Different quantum f-divergences and the reversibility of quantum operations

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Abstract

The concept of classical f-divergences gives a unified framework to construct and study measures of dissimilarity of probability distributions; special cases include the relative entropy and the Rényi divergences. Various quantum versions of this concept, and more narrowly, the concept of Rényi divergences, have been introduced in the literature with applications in quantum information theory; most notably Petz' quasi-entropies (standard f-divergences), Matsumoto's maximal f-divergences, measured f-divergences, and sandwiched and α-z-Rényi divergences.

In this paper we give a systematic overview of the various concepts of quantum f-divergences, with a main focus on their monotonicity under quantum operations, and the implications of the preservation of a quantum f-divergence by a quantum operation. In particular, we compare the standard and the maximal f-divergences regarding their ability to detect the reversibility of quantum operations. We also show that these two quantum f-divergences are strictly different for non-commuting operators unless f is a polynomial, and obtain some analogous partial results for the relation between the measured and the standard f-divergences.

We also study the monotonicity of the α-z-Rényi divergences under the special class of bistochastic maps that leave one of the arguments of the Rényi divergence invariant, and determine domains of the parameters α, z where monotonicity holds, and where the preservation of the α-z-Rényi divergence implies the reversibility of the quantum operation.

Keywords and phrases: Quantum f-divergences, sandwiched Rényi divergences, α-z-Rényi divergences, maximal f-divergences, measured f-divergences, monotonicity inequality, reversibility of quantum operations.

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1 Introduction

Quantum divergences give measures of dissimilarity of quantum states (or, more generally, positive semidefinite operators on a Hilbert space). While from a purely mathematical point of view, any norm on the space of operators would do this job, for information theoretic applications it is often more beneficial to consider other types of divergences, that are more naturally linked to the given problems. Undisputably the most important such divergence is *Umegaki's relative entropy* [71], defined for two positive operators ϱ, σ as[1]

$$S(\varrho\|\sigma) := \operatorname{Tr} \varrho(\log \varrho - \log \sigma). \tag{1.1}$$

The operational significance of this quantity was established in [36, 60], as an optimal error exponent in the hypothesis testing problem of Stein's lemma. Moreover, the relative entropy

[1] In the Introduction we assume all positive operators to be invertible for simplicity; the precise definitions for not necessarily invertible positive semidefinite operators will be given later in the paper.

serves as a parent quantity to many other measures of information and correlation, like the von Neumann entropy, the conditional entropy and the coherent information, the mutual information, the Holevo capacity, and more, each of which quantifies an optimal achievable rate in a certain quantum information theoretic problem; see, e.g., [72].

The relative entropy and its derived quantities mentioned above appear in the so-called first order versions of coding theorems, typically as the optimal exponent of some operational quantity (e.g., the coding rate or the compression rate) under the assumption that a certain error probability vanishes in the asymptotic treatment of the problem. In a more detailed analysis of these problems, one can try to give a quantitative description of the interplay between the relevant error probability and the operational quantity of interest (e.g., the coding rate) by fixing the asymptotic rate of one and optimzing the rate of the other. As it turns out, in every case when such a quantification has been found, it is given in terms of two different families of divergences: the *(conventional) Rényi divergences*

$$D_\alpha(\varrho\|\sigma) := \frac{1}{\alpha-1}\log\frac{\operatorname{Tr}\varrho^\alpha\sigma^{1-\alpha}}{\operatorname{Tr}\varrho}, \tag{1.2}$$

or the recently discovered *sandwiched Rényi divergences* [56, 73]

$$D_\alpha^*(\varrho\|\sigma) := \frac{1}{\alpha-1}\log\frac{\operatorname{Tr}(\sigma^{\frac{1-\alpha}{2\alpha}}\varrho\sigma^{\frac{1-\alpha}{2\alpha}})^\alpha}{\operatorname{Tr}\varrho}; \tag{1.3}$$

see, e.g., [7, 17, 27, 28, 29, 52, 53, 57]. Both families are defined for any $\alpha > 0$, $\alpha \neq 1$, and the values for $\alpha \in \{0, 1, +\infty\}$ can be obtained by taking the respective limit in α. In particular, the limit for $\alpha \to 1$ gives $\frac{1}{\operatorname{Tr}\varrho}S(\varrho\|\sigma)$. It is important to note that these two families coincide for commuting ϱ and σ. A two-parameter unification of these two families is given by the so-called α-z-Rényi divergences, introduced in [6, 39] as

$$D_{\alpha,z}(\varrho\|\sigma) := \frac{1}{\alpha-1}\log\frac{\operatorname{Tr}(\sigma^{\frac{1-\alpha}{2z}}\varrho^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}})^z}{\operatorname{Tr}\varrho}, \qquad \alpha, z > 0,\ \alpha \neq 1. \tag{1.4}$$

The previous two families are embedded as $D_{\alpha,1} = D_\alpha$ and $D_{\alpha,\alpha} = D_\alpha^*$ for every α.

