MAPS ON DENSITY OPERATORS PRESERVING QUANTUM f-DIVERGENCES

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Abstract. For an arbitrary strictly convex function f defined on the non-negative real line we determine the structure of all transformations on the set of density operators which preserve the quantum f-divergence.

1. Introduction and statement of the result

Relative entropy is one of the most important numerical quantities appearing in quantum information theory. It is used as a measure of distinguishability between quantum states, or their mathematical representatives, the density operators. In fact, there are several concepts of relative entropy, among which the most common one is due to Umegaki. In [7] Molnár described the general form of all bijective transformations on the set of density operators which preserve that kind of relative entropy. The motivation to explore the structure of those transformations came from the fundamental theorem of Wigner concerning quantum mechanical symmetry transformations which are bijective maps on pure states (rank-one projections on a Hilbert space) preserving the quantity of transition probability. Roughly speaking, Wigner's theorem states that any such transformation is implemented by either a unitary or an antiunitary operator on the underlying Hilbert space. In [7] the author showed that the same conclusion holds for those bijective transformations on the set of density operators which preserve the relative entropy. Later, in [8] Molnár and Szokol have significantly extended this result by removing the bijectivity condition. We remark that recently there has been considerable interest in investigations relating to "preserver" transformations on different kinds of mathematical structures. Those are maps which preserve a given numerical quantity, or a given relation, or a given operation, etc. relevant for the underlying structure. In physics such transformations are usually viewed as sorts of symmetries. For one of the nicest recent results in that area of research we refer to the paper [14] by Šemrl.

The authors were supported by the "Lendület" Program (LP2012-46/2012) of the Hungarian Academy of Sciences. The first and second author were supported by the Hungarian Scientific Research Fund (OTKA) Reg.No. K81166 NK81402. The second and third author were supported by the TÁMOP-4.2.2/B-10/1-2010-0024 project co-financed by the European Union and the European Social Fund.

The aim of this paper is to give a far-reaching generalization of the results in [7, 8]. Namely, here we describe all transformations on the set of density operators which preserve the quantum f-divergence with respect to an arbitrary strictly convex function f defined on the non-negative real line.

Classical f-divergences between probability distributions were introduced by Csiszár [2], and by Ali and Silvey [1] independently. They are widely used in information theory and statistics as distinguishability measures among probability distributions (see, e.g., [5]). Their quantum theoretical analogues, quantum f-divergences which play a similar role in quantum information theory and quantum statistics (see, e.g., [13]) were defined by Petz [10], [11]. This concept is an essential common generalization and extension of several notions of quantum relative entropy including Umegaki's and Tsallis' relative entropies. Sometimes quantum f-divergences are also called quasi-entropies [12].

We define that concept following the approach given in [4]. We begin with some necessary notation. Let H be a finite dimensional complex Hilbert space. We denote by $B(H)$ the algebra of all linear operators on H and by $B(H)^+$ the cone of all positive semi-definite operators on H. Next, $S(H)$ stands for the set of all density operators which are the elements of $B(H)^+$ having unit trace. We recall that $B(H)$ is a complex Hilbert space with the Hilbert-Schmidt inner product $\langle ., . \rangle_{\mathrm{HS}} \colon B(H) \times B(H) \to \mathbb{C}$ defined by

$$\langle A, B \rangle_{\mathrm{HS}} = \operatorname{Tr} AB^* \quad (A, B \in B(H)),$$ [1]

where Tr denotes the usual trace functional on $B(H)$. For any $A \in B(H)$, let $L_A, R_A \colon B(H) \to B(H)$ be the left and the right multiplication operators defined as

$$L_A T = AT, \; R_A T = TA \quad (T \in B(H)).$$

We remark that $L_A R_B = R_B L_A$ holds for every $A, B \in B(H)$. If $A, B \in B(H)^+$, then L_A and R_B are positive Hilbert space operators, hence so is $L_A R_B$.

Let now $f \colon [0, \infty[\to \mathbb{R}$ be a function which is continuous on $]0, \infty[$ and the limit

$$\alpha := \lim_{x \to \infty} \frac{f(x)}{x}$$

exists in $[-\infty, \infty]$. Following [4, 2.1 Definition], for $A, B \in B(H)^+$ with $\operatorname{supp} A \subset \operatorname{supp} B$ (supp denoting the orthogonal complement of the kernel of an operator) the f-divergence $S_f(A \| B)$ of A with respect to B is defined by

$$S_f(A \| B) = \left\langle \sqrt{B}, f(L_A R_{B^{-1}}) \sqrt{B} \right\rangle_{\mathrm{HS}}.$$

[1] We mention that, as one of the referees pointed out, opposed to the conventions in mathematics, in physics the inner product is usually assumed to be conjugate-linear in its first variable and linear in the second. Accordingly, $\langle A, B \rangle_{\mathrm{HS}}$ would be defined as $\operatorname{Tr} A^* B$. However, in this paper we follow the common mathematical convention which is going to cause no confusion.

