac{1}{4}\tau_T(X) = 1 - \beta^2 - (\alpha - \gamma)^2 - 2(\alpha - \gamma)(\alpha + \gamma - 1)x_3 \qquad (108)$$

and the tangle becomes affine on the Bloch ball.

Case C: If $|\beta| < |\alpha + \gamma - 1|$ then $w = (\alpha + \gamma - 1)^2$ and we obtain

$$\frac{1}{4}\tau_T(X) = 1 - (\alpha + \gamma - 1)^2 - (\alpha - \beta)^2 - 2(\alpha - \gamma)(\alpha + \gamma - 1)x_3 + [(\alpha + \gamma - 1)^2 - \beta^2](x_1^2 + x_2^2) \quad (109)$$

6. Symmetries

The use of symmetries is almost obligatory in the treatment of roofs. We present only a small, hopefully helpful, part of it, mainly abstracted from [10,26,27,54,55]. See also [45].

Let $\Omega(\mathcal{H})$ be the space of states supported by the Hilbert space $\mathcal{H}$ of dimension d, and g a real continuous function on Ω^{pure}.

A symmetry of Ω is a transformation

$$\omega \to \omega^V := V\omega V^{-1} \qquad (110)$$

V is a unitary or an anti-unitary operator *inducing* the symmetry (110).

We need the group Γ of all V such that

$$\pi \in \Omega^{\text{pure}} \implies g(\pi^V) = g(\pi) \qquad (111)$$

Γ is the *invariance group of g*. A quite obvious statement reads

Proposition 6.1:

If Γ is the invariance group of g, then

$$g^{\cup}(\omega^V) = g^{\cup}(\omega), \quad g^{\cap}(\omega^V) = g^{\cap}(\omega) \qquad (112)$$

for all $V \in \Gamma$ and all $\omega \in \Omega$.

Let K be a convex leaf of $g^{\cup}$. Obviously,

$$K^V = \{\omega^V \mid \omega \in K\} \qquad (113)$$

is a convex leaf of $g^{\cup}$ again. Hence, $K \to K^V$ permutes the convex leaves.

An interesting subgroup of Γ is the stabilizer group

$$\Gamma_K = \{V \in \Gamma \mid K^V = K\} \tag{114}$$

This is a compact group with an invariant Haar measure. say $d_K V$. We can perform the invariant integration ("twirling") over Γ_K,

$$\omega \longrightarrow \omega^K = \int \omega^V d_K V \tag{115}$$

There is only one Γ_K-invariant element in the convex hull of all ω^V. It is ω^K.

The map $\omega \to \omega^K$ contracts K onto the set

$$K^{\text{stable}} = \{\omega \in K \mid \omega = \int \omega^V d_K V\} \tag{116}$$

This set, being convex and compact, is the convex hull of its *extremal invariant states.* Extremal invariant states can be represented by π^K with pure $\pi \in K$. Invariant states which are not extremal, cannot be represented in such a way.

Proposition 6.2:

Let K be a convex leaf of $g^{\cup}$ and Γ_K its stabilizer group. Then $K \cap \Omega^{\text{pure}}$ consists of Γ_K-orbits. Every extremal Γ_K-invariant state of K is of the form π^K, π pure. Every Γ_K-invariant states of K is a convex combination of extremal Γ_K-invariant states.

6.1. Entanglement of the Diagonal Channel

In example 3.2 we considered the concave roof of (46),

$$g(\pi) = S(\text{diag}(\pi)), \quad \pi \in \Omega(\mathcal{H})$$

Now we look at the convex roof $g^{\cup}$, *i.e.*, at the entanglement E_D of $D(\omega) = \text{diag}(\omega)$.

With the exception of $d = 2$ one does not know the structure of E_D. But there are some insights on highly symmetric, "isotropic" quantum states.

The channel D will be described by the help of a basis $|j\rangle$, $j = 1, \ldots, d$. To it we associate the vector

$$|\psi\rangle = \frac{1}{\sqrt{d}} \sum |j\rangle \tag{117}$$

The invariance group, Γ, of (117) consists of the permutations of the chosen basis, eventually followed by the conjugation Θ defined by $\Theta|j\rangle = |j\rangle$ for all j. The density operator ω commutes with Γ if its matrix elements satisfy

$$\langle j|\omega|j\rangle = \frac{1}{d}, \quad \langle j|\omega|k\rangle = \frac{x}{d} \tag{118}$$

for all j and all $k \neq j$. x is a real number in the range

$$-\frac{1}{d-1} \le x \le 1 \tag{119}$$

The restriction is due to the positivity of ω. One often uses the *fidelity parameter, F*,

$$0 \leq F := \langle \psi | \omega | \psi \rangle = \frac{(d-1)x + 1}{d-1} \leq 1 \tag{120}$$

and we denote the corresponding Γ-invariant density operator by ω_F.