In the classical case, both the relative entropy and the Rényi divergences can be expressed as f-divergences, introduced by Csiszár [18] and Ali and Silvey [1] for two probability distributions p, q on a finite set $\mathcal{X}$ and a convex function $f : (0, +\infty) \to \mathbb{R}$ as

$$S_f(p\|q) := \sum_{x\in\mathcal{X}} q(x) f\left(\frac{p(x)}{q(x)}\right). \tag{1.5}$$

The relative entropy corresponds to $f(t) := \eta(t) := t\log t$, while the Rényi divergences can be expressed as $D_\alpha(p\|q) = \frac{1}{\alpha-1}\log S_{f_\alpha}(p\|q)$, $f_\alpha(t) := \operatorname{sign}(\alpha-1)t^\alpha$. Moreover, various other divergences for probability distributions can be cast in this form; among others, the variational distance and the χ^2-divergence. An advantage of this general formulation is that important properties of the various divergences, like joint convexity and monotonicity under stochastic maps, can be derived from (1.5) and the convexity of f, thus providing a unified framework to study the different divergences.

Motivated by the success of the classical f-divergences, various quantum generalizations of the concept have been put forward in the literature. The closest in properties to the classical version are probably the *standard f-divergences*, that are a special case of Petz' quasi-entropies [62, 63] (see also [34]), and are defined as

$$S_f(\varrho\|\sigma) := \operatorname{Tr}\sigma^{1/2} f(L_\varrho R_{\sigma^{-1}})(\sigma^{1/2}), \tag{1.6}$$

where L_ϱ and $R_{\sigma^{-1}}$ are the left and the right multiplication operators by ϱ and σ^{-1}, respectively. The choices $f = \eta$ and $f = f_\alpha$ give rise to the Umegaki relative entropy (1.1) and the conventional Rényi divergences (1.2), just as in the classical case. An alternative version, that coincides with the above for commuting ϱ and σ, has been introduced by Petz and Ruskai in [68] as

$$\widehat{S}_f(\varrho\|\sigma) := \operatorname{Tr} \sigma f(\sigma^{-1/2}\varrho\sigma^{-1/2}).$$

It has been shown recently by Matsumoto [50] that this notion of quantum f-divergence is maximal among the monotone quantum f-divergences, and, moreover, it can be expressed in the form of a natural optimization of the f-divergences of classical distribution functions that can be mapped into the given quantum operators (see Section 3.1 for details). Hence, following Matsumoto's terminology, we will refer to them as *maximal f-divergences*.

The relative entropy and the standard and the sandwiched Rényi divergences take strictly positive values on pairs of unequal quantum states, supporting their interpretation as measures of distinguishability; for the standard f-divergences the same holds for every strictly convex f with the normalization $f(1) = 0$ [34, Proposition A.4]. For any measure D of distinguishability of states, it is natural to assume that stochastic operations do not increase the distinguishability, i.e., the monotonicity inequality

$$D(\Phi(\varrho)\|\Phi(\sigma)) \leq D(\varrho\|\sigma) \tag{1.7}$$

holds for any states (or, more generally, positive operators) ϱ, σ, and quantum operation Φ. For physical applications, the latter is usually defined as a completely positive and trace-preserving (CPTP) map, although from a purely mathematical point it is also interesting to study monotonicity under maps with weaker positivity properties [34, 55, 62, 63]. The monotonicity inequality is also called the data-processing inequality in information theory, and it is often considered as a primary requirement for a quantum quantity to be called a divergence. It is well-known that the standard Rényi divergences satisfy monotonicity exactly when $\alpha \in [0, 2]$ [34, 48, 63, 70], and the sandwiched Rényi divergences when $\alpha \in [1/2, +\infty]$ [8, 14, 24, 33, 56, 73]; this gives a further insight into why one needs two separate families of Rényi divergences in the quantum case. Domains of the parameters α, z where the α-z-Rényi divergences satisfy monotonicity have been determined in [14, 33] (see also [6, Theorem 1]), but a complete characterization of all α, z values for which monotonicity holds is still missing.