In the general case we set

$$S_f(A\|B) = \lim_{\varepsilon\to 0^+} S_f(A\|B+\varepsilon I),$$

where I is the identity operator on H. By [4, 2.2 Proposition] the limit above exists in $[-\infty,\infty]$. We next recall a useful formula which will play an important role in our arguments. Let $A, B \in B(H)^+$ and for any $\lambda \in \mathbb{R}$ denote by P_λ, respectively by Q_λ the projection on H projecting onto the kernel of $A-\lambda I$, respectively onto the kernel of $B-\lambda I$. According to [4, 2.3 Corollary] we have

$$(1) \qquad S_f(A||B) = \sum_{a\in\sigma(A)} \left(\sum_{b\in\sigma(B)\setminus\{0\}} bf\left(\frac{a}{b}\right) \operatorname{Tr} P_a Q_b + \alpha a \operatorname{Tr} P_a Q_0 \right),$$

where $\sigma(.)$ stands for the spectrum of elements in $B(H)$ and the convention $0\cdot(-\infty) = 0\cdot\infty = 0$ is used.

A few important examples of quantum f-divergences between density operators follow. Let $A, B \in S(H)$.

(i) If

$$f(x) = \begin{cases} x\log x, & x>0 \\ 0, & x=0, \end{cases}$$

then

$$S_f(A\|B) = \begin{cases} \operatorname{Tr} A(\log A - \log B), & \operatorname{supp} A \subset \operatorname{supp} B \\ \infty, & \text{otherwise} \end{cases}$$

which is just the usual Umegaki relative entropy of A with respect to B.

(ii) Let $q \in]0,1[$ and define the function $f_q\colon [0,\infty[\to \mathbb{R}$ by $f_q(x) = (1-x^q)/(1-q)$ $(x\geq 0)$. Then

$$S_{f_q}(A\|B) = \frac{1-\operatorname{Tr} A^q B^{1-q}}{1-q}$$

which is the quantum Tsallis relative entropy (see, e.g., [3]) of A with respect to B.

(iii) If $f(x) = (\sqrt{x}-1)^2$ $(x\geq 0)$, then $S_f(A\|B) = \left\|\sqrt{A}-\sqrt{B}\right\|_{\mathrm{HS}}^2$, where $\|.\|_{\mathrm{HS}}$ stands for the Hilbert-Schmidt norm.

We can now formulate the main result of the paper which describes the structure of all transformations on $S(H)$ leaving a given quantum f-divergence invariant. First observe that for any unitary or antiunitary operator U on H the transformation $A \mapsto UAU^*$ preserves the f-divergence on $S(H)$, i.e., we have $S_f(UAU^*\|UBU^*) = S_f(A\|B)$ for any $A, B \in S(H)$ (here the function f is as above). The theorem below states that for a strictly convex function f the reverse statement is also true: All transformations on $S(H)$ which leave the f-divergence invariant are of the preceding form, i.e., they are all implemented by unitary or antiunitary operators. Apparently, this is a Wigner-type result concerning transformations of the space $S(H)$ of density operators. Let us point out the fact that any convex function $f : [0, \infty[\to \mathbb{R}$ satisfies the requirements given in the definition of f-divergence: it is continuous on the open interval $]0, \infty[$ and since the difference quotient $(f(x) - f(0))/(x - 0)$ is increasing, the limit $\lim_{x\to\infty} f(x)/x$ exists and is finite or equal to ∞. The precise formulation of our result is as follows.

Theorem. *Assume that* $f : [0, \infty[\to \mathbb{R}$ *is a strictly convex function and* $\phi\colon S(H) \to S(H)$ *is a transformation satisfying*

$$S_f(\phi(A)||\phi(B)) = S_f(A||B) \quad (A, B \in S(H)).$$

Then there is either a unitary or an antiunitary operator U *on* H *such that* ϕ *is of the form*

$$\phi(A) = UAU^* \qquad (A \in S(H)).$$

We emphasize that the bijectivity or the surjectivity of the transformation ϕ is not assumed in the theorem and we do not require any sort of linearity either. Let us make a remark also on the convexity assumption above. When they consider f-divergence in the classical setting, it is practically always assumed that the function f is convex. The main reason is that this condition guarantees the joint convexity and information monotonicity of the f-divergence which are significant properties. As for quantum f-divergence, to obtain similar important properties one needs to assume that f is operator convex (see, e.g., [4]). Therefore, our condition that f is a convex function is very natural and not restrictive. As for strict convexity, it is easy to see that if f is affine then $S_f(.\|.)$ is constant. Hence in that case every selfmap of $S(H)$ preserves the f-divergence which is obviously out of interest. Observe that the functions appearing in (i)-(iii) are all strictly convex.

2. Proof

In this section we present the proof of our result. First we recall the notion of orthogonality of operators. The self-adjoint operators $A, B \in B(H)$ are said to be orthogonal if and only if $AB = 0$, which is equivalent to the fact that A and B have mutually orthogonal ranges. In what follows let $n = \dim H$ and denote by $P_1(H)$ the set of all rank-one projections on H.