We choose an allowed value F and write K_ω or $K(F)$ for the complete convex leaf of ω_F with respect to E_D. Now we state the following:

$$\rho \in K_\omega \Rightarrow \Theta\rho = \rho\Theta \tag{121}$$

Θ is the conjugation about the basis $\{|j\rangle\}$.

Proof: It suffices to prove the assertion for pure states. We assume that the pure states π and $\pi' = \Theta\pi\Theta$ are both in K_ω. The diagonal parts of them and of $\rho = (1/2)(\pi + \pi')$ are the same. It follows $S_D(\rho) = S_D(\pi) = S_D(\pi')$ and, because we are inside a convex leaf, we get also $g^\cup(\rho) = S_D(\rho)$. Hence, by proposition 3.2, $S_D = E_D$ on the whole face containing π and π'. This is a contradiction if $\pi \neq \pi'$.

Indeed, we proved something more:

Proposition 6.3:

Any two different pure states contained in a convex leaf of E_D must have different diagonal parts.

The Γ-invariant density operators are ordered by the fidelity parameters as indicated by (120). The more, $F \to \omega_F$ is convexly linear in F. This fact allows to apply proposition 6.2.

Proposition 6.4:

Let $K(F)$ denote the compact convex leaf of E_D belonging to the Γ-invariant density operator ω_F. There is a subset R of the unit interval as follows:
a) Either we have $F \in R$. Then $K(F)$ consists of flat roof points only. There is no other maximal symmetrical state in $K(F)$ than ω_F.
b) Or there are $F^-, F^+ \in R$ such that $K(F)$ is the convex hull of $K(F^-) \cap K(F^+)$.

In the case $d = 3$ and if

$$\frac{1}{2} \leq F \leq F^{**}, \quad F^{**} = \frac{8}{9}$$

or $F = 0$ case a) is true. There is an optimal vector of the form $a|1\rangle + b|2\rangle + b|3\rangle$ for any of these F-values. $K_\omega = K(F)$ contains not more than three pure states. They become permuted by the action of the invariance group Γ.

For more details, also in higher dimensions, see [55].

6.2. An Embedding

There are numerous relations between different channels. Some of them provide insight in roof structures. Our main interest is again in the diagonal channels.

Let $\mathcal{H}$ and $\mathcal{H}'$ be Hilbert spaces of dimensions d and $d' > d$. There are embeddings of $\mathcal{H}$ into $\mathcal{H}'$ which relate the entanglement E_D and $E_{D'}$ of the corresponding diagonal maps, D and D'.

For their description we first choose d integers, $m_1, \ldots, m_d$, such that $d' = m_1 + \ldots + m_d$ and enumerate the basis vectors of $\mathcal{H}'$ as

$$|jk\rangle, \quad j = 1, \ldots, d, \quad k = 1, \ldots, m_j \tag{122}$$

We further choose numbers

$$y_{j,k}, \quad j = 1, \ldots, d, \quad k = 1, \ldots, m_j \tag{123}$$

satisfying

$$\sum_{k=1}^{m_j} |y_{jk}|^2 = 1, \quad j = 1, \ldots, d \tag{124}$$

These data provide a unitary embedding

$$|j\rangle \rightarrow V|j\rangle = \sum_{j=1}^{d} y_{jk}|j, k\rangle \tag{125}$$

From

$$\mathrm{diag}(X) = \{x_{11}, \ldots, x_{dd}\} \tag{126}$$

we get

$$\mathrm{diag}(VXV^\dagger) = \{|y_{11}|^2 x_{11}, \ldots, |y_{1m_1}|^2 x_{11}, |y_{21}|^2 x_{22}, \ldots |y_{2m_1}|^2 x_{22}, \ldots\} \tag{127}$$