As with any inequality, it is natural to ask when the monotonicity inequality (1.7) holds as an equality, i.e., when does a quantum operation preserve the distinguishability of two states (as measured by a certain quantum divergence). It is clear that this is the case for any monotone divergence whenever Φ is reversible on $\{\varrho, \sigma\}$ in the sense that there exists a quantum operation Ψ such that $\Psi(\Phi(\varrho)) = \varrho$ and $\Psi(\Phi(\sigma)) = \sigma$. It is a highly non-trivial observation with far-reaching consequences that for a large class of divergences the converse is also true. This line of research was initiated by Petz [64, 65], who showed this converse for the relative entropy and the standard Rényi divergence with parameter 1/2, and determined a canonical reversion map. His results were later extended to standard Rényi divergences with other parameter values [42, 43], and more general standard f-divergences in [34, 40]. Various other, mainly algebraic, characterizations of the preservation of the relative entropy were given, e.g., in [67, 69]. In [30], a structural characterization of the equality case of the strong subadditivity of entropy (a special case of the monotonicity of the relative entropy) was presented, which was used to give a constructive description of quantum Markov states. This was later extended in [54] to a structural characterization of triples (Φ, ϱ, σ) such that Φ is reversible on $\{\varrho, \sigma\}$. Also, the equality case in the joint convexity (another special instance of monotonicity) of various quasi-entropies was clarified in [45]. The above characterizations are all related to quantum f-divergences of the form (1.6), in particular, mainly to the standard Rényi relative entropies (1.2). Very recently, an algebraic characterization of the preservation of the sandwiched Rényi divergences (1.3) with parameter values $\alpha > 1/2$ was given in [47], based on the variational formula of [24]. Moreover, in [41] it was shown that the preservation of a sandwiched Rényi divergence with $\alpha > 1$ implies reversibility. This was based on the complex interpolation method in non-commutative L_p spaces, following the approach of [8].

In this paper we give a systematic overview of the various concepts of quantum f-divergences, with a main focus on their monotonicity under quantum operations, and the implications of the preservation of a quantum f-divergence by a quantum operation. After summarizing the necessary preliminaries in Section 2, we give a detailed overview of the standard and the maximal f-divergences in Section 3. Unlike in previous works, we define these f-divergences for operator convex functions on $(0, +\infty)$ that need not have a finite limit from the right at 0, and establish the relevant continuity properties to make sense of the definition. In the introduction of the maximal f-divergences in Section 3.3, we deviate from Matsumoto's treatment in that we take the notion of the operator perspective as our starting point. To define the maximal f-divergences for not necessarily invertible operators, we establish the extension of the operator perspective for certain settings with non-invertible operators in Propositions 3.25 and 3.26, that seems to be new and probably interesting in itself. It is easy to see, as we show in Proposition 3.12, that even with this more general definition, the standard f-divergences are monotone under the same class of positive trace-preserving maps as considered before in [34], while the maximal f-divergences are monotone under arbitrary positive maps, as follows from standard facts in matrix analysis.

We summarize the known characterizations for the preservation of the standard f-divergences by positive trace-preserving maps in Theorems 3.18 and 3.19. Theorem 3.18 contains a slight extension as compared to previous results, as we show that ordinary positivity of the reversion map (as opposed to a stronger positivity criterion in [34, Theorem 5.1]) is sufficient for the preservation of any f-divergence; this is possible due to the recent developments in this direction in [8, 55]. In Theorem 3.34, we give a slight extension of Matsumoto's prior results on the characterization of the preservation of the maximal f-divergences by quantum operations. In particular, we remove a technical restriction on the function f in [50, Lemma 12], and show that the preservation of any maximal f-divergence with a non-linear operator convex function f implies the preservation of any other maximal f-divergence. In particular, the choice $f_2(t) = t^2$ implies that the preservation of a maximal f-divergence with any non-linear operator convex function f is equivalent to the preservation of the standard f-divergence S_{f_2} (as $S_{f_2} = \widehat{S}_{f_2}$), which in turn is known not to imply reversibility, as was shown in [34, Remark 5.4]. Hence, we conclude that the preservation of the maximal f-divergences has strictly weaker consequences than the preservation of the standard f-divergences. We discuss this difference in more detail in Section 4.2. In particular, we give (in Example 4.8) a simple explicit construction for a channel Φ and two states ϱ, σ on $\mathbb{C}^3$ such that Φ preserves all the maximal f-divergences of ϱ and σ, but does not preserve any of their standard f-divergences whenever f satisfies some mild technical condition. On the other hand, we show in Proposition 4.10 that for unital qubit channels, preservation of the maximal f-divergences is equivalent to the preservation of the standard f-divergences, and we show in Proposition 4.11 that the same holds whenever the outputs of the channel commute with each other.