Proof. Observe that for any real number a and operators $A, B \in S(H)$ we have $S_{f+a}(A\|B) = S_f(A\|B) + a$. Therefore without any loss of generality we may and do assume that $f(0) = 0$. According to the value of α, we divide the proof into two cases.

CASE I. We assume that α is finite. First we show that ϕ preserves the orthogonality in both directions, i.e. it satisfies

$$\phi(A)\phi(B) = 0 \iff AB = 0$$

for any $A, B \in S(H)$. To see this we need the following characterization of orthogonality. For any $A, B \in S(H)$ we have

$$AB = 0 \iff S_f(A||B) = \alpha. \tag{2}$$

Indeed, if $AB = 0$, then a straightforward calculation using the formula (1) shows that $S_f(A||B) = \alpha$. Suppose now that the right-hand side of (2) holds. On the one hand, we have

$$S_f(A||B) = \sum_{a\in\sigma(A)\setminus\{0\}} \sum_{b\in\sigma(B)\setminus\{0\}} bf\left(\frac{a}{b}\right) \operatorname{Tr} P_a Q_b + \sum_{a\in\sigma(A)\setminus\{0\}} \alpha a \operatorname{Tr} P_a Q_0.$$

On the other hand, we have

$$\alpha = \alpha \operatorname{Tr} A = \alpha \sum_{a\in\sigma(A)\setminus\{0\}} a \operatorname{Tr} P_a.$$

Since the left-hand sides of the previous two equalities are equal, using the fact that

$$\sum_{b\in\sigma(B)} Q_b = I$$

we easily infer that

$$\sum_{a\in\sigma(A)\setminus\{0\}} \sum_{b\in\sigma(B)\setminus\{0\}} bf\left(\frac{a}{b}\right) \operatorname{Tr} P_a Q_b = \alpha \sum_{a\in\sigma(A)\setminus\{0\}} \sum_{b\in\sigma(B)\setminus\{0\}} a \operatorname{Tr} P_a Q_b.$$

This yields that

$$\sum_{a\in\sigma(A)\setminus\{0\}} \sum_{b\in\sigma(B)\setminus\{0\}} \left(\alpha a - bf\left(\frac{a}{b}\right)\right) \operatorname{Tr} P_a Q_b = 0. \tag{3}$$

Let $a \in \sigma(A)\setminus\{0\}$ and $b \in \sigma(B)\setminus\{0\}$ and consider the quantity

$$\alpha a - bf\left(\frac{a}{b}\right) = b\left(\alpha\frac{a}{b} - f\left(\frac{a}{b}\right)\right). \tag{4}$$

It follows from the strict convexity of f that the function $f_1\colon]0,\infty[\to \mathbb{R}$ defined by

$$f_1(x) = \frac{f(x) - f(0)}{x - 0} = \frac{f(x)}{x} \quad (x > 0) \tag{5}$$

is strictly increasing. Therefore, for any $x > 0$ we have

$$f(x)/x < \lim_{s\to\infty} f_1(s) = \alpha \tag{6}$$

and hence

$$f(x) < \alpha x \tag{7}$$

which implies that the quantity in (4) is positive. On the other hand, since $P_a, Q_b \in B(H)^+$ we have $\operatorname{Tr} P_a Q_b \geq 0$. It follows that the terms of the sum on the left-hand side of (3) are nonnegative. We conclude that $\operatorname{Tr} P_a Q_b = 0$ holds for all $a \in \sigma(A)\setminus\{0\}$ and $b \in \sigma(B)\setminus\{0\}$ which implies that $AB = 0$. This completes the proof of the equivalence in (2). Since ϕ preserves the f-divergence, it then follows that ϕ preserves the orthogonality in both directions.

Apparently, we can characterize the elements of $P_1(H)$ as those operators in $S(H)$ which belong to a set of n pairwise orthogonal density operators on H. By the orthogonality preserving property of ϕ, we infer that it maps $P_1(H)$ into itself. We claim that ϕ preserves the transition probability (the trace of products) on $P_1(H)$. To prove this, let $P, Q \in P_1(H)$ be arbitrary. A straightforward calculation gives that

$$S_f(P||Q) = (f(1) - \alpha) \operatorname{Tr} PQ + \alpha$$

and similarly

$$S_f(\phi(P)||\phi(Q)) = (f(1) - \alpha) \operatorname{Tr} \phi(P)\phi(Q) + \alpha.$$

By (7) one has $f(1) - \alpha \neq 0$ and it follows that

$$\operatorname{Tr} \phi(P)\phi(Q) = \operatorname{Tr} PQ.$$

This means that the restriction of ϕ to $P_1(H)$ preserves the transition probability. The non-surjective version of Wigner's theorem (see, e.g., [6, Theorem 2.1.4]) describes the structure of all such maps. Since H is finite dimensional, we obtain that there exists either a unitary or an antiunitary operator U on H such that

$$\phi(P) = UPU^* \quad (P \in P_1(H)).$$

Consider the transformation $\psi \colon S(H) \to S(H)$ defined by $\psi(A) = U^*\phi(A)U$ $(A \in S(H))$. It is clear that this map preserves the quantum f-divergence and has the additional property that it acts as the identity on $P_1(H)$. Define the function $f_2 \colon [0, \infty[\to \mathbb{R}$ by

$$f_2(x) = \begin{cases} xf\left(\frac{1}{x}\right), & x > 0 \\ \alpha, & x = 0. \end{cases}$$