One obtains for the entropy of the diagonal channel

$$S_{D'}(VXV^\dagger) = \sum_{k=1}^{m_1} \eta(|y_{1k}|^2 x_{11}) + \sum_{k=1}^{m_2} \eta(|y_{2k}|^2 x_{22}) + \ldots \tag{128}$$

The functional equation $\eta(xy) = y\eta(x) + x\eta(y)$ allows to rewrite the first sum in (128) into the form

$$\sum |y_{1k}|^2 \eta(x_{11}) + x_{11} \sum \eta(|y_{1k}|^2)$$

and we get finally

$$S_{D'}(V\omega V^\dagger) = S_D(\omega) + \sum_{j=1}^{m} \langle j|\omega|j\rangle \sum_{k=1}^{m_j} \eta(|y_{jk}|^2) \tag{129}$$

A convex roof remains a convex roof if we add a function linear in ω. Plugging (129) into (25) directly provides:

Proposition 6.5:

If $\mathcal{H}$ is embedded unitarily in $\mathcal{H}'$ according to (125), then the entanglements of the diagonal channels are related by

$$E_{D'}(V\omega V^\dagger) = E_D(\omega) + l(\omega) \tag{130}$$

and the linear function is given by

$$l(\omega) = \sum_{j=1}^{m} \langle j|\omega|j\rangle \sum_{k=1}^{m_j} \eta(|y_{jk}|^2) \tag{131}$$

Optimal decompositions are mapped onto optimal decomposition and convex leaves onto convex leaves.

A particular simple example is the embedding

$$V|0\rangle = |1\rangle, \quad V|1\rangle = \frac{1}{\sqrt{2}}(|2\rangle + |3\rangle) \tag{132}$$

of $\mathcal{H}_2$ into $\mathcal{H}_3$. Pairs of pure state vectors, yielding flat optimal decompositions for the entanglement of D_2, are

$$a_0|0\rangle + a_1|1\rangle, \quad a_1^*|0\rangle + a_0^*|1\rangle \tag{133}$$

A particular case is $a_0 = \sqrt{1/3}$, $a_1 = \sqrt{2/3}$. Applying the map (132) results in the optimal pair

$$\sqrt{\frac{1}{3}}(|1\rangle + |2\rangle + |3\rangle), \quad \sqrt{\frac{2}{3}}|1\rangle + \sqrt{\frac{1}{6}}(|2\rangle + |3\rangle) \tag{134}$$

Call π_0 and π_1 the pure states determined by the vectors (134). Then

$$\mathrm{diag}(\pi_0) = \{\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\}, \quad \mathrm{diag}(\pi_1) = \{\frac{2}{3}, \frac{1}{6}, \frac{1}{6}\} \tag{135}$$

and the fidelity parameters (120) are 1 and $F^{**} = 8/9$. Returning to the remarks after proposition 6.4, we see a reason why this value should be a bifurcation point for the behavior of maximal symmetric states and their convex leaves.

6.3. A Further Embedding

There are strong relations between the entanglement of the diagonal channels and the entanglement of formation, governed by embedding procedures. A nice and quite simple one is

$$V|j\rangle = |jj\rangle = |j\rangle \otimes |j\rangle \tag{136}$$

V is a unitary map of $\mathcal{H}$ onto the subspace $\mathcal{H}'$ of $\mathcal{H}^a \otimes \mathcal{H}^b$ with basis $\{|jj\rangle\}$. The embedding is of interest because of

$$D(X) := \mathrm{diag}(X) = \mathrm{Tr}_b(VXV^\dagger), \quad X \in \mathcal{B}(\mathcal{H}) \tag{137}$$

The relation implies

$$E((V\omega V^\dagger)) = E_D(\omega), \quad \omega \in \Omega(\mathcal{H}) \tag{138}$$

and relates the entanglement E_D of a diagonal map to the entanglement of formation E for bipartite states supported by $\mathcal{H}'$. This is true for all dimensions $d = \dim \mathcal{H}$. The vector (117) becomes a completely entangled one, say $|e\rangle$, if transformed by (136).