Section 4 is devoted to the comparison of three different notions of quantum f-divergences: the standard f-divergence, the maximal f-divergence and the measured (minimal) f-divergence. In Section 4.1 we use Matsumoto's reverse tests and the characterization of the preservation of standard f-divergences to show that for non-commuting states, their maximal f-divergences are strictly larger than their standard f-divergences for all operator convex functions with a large enough support of their representing measure in a canonical integral representation (given in [34, Theorem 8.1]). Moreover, for qubit operators this condition can be dropped, as we show in Proposition 4.7. Section 4.2 is devoted to the comparison of the standard and the maximal f-divergences regarding their ability to detect the reversibility of quantum operations, as explained above. Finally, in Section 4.3, we discuss the measured f-divergences, and show that for any pair of non-commuting operators, their measured f-divergence is strictly smaller than their standard f-divergence, provided again some technical conditions on the size of the support of the representing measure of f are satisfied. We also review, and give a slight extension of recent results on the ordering of the standard, the sandwiched, the measured, and the regularized measured Rényi divergences, in Proposition 4.24. We close this section by a Pinsker inequality on the projectively measured f-divergences, given in Proposition 4.28.

In the last section, Section 5, we consider the behaviour of the α-z-Rényi divergences under bistochastic maps that leave one of the arguments of the Rényi divergence invariant, and determine domains of α, z values where monotonicity holds, and where the preservation of the α-z-Rényi divergence implies the reversibility of the quantum operation. This setup contains dephasing maps, i.e., (block-)diagonalization of one operator in a basis in which the other operator is already (block-)diagonal, or, more generally, conditional expectations onto a subalgebra that contains one of the arguments of the Rényi divergence. A particular example is the pinching by the eigenprojectors of the second argument of the Rényi divergence; the behaviour of the sandwiched Rényi divergences ($z = \alpha$ case) under these maps played an important role in establishing their operational significance in quantum state discrimination [52]. The α, z values where we establish monotonicity contain domains where the monotonicity of the α-z-Rényi divergences is either not known or does not hold for general maps. The analysis of the implications of the preservation of the α-z-Rényi divergences is completely new, as this has only been carried out so far for the standard Rényi divergences [34, 42, 43, 65], and, very recently, for the sandwiched Rényi divergences for a part of the parameter range where they are monotone [41].

We give supplementary material and some longer proofs in Appendices A–E.

2 Preliminaries

2.1 Notations

Throughout the paper, $\mathcal{H}, \mathcal{K}$ will denote finite-dimensional Hilbert spaces. For any finite-dimensional Hilbert space $\mathcal{H}$, $\mathcal{B}(\mathcal{H})$ will denote the algebra of linear operators on $\mathcal{H}$, and $\mathcal{B}(\mathcal{H})_{\mathrm{sa}}$ the real subspace of self-adjoint operators in $\mathcal{B}(\mathcal{H})$. The identity operator on $\mathcal{H}$ is denoted by $I_{\mathcal{H}}$ (or simply I). The spectrum of an operator $X \in \mathcal{B}(\mathcal{H})$ is denoted by $\mathrm{spec}(X)$.

We write $\mathcal{B}(\mathcal{H})_+$ for the set of positive linear operators on $\mathcal{H}$. We write $\varrho > 0$ when $\varrho \in \mathcal{B}(\mathcal{H})_+$ is invertible, and denote the set of invertible positive operators by $\mathcal{B}(\mathcal{H})_{++}$. For $\varrho \in \mathcal{B}(\mathcal{H})_+$ with spectral decomposition $\varrho = \sum_{a\in\mathrm{spec}(\varrho)} aP_a$, we define its real powers by $\varrho^t := \sum_{a\in\mathrm{spec}(\varrho),\, a>0} a^t P_a$, $t \in \mathbb{R}$. In particular, ϱ^{-1} stands for the generalized inverse of ϱ, and ϱ^0 is the support projection of ϱ, i.e., the projection onto the support of ϱ.

The usual trace functional on $\mathcal{B}(\mathcal{H})$ is denoted by Tr. We always consider $\mathcal{B}(\mathcal{H})$ as the Hilbert space with the *Hilbert-Schmidt inner product*

$$\langle X, Y\rangle_{\mathrm{HS}} := \mathrm{Tr}\, X^*Y, \qquad X, Y \in \mathcal{B}(\mathcal{H}).$$

For a linear operator $\varrho \in \mathcal{B}(\mathcal{H})$, the *left multiplication* L_ϱ and the *right multiplication* R_ϱ are the linear operators on $\mathcal{B}(\mathcal{H})$ defined by

$$L_\varrho X := \varrho X, \quad R_\varrho X := X\varrho, \qquad X \in \mathcal{B}(\mathcal{H}).$$

If $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, then both L_ϱ and R_ϱ are positive operators on the Hilbert space $\mathcal{B}(\mathcal{H})$, which are commuting, i.e., $L_\varrho R_\sigma = R_\sigma L_\varrho$.