Let $A \in S(H)$ be fixed and $Q \in P_1(H)$ be arbitrary. Using (1), we easily have

$$S_f(Q||A) = \operatorname{Tr} Q f_2(A)$$

and similarly

$$S_f(Q||\psi(A)) = \operatorname{Tr} Q f_2(\psi(A)).$$

By the properties of ψ, the left-hand sides of the above equalities coincide, therefore

$$\operatorname{Tr} f_2(\psi(A))Q = \operatorname{Tr} f_2(A)Q$$

holds for every rank-one projection Q on H. It easily follows that $f_2(\psi(A)) = f_2(A)$. Observe that $f_2(x) = f_1(1/x)$ $(x > 0)$. Since f_1 is clearly injective, so is f_2 on $]0, \infty[$. Moreover, by (6) we have $f_1(x) < \alpha$ $(x > 0)$ and then we obtain that f_2 is injective on the whole interval $[0, \infty[$. It then follows that

$$A = \psi(A) = U^*\phi(A)U \quad (A \in S(H))$$

and this completes the proof in CASE I.

CASE II. We now assume that α is infinite. The basic strategy of the argument below is close to that of the proof of [8, Theorem]. However, due to the fact that here we consider general divergences, we necessarily face many problems which are of different levels of difficulties. Although at some parts in our argument we may directly refer to parts of the proof of [8, Theorem], for the sake of understandability, readability and completeness we present practically all necessary details.

As mentioned before the formulation of Theorem, the possibility $\alpha = -\infty$ is ruled out by the convexity of the function f. Therefore, $\alpha = \infty$. We show that ϕ preserves the rank, i.e. for any $A \in S(H)$ the rank of $\phi(A)$ equals the rank of A. In order to see it, let $A, B \in S(H)$ be arbitrary. Using (1) it is easy to check that $S_f(A\|B) < \infty$ holds if and only if $\operatorname{supp} A \subset \operatorname{supp} B$. It follows that

$$\operatorname{supp} \phi(A) \subset \operatorname{supp} \phi(B) \iff \operatorname{supp} A \subset \operatorname{supp} B$$

and next that

$$\operatorname{supp} \phi(A) \subsetneq \operatorname{supp} \phi(B) \iff \operatorname{supp} A \subsetneq \operatorname{supp} B. \tag{8}$$

Observe that the rank of A is k if and only if there is a strictly increasing chain (with respect to inclusion) of supports of n density operators on H such that its kth element is $\operatorname{supp} A$. Using this characterization and (8) we see that ϕ leaves the rank of operators invariant. In particular

$$\phi(P_1(H)) \subset P_1(H). \tag{9}$$

We next verify that ϕ is injective. Indeed, it is an immediate consequence of the following assertion. For any $A, B \in S(H)$ we have $f(1) \leq S_f(A\|B)$ and equality appears if and only if $A = B$. For the proof, it is clear that if the support of A is not contained in that of B, then this inequality holds and it is strict. Otherwise we have

$$S_f(A\|B) = \sum_{a \in \sigma(A)} \sum_{b \in \sigma(B) \setminus \{0\}} (b \operatorname{Tr} P_a Q_b) f\left(\frac{a}{b}\right).$$

Observe that the numbers $b \operatorname{Tr} P_a Q_b$ ($a \in \sigma(A)$, $b \in \sigma(B) \setminus \{0\}$) are non-negative and their sum is 1. Thus, by the convexity of f it follows easily that

$$f(1) = f\left(\sum_{a \in \sigma(A)} \sum_{b \in \sigma(B) \setminus \{0\}} b\frac{a}{b} \operatorname{Tr} P_a Q_b\right) \leq S_f(A\|B) \tag{10}$$

and this yields the desired inequality. Moreover, since f is strictly convex, in the above inequality we have equality exactly when for any $a \in \sigma(A)$ and $b \in \sigma(B) \setminus \{0\}$ satisfying $b \operatorname{Tr} P_a Q_b > 0$, the value a/b is constant. Since the sum of the numbers $b(a/b) \operatorname{Tr} P_a Q_b$ over such values of a and b equals 1, we get that this constant is 1. By the previous observations we easily obtain that for any $a \in \sigma(A)$ and $b \in \sigma(B) \setminus \{0\}$ at least one of the relations $a = b$, $P_a Q_b = 0$ must hold. One can simply check that under the condition

$\operatorname{supp} A \subset \operatorname{supp} B$ which we have supposed above, the latter property is equivalent to the equality $A = B$. We conclude that ϕ is injective.