The crucial point is now that invariance group Γ_e of $|e\rangle = V|\psi\rangle$ is much larger than $V\Gamma V^\dagger$, the invariance group of $|\psi\rangle$. Γ_e contains the local unitary operators $U \otimes \bar{U}$ and the swap operation. The involution $V\Theta\rangle^\dagger = \Theta \otimes \Theta$ is defined originally only on $\mathcal{H}'$. The canonical extension to an involution Θ_e of all $\mathcal{H}^a \otimes \mathcal{H}^b$ can be gained by

$$\Theta_e|jk\rangle = |kj\rangle \tag{139}$$

and the requirement of anti-linearity. Θ_e satisfies

$$\Theta_e(X \otimes \mathbf{1})|e\rangle = (X^\dagger \otimes \mathbf{1})|e\rangle \tag{140}$$

for all $X \in \mathcal{B}(\mathcal{H}^a)$ [57].

Now one tries to enlarge convex leaves in $\mathcal{H}'$ by transforming them with operators from a suitable larger group $\Gamma' \subset \Gamma_e$. The involution Θ_e is a symmetry of the entanglement of formation. If a bipartite state ρ commutes with Θ_e, all elements of the convex leaf of ρ must commute with Θ_e.

One can understand quite well why E_D for maximal symmetric states are so similar to the entanglement of formation for isotropic states. A detailed discussion is not in the frame of the present paper. However, an essential point in the considerations above is in the relation between the entanglement of diagonal channels and the entanglement of formation. This may be of use in future research: It seems easier to imagine the structure of the diagonal channel as that of the partial trace. Nevertheless, the degree of difficulty is about the same.

7. Summary and Outlook

Given values $g(\pi)$ for pure states π, the direct way of solving the convex roof problem is the search for optimal decompositions. The most prominent and successful examples are the concurrence and the entanglement of formation for 2-qubit bipartite quantum systems. The method goes back to Wootters and is described in section 4. With it one gets analytical expressions and flat optimal decompositions. The flatness of the convex (and concave) roofs inherited from Wootters' method is rendering its use in higher dimensions.

A quite different way is to look for a maximal convex extension G of g: If for any other extension G' of g we find $G'(\omega) > G(\omega)$ for a state $\omega \in \Omega$, then G' cannot be convex.

A further, and more efficient reformulation of the convex roof problem asks for roof points, (see definition 2.1a), of a convex extension G of g. At a roof point ω of a convex extension G one gets $G(\omega) = g^{\cup}(\omega)$ and the problem is solved for the particular state ω. Similarly, if G would be a concave extension of g, then $G(\omega) = g^{\cap}(\omega)$ for a roof point of G.

This way of proving is used in the chapter on the "subtraction procedure". One of its merits is the control on the concurrence and on the 1-tangle of any rank two density operator of a $2 \times m$ bipartite quantum system. The same is with the slightly more general class of stochastic, (just positive and trace preserving), 1-qubit channels.

Therefore, there is some hope to get the concurrence (and the 1-tangle) for all states of any $2 \times m$ bipartite quantum system explicitly.

But even if this becomes true, it does not provide us with the entanglement of formation of a 2×3 system: The concurrence ceases to be flat. However, by proposition 4.1 one can obtain reasonable lower bounds.

Wootters' and the subtraction method seem to be quite different in spirit. Uniting the strength of both, would be very useful. Also one should look at the subtraction method in more general terms. One can get at least lower bounds on the concurrence for higher dimensional system as shown by two examples in [52]. A more systematic study of the issue seems prospective.

The use of symmetries is well know and efficient in general. In convex roof construction the symmetries of g as of a function on the pure states is what counts. If a state ω is invariant with respect to a symmetry group Γ, its convex leaf, (see definitions 3.2), is the convex hull of a set of Γ-orbits consisting of pure states. The shapes of the leaves can be quite different. However, one would suppose a smooth

change of the leaves with the exception of some bifurcation points (or lines ...) at which the dimension of the leaves is changing. Some help comes from embedding a lower dimensional problem into a higher dimensional one. This is shown for the entanglement of the diagonal channel: E_T can be computed in any dimension on 2-dimensional subspaces which contain at least one pure diagonal state. On these subspaces E_T is the sum of a flat convex roof and a linear function. The study of more examples is certainly desirable.

At this point we can return to the concurrence of the stochastic 1-qubit maps. For them C_T is the restriction of a Hilbertian semi-norm to the state space. The proof of proposition 5.1 shows a one to one correspondence between the structure of the foliation and the null-space of the semi-norm. Two stochastic 1-qubit maps come with the same pattern of their convex leaves if the null-spaces of their semi-norms are identical. Indeed, it is the first class of channels and roofs with a complete classification of their convex leaves and their foliation.

Acknowledgements

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