2.2 Operator convex and operator monotone functions

In the rest of the paper, unless otherwise stated, we always assume that $f : (0, +\infty) \to \mathbb{R}$ is a continuous function such that the limits

$$f(0^+) := \lim_{x \searrow 0} f(x) \quad \text{and} \quad f'(+\infty) := \lim_{x\to+\infty} \frac{f(x)}{x}$$

exist in $\mathbb{R} \cup \{\pm\infty\}$, and they are not both infinity with opposite signs. These assumptions are obviously satisfied when f is convex, in which case the limits exist in $(-\infty, +\infty]$, and if f is a differentiable convex function then in fact $f'(+\infty) = \lim_{x\to+\infty} f'(x)$.

A function $f : (0, +\infty) \to \mathbb{R}$ is called an *operator convex* function if the operator inequality

$$f(tA + (1-t)B) \le tf(A) + (1-t)f(B), \qquad 0 \le t \le 1$$

holds for every $A, B \in \mathcal{B}(\mathcal{H})_{++}$ of any (even infinite-dimensional) $\mathcal{H}$, where $f(A)$ etc. are defined via usual functional calculus. Also, a function $h : (0, +\infty) \to \mathbb{R}$ is said to be *operator monotone* if $A \le B$ implies $h(A) \le h(B)$ for every $A, B \in \mathcal{B}(\mathcal{H})_{++}$ of any $\mathcal{H}$. For the general theory of operator monotone and operator convex functions, see, e.g., [11, 32]. For the rest of the paper, we will mainly follow the convention that h denotes an operator monotone function, and f an operator convex, or at least convex, function.

Operator monotone and operator convex functions can be decomposed to simpler functions via integral representations, a few of which we recall here for later use. Every non-negative operator monotone function h on $(0, \infty)$ can be uniquely written as

$$h(x) = a + bx + \int_{(0,+\infty)} \frac{x(1+s)}{x+s}\, d\nu_h(s), \qquad x \in (0, +\infty), \tag{2.1}$$

with $a = h(0^+)$, $b = h'(+\infty) = \lim_{x\to+\infty} h(x)/x$, and a finite positive measure ν_h on $(0, +\infty)$ (see [32, Theorem 2.7.11]).

When $f : (0, +\infty) \to \mathbb{R}$ is operator convex, it can be written [48] (see also [25, (5.2)] for a more general form) as

$$f(x) = f(1) + f'(1)(x-1) + c(x-1)^2 + \int_{[0,+\infty)} \frac{(x-1)^2}{x+s}\, d\lambda(s), \quad x \in (0, +\infty), \tag{2.2}$$

with $c \ge 0$ and a positive measure λ on $[0, +\infty)$ satisfying $\int_{[0,+\infty)} (1+s)^{-1}\, d\lambda(s) < +\infty$. When $f(0^+) < +\infty$, and hence f extends by continuity to an operator convex function on $[0, +\infty)$, an alternative integral representation can be obtained [34, Theorem 8.1] as

$$f(x) = f(0^+) + ax + bx^2 + \int_{(0,+\infty)} \left(\frac{x}{1+s} - \frac{x}{x+s} \right) d\mu_f(s), \qquad x \in (0, +\infty), \tag{2.3}$$

with $a \in \mathbb{R}$, $b \ge 0$ and a positive measure μ_f on $(0, +\infty)$ satisfying $\int_{(0,+\infty)} (1+s)^{-2}\, d\mu_f(s) < +\infty$. In the more restrictive case when $f(0^+) < +\infty$ and $f'(+\infty) < +\infty$, yet another integral representation was given in [34, Theorem 8.4] as

$$f(x) = f(0^+) + f'(+\infty)x - \int_{(0,+\infty)} \frac{x(1+s)}{x+s}\, d\nu(s) \tag{2.4}$$

with a finite positive measure ν on $(0, +\infty)$. Note that the coefficients c, a, b and the representing measures λ, μ_f, ν are uniquely determined by f in each of the above integral representations. We make the dependence of μ on f explicit in (2.3) for the convenience of later references. Moreover, the representing measures in the above are explicitly related to each other. Indeed, for f with expression (2.2), $f(0^+) < +\infty$ if and only if $\int_{[0,+\infty)} s^{-1}\,d\lambda(s) < +\infty$ (in particular, $\lambda(\{0\}) = 0$), and in this case, the relation $(1+s)^{-2}\,d\mu_f(s) = s^{-1}\,d\lambda(s)$ holds (the proof of this is left to the reader). Also, for f with expression (2.3) (hence $f(0^+) < +\infty$), $f'(+\infty) < +\infty$ if and only if $b = 0$ and $\int_{(0,+\infty)}(1+s)^{-1}\,d\mu_f < +\infty$, and in this case, $d\nu(s) = (1+s)^{-1}\,d\mu_f(s)$ (see the proof of [34, Theorem 8.4]). Thus, the support of the representing measure for f is independent of the possible choice of the above integral expressions.