We derive a formula which will be used several times in the rest of the proof. Define the function $f_3 \colon]0, \infty[\to \mathbb{R}$ by

$$f_3(x) = x f\left(\frac{1}{x}\right) = f_1\left(\frac{1}{x}\right) \quad (x > 0),$$

where f_1 is the function that has appeared in (5). Easy computation shows that for any $A \in S(H)$ and $P \in P_1(H)$ with $\operatorname{supp} P \subset \operatorname{supp} A$ we have

$$S_f(P||A) = \operatorname{Tr} P|_{\operatorname{supp} A} f_3(A|_{\operatorname{supp} A}). \tag{11}$$

In the next part of our argument H is assumed to be 2-dimensional. We claim that for any $A \in S(H)$ we have

$$[\min \sigma(A), \max \sigma(A)] \subset [\min \sigma(\phi(A)), \max \sigma(\phi(A))]$$

meaning that ϕ can only enlarge the convex hull of the spectrum of the elements of $S(H)$. To verify this property, first observe that by (9) the inclusion above holds for all $A \in P_1(H)$. Now pick a rank-two operator $A \in S(H)$ and set $\lambda = \max \sigma(A) \in [1/2, 1[$. Then there are mutually orthogonal projections $P, Q \in P_1(H)$ such that $A = \lambda P + (1-\lambda) Q$. Applying (11) we easily get that for any $R \in P_1(H)$

$$S_f(R||A) = f_3(\lambda) \operatorname{Tr} RP + f_3(1-\lambda) \operatorname{Tr} RQ. \tag{12}$$

We have seen that f_1 is strictly increasing, so f_3 is strictly decreasing and thus $f_3(\lambda) \leq f_3(1-\lambda)$. It follows that as R runs through the set $P_1(H)$, the quantity $S_f(R||A)$ runs through $[f_3(\lambda), f_3(1-\lambda)]$. Similarly, we infer that for any $R \in P_1(H)$ the number $S_f(\phi(R)\|\phi(A))$ belongs to $[f_3(\mu), f_3(1-\mu)]$, where $\mu = \max \sigma(\phi(A))$. Since ϕ preserves f-divergence, we obtain that

$$f_3(\mu) \leq f_3(\lambda) \leq f_3(1-\lambda) \leq f_3(1-\mu).$$

Due to the fact that f_3 is strictly decreasing this implies

$$\min \sigma(\phi(A)) \leq \min \sigma(A) \leq \max \sigma(A) \leq \max \sigma(\phi(A))$$

which verifies our claim.

In the most crucial part of the proof that follows we show that $\phi\left(\frac{1}{2}I\right) = \frac{1}{2}I$. Assume on the contrary that there is a number $\lambda_1 \in]1/2, 1[$ and mutually orthogonal projections $P_1, Q_1 \in P_1(H)$ such that

$$\phi\left(\frac{1}{2}I\right) = \lambda_1 P_1 + (1-\lambda_1) Q_1. \tag{13}$$

By (12) for any $R \in P_1(H)$ one has $S_f\left(R \middle\| \frac{1}{2}I\right) = f_3\left(\frac{1}{2}\right)$ and then we deduce that

$$\begin{aligned} f_3\left(\frac{1}{2}\right) = S_f\left(\phi(R) \middle\| \phi\left(\frac{1}{2}I\right)\right) &= f_3(\lambda_1) \operatorname{Tr} \phi(R) P_1 \\ &\quad + f_3(1-\lambda_1) \operatorname{Tr} \phi(R) Q_1. \end{aligned} \tag{14}$$

Because $1 = \operatorname{Tr}\phi(R) = \operatorname{Tr}\phi(R)P_1 + \operatorname{Tr}\phi(R)Q_1$, this gives us that $f_3\left(\frac{1}{2}\right)$ is a convex combination of $f_3(\lambda_1)$ and $f_3(1-\lambda_1)$. Since these two latter numbers are different (f_3 is strictly decreasing), we infer that $\operatorname{Tr}\phi(R)P_1$ has the same value for any $R \in P_1(H)$ and the same holds for $\operatorname{Tr}\phi(R)Q_1$, too. We next prove that

$$\operatorname{Tr}\phi(R)P_1 > \operatorname{Tr}\phi(R)Q_1. \tag{15}$$

To this end, we first show that f_3 is strictly convex. According to [9, Lemma 1.3.2], a real-valued function g defined on an interval J is strictly convex if and only if for any elements $x_1 < x_2 < x_3$ in J we have

$$\det\begin{pmatrix} 1 & x_1 & g(x_1) \\ 1 & x_2 & g(x_2) \\ 1 & x_3 & g(x_3) \end{pmatrix} > 0.$$

It is easy to check that for any positive reals $x_1 < x_2 < x_3$ we have

$$\frac{1}{x_1x_2x_3}\det\begin{pmatrix} 1 & x_1 & f_3(x_1) \\ 1 & x_2 & f_3(x_2) \\ 1 & x_3 & f_3(x_3) \end{pmatrix} = \det\begin{pmatrix} 1 & 1/x_3 & f(1/x_3) \\ 1 & 1/x_2 & f(1/x_2) \\ 1 & 1/x_1 & f(1/x_1) \end{pmatrix}$$

and the latter number is positive due to the strict convexity of f. This proves that f_3 is also strictly convex. Using that property and the fact that f_3 is strictly decreasing, referring to (14) one can verify in turn that $\operatorname{Tr}\phi(R)P_1 \neq \frac{1}{2}$ and then that $\operatorname{Tr}\phi(R)P_1 > \frac{1}{2}$. Therefore, we obtain $\operatorname{Tr}\phi(R)P_1 > \operatorname{Tr}\phi(R)Q_1$. In fact, in any representation of $f_3\left(\frac{1}{2}\right)$ as a convex combination of $f_3(t)$ and $f_3(1-t)$ ($t \in]1/2, 1[$), the coefficient of the former term is greater than the coefficient of the latter one.

Now choose unit vectors u and v from the ranges of P_1 and Q_1. It is easy to check that the matrix of an element of $P_1(H)$ with respect to the basis $\{u, v\}$ is of the form

$$\begin{pmatrix} a & \varepsilon\sqrt{a(1-a)} \\ \bar{\varepsilon}\sqrt{a(1-a)} & 1-a \end{pmatrix},$$

where $a \in [0,1]$ and $\varepsilon \in \mathbb{C}$ with $|\varepsilon| = 1$. It follows from what we have observed above that when R runs through the set $P_1(H)$, the number $a = \operatorname{Tr}\phi(R)P_1$ in the matrix representation of $\phi(R)$ remains constant, and since f_3 is clearly injective, a is different from the numbers $0, 1$. Now we can rewrite (14) in the form

$$af_3(\lambda_1) + (1-a)f_3(1-\lambda_1) = f_3\left(\frac{1}{2}\right). \tag{16}$$

Next let us consider $\phi\left(\phi\left(\frac{1}{2}I\right)\right)$. We have

$$\phi\left(\phi\left(\frac{1}{2}I\right)\right) = \lambda_2 P_2 + (1-\lambda_2)Q_2,$$

for some $\frac{1}{2} \leq \lambda_2 < 1$ and mutually orthogonal elements P_2, Q_2 of $P_1(H)$. In fact, as ϕ can only enlarge the convex hull of the spectrum and $\lambda_1 > \frac{1}{2}$, it follows that $\lambda_2 > \frac{1}{2}$. Pick an arbitrary rank-one projection R on H and set $R_2 = \phi(\phi(R))$. Since ϕ preserves $S_f(.\|.)$, by (14) we have

(17)
$$f_3\left(\frac{1}{2}\right) = S_f\left(\phi(\phi(R))\middle\|\phi\left(\phi\left(\frac{1}{2}I\right)\right)\right)$$
$$= S_f(R_2\|\lambda_2 P_2 + (1-\lambda_2)Q_2) = f_3(\lambda_2)\operatorname{Tr} R_2P_2 + f_3(1-\lambda_2)\operatorname{Tr} R_2Q_2.$$

Here $\lambda_2 > \frac{1}{2}$ is fixed. Since we have $\operatorname{Tr} R_2P_2 + \operatorname{Tr} R_2Q_2 = 1$, it follows just as above that the numbers $\operatorname{Tr} R_2P_2$ and $\operatorname{Tr} R_2Q_2$ are also fixed, they do not change when R varies. Moreover, we necessarily have

$$\operatorname{Tr} R_2P_2 > \operatorname{Tr} R_2Q_2. \tag{18}$$

Consider a unit vector from the range of P_2. Let x, y be its coordinates with respect to the basis $\{u, v\}$ appearing in the previous paragraph. It is easy to see that the representing matrix of P_2 is

$$\begin{pmatrix} x \\ y \end{pmatrix}\begin{pmatrix} \overline{x} \\ \overline{y} \end{pmatrix}^t,$$

where ^{t} denotes the transposition. Moreover, since R_2 is a rank-one projection which is the image (under ϕ) of a rank-one projection, its matrix representation is of the form

$$\begin{pmatrix} a & \varepsilon\sqrt{a(1-a)} \\ \overline{\varepsilon}\sqrt{a(1-a)} & 1-a \end{pmatrix},$$

where a is the same as in (16), and $\varepsilon \in \mathbb{C}$ with $|\varepsilon| = 1$ may vary. We have

$$\operatorname{Tr} R_2P_2 = \operatorname{Tr}\left[\begin{pmatrix} a & \sqrt{a(1-a)}\varepsilon \\ \sqrt{a(1-a)}\overline{\varepsilon} & 1-a \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix}\begin{pmatrix} \overline{x} \\ \overline{y} \end{pmatrix}^t\right].$$

Elementary computations show that the latter quantity equals

$$ax\overline{x} + \sqrt{a(1-a)}\varepsilon\overline{x}y + \sqrt{a(1-a)}\overline{\varepsilon}x\overline{y} + (1-a)y\overline{y} =$$
$$a|x|^2 + (1-a)|y|^2 + 2\sqrt{a(1-a)}\Re(\varepsilon\overline{x}y).$$