2.3 Non-commutative perspectives and operator connections

For any function $\varphi : (0, +\infty) \to \mathbb{R}$, its *perspective* $P_\varphi : (0, +\infty) \times (0, +\infty) \to \mathbb{R}$ is defined by

$$P_\varphi(x, y) := y\varphi\left(\frac{x}{y}\right), \qquad x, y \in (0, +\infty).$$

By definition, $\varphi(x) = P_\varphi(x, 1)$ for all $x \in (0, +\infty)$, and the *transpose* $\widetilde{\varphi}$ of φ is defined as

$$\widetilde{\varphi}(y) := P_\varphi(1, y) = y\varphi\left(\frac{1}{y}\right), \qquad y \in (0, +\infty).$$

Thus, φ and $\widetilde{\varphi}$ can be considered as marginals of the two-variable function P_f.

When f is as at the beginning of the previous section, we can extend P_f to $[0, +\infty) \times [0, +\infty)$ by

$$P_f(x, y) := \lim_{\varepsilon \searrow 0}(y+\varepsilon) f\left(\frac{x+\varepsilon}{y+\varepsilon}\right) = \begin{cases} yf(xy^{-1}), & \text{if } x, y > 0, \\ yf(0^+), & \text{if } x = 0, \\ xf'(+\infty), & \text{if } y = 0, \end{cases} \tag{2.5}$$

with the convention $0 \cdot \infty := 0$. It is straightforward to see that

$$\widetilde{f}(0^+) = f'(+\infty), \qquad \widetilde{f}'(+\infty) = f(0^+). \tag{2.6}$$

It is well-known that the transpose $\widetilde{h}$ of a non-negative operator monotone function h on $(0, +\infty)$ is operator monotone again. Similarly, the transpose $\widetilde{f}$ of an operator convex function f on $(0, +\infty)$ is operator convex again. For these assertions, see Propositions A.1 and A.2 of Appendix A.

For a function φ on $(0, +\infty)$, its *non-commutative* (or *operator*) *perspective* P_φ is defined as the two-variable operator function

$$P_\varphi : (A, B) \in \mathcal{B}(\mathcal{H})_{++} \times \mathcal{B}(\mathcal{H})_{++} \longmapsto B^{1/2}\varphi(B^{-1/2}AB^{-1/2})B^{1/2} \tag{2.7}$$

for every finite-dimensional Hilbert space $\mathcal{H}$. The following simple observation will be useful:

Lemma 2.1. Let $\varphi : (0, +\infty) \to \mathbb{R}$ be any function and $\widetilde{\varphi}$ be the transpose of φ. For every $A, B \in \mathcal{B}(\mathcal{H})_{++}$,

$$P_{\widetilde{\varphi}}(A, B) = P_\varphi(B, A).$$

Proof. By definition,

$$\begin{aligned}
P_{\widetilde{\varphi}}(A,B) &= B^{1/2}\widetilde{\varphi}(B^{-1/2}AB^{-1/2})B^{1/2} \\
&= B^{1/2}(B^{-1/2}AB^{-1/2})\varphi(B^{1/2}A^{-1}B^{1/2})B^{1/2} \\
&= AB^{-1/2}\varphi(XX^*)XA^{1/2} = AB^{-1/2}X\varphi(X^*X)A^{1/2} \\
&= A^{1/2}\varphi(A^{-1/2}BA^{-1/2})A^{1/2} = P_\varphi(B,A),
\end{aligned}$$

where $X := B^{1/2}A^{-1/2}$. □

The following are basic properties of operator perspectives. The proof of (1) is due to [21, 22, 23]. We give a small extension of the next lemma in Appendix A.

Lemma 2.2. Let $\varphi:\ (0,+\infty)\to\mathbb{R}$.

(1) P_φ is jointly operator convex on $\mathcal{B}(\mathcal{H})_{++}\times\mathcal{B}(\mathcal{H})_{++}$ for every finite-dimensional Hilbert space $\mathcal{H}$ if and only if φ is operator convex.

(2) P_φ is monotone non-decreasing in both of its arguments on $\mathcal{B}(\mathcal{H})_{++}\times\mathcal{B}(\mathcal{H})_{++}$ for every finite-dimensional Hilbert space $\mathcal{H}$ if and only φ is a non-negative operator monotone function.