As we have already noted, the value of $\operatorname{Tr} R_2P_2$ does not change when R varies and a is also constant. Therefore, we obtain that the value of

$$a|x|^2 + (1-a)|y|^2 + 2\sqrt{a(1-a)}\Re(\varepsilon\overline{x}y)$$

is constant for infinitely many values of ε (by the injectivity of ϕ we see that R_2 runs through a set of continuum cardinality, so there is such a large set for the values of ε, too). It follows that $\Re(\varepsilon\overline{x}y)$ is constant for infinitely many values of ε which clearly implies that $\overline{x}y = 0$. Therefore, the column vector

$$\begin{pmatrix} x \\ y \end{pmatrix}$$

is a scalar multiple of

$$\begin{pmatrix}1\\0\end{pmatrix} \text{ or } \begin{pmatrix}0\\1\end{pmatrix}.$$

Obviously, this can happen only when $P_2 = P_1$ or $P_2 = Q_1$. Using the fact that R_2 is the image of a rank-one projection under ϕ, it follows from (15) that

$$\operatorname{Tr} R_2 P_1 > \operatorname{Tr} R_2 Q_1. \tag{19}$$

Therefore the equality $P_2 = Q_1$ is excluded due to (18). Consequently, $P_2 = P_1$ and $Q_2 = Q_1$ and hence we obtain

$$\phi\left(\phi\left(\frac{1}{2}I\right)\right) = \lambda_2 P_1 + (1-\lambda_2)Q_1. \tag{20}$$

From (17) we have

$$f_3(\lambda_2) \operatorname{Tr} R_2 P_1 + f_3(1-\lambda_2) \operatorname{Tr} R_2 Q_1 = f_3\left(\frac{1}{2}\right).$$

On the other hand, referring to the preceding paragraph we see that $\operatorname{Tr} R_2 P_1 = a$ and $\operatorname{Tr} R_2 Q_1 = 1-a$, thus it follows that

$$a f_3(\lambda_2) + (1-a) f_3(1-\lambda_2) = f_3\left(\frac{1}{2}\right). \tag{21}$$

We assert that the equation

$$a f_3(\lambda) + (1-a) f_3(1-\lambda) = f_3\left(\frac{1}{2}\right) \tag{22}$$

has at most two solutions in $]0,1[$. Indeed, consider the function

$$\lambda \mapsto a f_3(\lambda) + (1-a) f_3(1-\lambda) \quad (\lambda \in]0,1[).$$

Since f_3 is strictly convex, the same holds for this function, too. Therefore it is obvious that it cannot take the same values at three different places. Hence (22) does not have three different solutions in $]0,1[$. But by (16) and (21) λ_1, λ_2 and clearly $\frac{1}{2}$ too are solutions. Since $\lambda_2 \geq \lambda_1 > \frac{1}{2}$, it then follows that $\lambda_2 = \lambda_1$ and referring to (13) and (20) we see that $\phi\left(\phi\left(\frac{1}{2}I\right)\right) = \phi\left(\frac{1}{2}I\right)$. Since ϕ is injective, this gives us that $\phi\left(\frac{1}{2}I\right) = \frac{1}{2}I$. Therefore, ϕ sends $\frac{1}{2}I$ to itself.

Now let $\frac{1}{2}I \neq A \in S(H)$ be a rank-two operator and denote by $\lambda \in]1/2,1[$ its maximal eigenvalue. We assert that $\sigma(\phi(A)) = \sigma(A)$. Let $f_4 \colon]0,1[\to \mathbb{R}$ be the function defined by

$$f_4(x) = \frac{f(2x) + f(2(1-x))}{2} \quad (x \in]0,1[).$$

Using the formula (1) we obtain $S_f\left(A \,\middle\|\, \frac{1}{2}I\right) = f_4(\lambda)$ and, similarly, $S_f\left(\phi(A) \,\middle\|\, \frac{1}{2}I\right) = f_4(\lambda')$, where $\lambda' = \max \sigma(\phi(A)) > \frac{1}{2}$. Since ϕ preserves the f-divergence and sends $\frac{1}{2}I$ to itself, it follows that $S_f\left(\phi(A) \,\middle\|\, \frac{1}{2}I\right) =$

$S_f\left(A \,\|\, \frac{1}{2}I\right)$, and hence that $f_4(\lambda) = f_4(\lambda')$. We have that f_4 is strictly convex and symmetric with respect to the middle point $\frac{1}{2}$ of its domain. By elementary properties of convex functions this implies that the restriction of f_4 to $]1/2, 1[$ is strictly increasing. We necessarily obtain that $\lambda = \lambda'$ and this yields that the spectrum of A coincides with that of $\phi(A)$. Therefore, ϕ is spectrum preserving.