Assume that h is a non-negative operator monotone function on $(0,+\infty)$, extended by continuity to $[0,\infty)$. Then $(A,B)\mapsto P_h(B,A)$ gives an *operator connection*, that we denote by τ_h, i.e., $A\,\tau_h\,B = P_h(B,A)$ (notice the reversed order of A and B). The general theory of operator connections was developed in an axiomatic way by Kubo and Ando [46]. The operator connection τ_h is extended to pairs of not necessarily invertible positive operators as

$$A\,\tau_h\,B := \lim_{\varepsilon\searrow 0}(A+\varepsilon I)\,\tau_h\,(B+\varepsilon I), \qquad A,B\in\mathcal{B}(\mathcal{H})_+, \tag{2.8}$$

and it is called an *operator mean* when h further satisfies $h(1)=1$. A main result of [46] says that the correspondence $h\leftrightarrow\tau_h$ is an order isomorphism between the non-negative operator monotone functions and the operator connections. Although $(A,B)\mapsto A\,\tau_h\,B$ is continuous for decreasing sequences in $\mathcal{B}(\mathcal{H})_+$, it is not necessarily so for general sequences. Nevertheless, we have the following slightly more general convergence property (whenever $\mathcal{H}$ is a finite-dimensional Hilbert space). This is easily seen from the joint monotonicity and the definition (2.8) of τ_h.

Lemma 2.3. Let $h:\ (0,+\infty)\to\mathbb{R}$ be a non-negative operator monotone function. For any $A,B\in\mathcal{B}(\mathcal{H})_+$, and any sequences $A_n,B_n\in\mathcal{B}(\mathcal{H})_+$ such that $A\le A_n\to A$ and $B\le B_n\to B$, the sequence $A_n\,\tau_h\,B_n = P_h(B_n,A_n)$ converges to $A\,\tau_h\,B$.

When h is a non-negative operator monotone function on $(0,+\infty)$, it admits a unique integral representation, given in (2.1), which in turn yields

$$A\,\tau_h\,B = aA + bB + \int_{(0,+\infty)} A\,\tau_{h_s}\,B\,d\nu_h(s), \qquad A,B\in\mathcal{B}(\mathcal{H})_+, \tag{2.9}$$

where $h_s(x) := x(1+s)/(x+s)$. In other notation, $A\,\tau_{h_s}\,B = \frac{1+s}{s}\{(sA):B\}$, where $A:B$ is the parallel sum of $A,B\in\mathcal{B}(\mathcal{H})_+$ (see [46]). We say that the operator connection τ_h is non-linear if h is non-linear (i.e., the measure ν_h is non-zero).

When f is an operator convex function on $(0,+\infty)$, the extension of its perspective to $\mathcal{B}(\mathcal{H})_+\times\mathcal{B}(\mathcal{H})_+$ is a non-trivial problem, that we will discuss in detail in Section 3.3.

2.4 Monotone metrics

Let $\mathcal{D}(\mathcal{H})$ denote the set of invertible density operators on $\mathcal{H}$, which is a smooth Riemannian manifold whose tangent space at any foot point is identified with

$$\mathcal{B}(\mathcal{H})_{\mathrm{sa}}^0 := \{X \in \mathcal{B}(\mathcal{H})_{\mathrm{sa}} : \mathrm{Tr}\, X = 0\}.$$

Let $\kappa : (0, +\infty) \to (0, +\infty)$ be an operator monotone decreasing function such that $x\kappa(x) = \kappa(x^{-1})$, $x > 0$. Since $h(x) := \kappa(x^{-1}) = x\kappa(x)$, $x > 0$, is operator monotone, the integral expression (2.1) of h gives that of κ as

$$\kappa(x) = \frac{a}{x} + b + \int_{(0,+\infty)} \frac{1+s}{x+s}\, d\nu_h(s) = b + \int_{[0,+\infty)} \frac{1+s}{x+s}\, \nu_\kappa(s), \tag{2.10}$$

where $\nu_\kappa := \nu_h + a\delta_0$. Associated with the function κ, a Riemannian metric on $\mathcal{D}(\mathcal{H})$ is defined by

$$\langle X, \Omega_\sigma^\kappa(Y)\rangle_{\mathrm{HS}}, \qquad X, Y \in \mathcal{B}(\mathcal{H})_{\mathrm{sa}}^0,\ \sigma \in \mathcal{D}(\mathcal{H}),$$

where

$$\Omega_\sigma^\kappa := R_{\sigma^{-1}}\kappa(L_\sigma R_{\sigma^{-1}}). \tag{2.11}$$