Select mutually orthogonal projections $P, Q \in P_1(H)$ and pick a number $\lambda \in]1/2, 1[$. Consider the operator $B = \lambda P + (1-\lambda)Q$. By the spectrum preserving property of ϕ we can choose another pair $P', Q' \in P_1(H)$ of mutually orthogonal projections such that $\phi(B) = \lambda P' + (1-\lambda)Q'$. We have learnt before that when R runs through the set of all rank-one projections, the quantity $S_f(R||B)$ runs through the interval $[f_3(\lambda), f_3(1-\lambda)]$. Using the equation (12) we easily see that $S_f(R\|B) = f_3(\lambda)$ if and only if $\operatorname{Tr} RP = 1$ which holds exactly when $R = P$. Therefore, we obtain

$$\begin{aligned} R = P \iff S_f(R\|B) = f_3(\lambda) \iff S_f(\phi(R)\|\phi(B)) = f_3(\lambda) \\ \iff S_f(\phi(R)\|\lambda P' + (1-\lambda)Q') = f_3(\lambda) \iff \phi(R) = P'. \end{aligned}$$

This gives us that $\phi(P) = P'$ and then we also obtain $\phi(Q) = Q'$. Consequently, ϕ preserves the orthogonality between rank-one projections. Moreover, we have

$$\phi(B) = \phi(\lambda P + (1-\lambda)Q) = \lambda\phi(P) + (1-\lambda)\phi(Q). \tag{23}$$

Next, we show that ϕ preserves also the nonzero transition probability between rank-one projections. Let P and R be different rank-one projections which are not orthogonal to each other. Choose a rank-one projection Q which is orthogonal to P. Pick $\lambda \in]1/2, 1[$. On the one hand, we have

$$S_f(R\|\lambda P + (1-\lambda)Q) = f_3(\lambda) \operatorname{Tr} RP + f_3(1-\lambda) \cdot \operatorname{Tr} RQ$$

and on the other hand, by (23), we compute

$$\begin{aligned} S_f(R\|\lambda P + (1-\lambda)Q) &= S_f(\phi(R)\|\lambda\phi(P) + (1-\lambda)\phi(Q)) \\ &= f_3(\lambda) \operatorname{Tr} \phi(R)\phi(P) + f_3(1-\lambda) \operatorname{Tr} \phi(R)\phi(Q). \end{aligned}$$

Comparing the right-hand sides, we infer

$$\operatorname{Tr} RP = \operatorname{Tr} \phi(R)\phi(P).$$

Consequently, ϕ preserves the transition probability between rank-one projections.

Above we have supposed that H is two-dimensional. Assume now that H is an arbitrary finite dimensional Hilbert space and $\phi : S(H) \to S(H)$ is a transformation which preserves the f-divergence. We show that ϕ preserves the transition probability between rank-one projections in this case too. In fact, we can reduce the general case to the previous one. To see this, first let H_2 be a two-dimensional subspace of H and $A_0 \in S(H)$ be such that $\operatorname{supp} A_0 = H_2$. Set $H_2' = \operatorname{supp} \phi(A_0)$. Since ϕ preserves the rank, H_2' is also two-dimensional. By what we have learnt at the beginning of the proof in CASE II, ϕ maps any element of $S(H)$ whose support is included in H_2 to an element of $S(H)$ whose support is included in H_2'. In that way ϕ gives rise to a transformation $\phi_0 : S(H_2) \to S(H_2')$ which preserves the f-divergence. Consider a unitary operator $V : H_2' \to H_2$. The transformation $V\phi_0(.)V^*$ maps $S(H_2)$ into itself and preserves the f-divergence. We have already seen that such a transformation necessarily preserves the transition probability between rank-one projections which implies that the same holds for ϕ_0 as well. Since for any two rank-one projections P, Q there exists a rank-two element $A_0 \in S(H)$ such that $\operatorname{supp} P, \operatorname{supp} Q \subset \operatorname{supp} A_0$, it follows that we have

$$\operatorname{Tr} PQ = \operatorname{Tr} \phi(P)\phi(Q).$$

By the non-surjective version of Wigner's theorem we infer that there is either a unitary or an antiunitary operator U on H such that

$$\phi(P) = UPU^* \quad (P \in P_1(H)).$$

Define the map $\psi\colon S(H) \to S(H)$ by $\psi(A) = U^*\phi(A)U$ $(A \in S(H))$. It is clear that ψ preserves $S_f(.\|.)$ and it acts as the identity on $P_1(H)$. Let $A \in S(H)$. Since ψ leaves the quantum f-divergence invariant, it preserves the inclusion between the supports of elements of $S(H)$ (see the first part of the proof in CASE II). This implies that for every rank-one projection P on H we have

$$\operatorname{supp} P \subset \operatorname{supp} A \Longleftrightarrow \operatorname{supp} P \subset \operatorname{supp} \psi(A).$$

We easily obtain that $\operatorname{supp} A = \operatorname{supp} \psi(A)$. Let P be an arbitrary rank-one projection which satisfies $\operatorname{supp} P \subset \operatorname{supp} A = \operatorname{supp} \psi(A)$. Using (11) and the equality $S_f(P||\psi(A)) = S_f(P||A)$ we deduce that

$$\operatorname{Tr} P f_3(\psi(A)) = \operatorname{Tr} P f_3(A).$$

It follows that $f_3(\psi(A))$ equals $f_3(A)$ on $\operatorname{supp} A$. Using the injectivity of f_3 we can infer that $\psi(A) = A$ and next that $\phi(A) = UAU^*$. This completes the proof of the theorem. □

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