This class of Riemannian metrics are called *monotone metrics* since the class was characterized by Petz [66] with the monotonicity property

$$\left\langle \Phi(X), \Omega_{\Phi(\sigma)}^\kappa(\Phi(X))\right\rangle_{\mathrm{HS}} \le \langle X, \Omega_\sigma^\kappa(X)\rangle_{\mathrm{HS}}, \qquad X \in \mathcal{B}(\mathcal{H})_{\mathrm{sa}}^0,\ \sigma \in \mathcal{D}(\mathcal{H}),$$

for every trace-preserving map $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ such that Φ^* is a Schwarz contraction. See also [38] for monotone Riemannian metrics. The description of Ω_σ^κ in (2.11) is from [38], that coincides with $\left[f(L_\sigma R_\sigma^{-1})R_\sigma\right]^{-1}$ in Petz' representation in [66, Theorem 5] for an operator monotone function $f(x) = 1/\kappa(x)$, $x > 0$, and the condition $x\kappa(x) = \kappa(x^{-1})$, $x > 0$, is equivalent to $f = \widetilde{f}$.

2.5 Positive maps

For a linear map $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$, where $\mathcal{H}$ and $\mathcal{K}$ are finite-dimensional Hilbert spaces, the *adjoint* map $\Phi^* : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ is defined in terms of the Hilbert-Schmidt inner products as

$$\langle \Phi(X), Y\rangle_{\mathrm{HS}} = \langle X, \Phi^*(Y)\rangle_{\mathrm{HS}}, \qquad X \in \mathcal{B}(\mathcal{H}),\ Y \in \mathcal{B}(\mathcal{K}).$$

The map Φ is said to be *positive* if $\Phi(A) \in \mathcal{B}(\mathcal{K})_+$ for all $A \in \mathcal{B}(\mathcal{H})_+$, and n*-positive*, for some $n \in \mathbb{N}$, if $\mathrm{id}_n \otimes \Phi : \mathcal{B}(\mathbb{C}^n) \otimes \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathbb{C}^n) \otimes \mathcal{B}(\mathcal{K})$ is positive, where id_n is the identity map on $\mathcal{B}(\mathbb{C}^n)$. A map Φ is said to be *completely positive* if it is n-positive for all $n \in \mathbb{N}$. It is easy to see that Φ is n-positive if and only if Φ^* is n-positive, and Φ is *trace-preserving* (i.e., $\mathrm{Tr}\,\Phi(X) = \mathrm{Tr}\, X$, $X \in \mathcal{B}(\mathcal{H})$) if and only if Φ^* is *unital* (i.e., $\Phi^*(I_\mathcal{K}) = I_\mathcal{H}$). A trace-preserving completely positive (CPTP) map is called a *quantum channel* (or simply a channel). We say that a positive map Φ is *bistochastic* if it is both unital and trace-preserving. The following is from [15, Theorem 2.1]:

Lemma 2.4. Let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a unital positive linear map, let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint, and f be an operator convex function defined on an interval containing $\mathrm{spec}(A)$. Then

$$f\left(\Phi(A)\right) \le \Phi\left(f(A)\right).$$

The *multiplicative domain* $\mathcal{M}_\Phi$ of a linear map $\Phi:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$ is defined as

$$\mathcal{M}_\Phi := \{X\in\mathcal{B}(\mathcal{H}):\, \Phi(XY)=\Phi(X)\Phi(Y),\ \Phi(YX)=\Phi(Y)\Phi(X),\, Y\in\mathcal{B}(\mathcal{H})\}. \tag{2.12}$$

Obviously, $\mathcal{M}_\Phi$ is an algebra, and if Φ is positive then it is also closed under the adjoint, and the restriction of Φ onto $\mathcal{M}_\Phi$ is a *-homomorphism. In particular, we have the following:

Lemma 2.5. For any unital positive map Φ and any normal element A in $\mathcal{M}_\Phi$, $\Phi(A)$ is also normal, and for any function φ on $\operatorname{spec}(A)\cup\operatorname{spec}(\Phi(A))$, we have

$$\varphi(\Phi(A))=\Phi(\varphi(A)).$$

We say that a linear map $\Phi:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{K})$ is a *Schwarz contraction* if it satisfies the *Schwarz inequality*

$$\Phi(X)^*\Phi(X)\le\Phi(X^*X),\qquad X\in\mathcal{B}(\mathcal{H}).$$

Obviously, every Schwarz contraction is positive, and it is known that every unital 2-positive map is a Schwarz contraction, while the converse is not true. If Φ is a Schwarz contraction, then its multiplicative domain can be characterized as

$$\mathcal{M}_\Phi=\{X\in\mathcal{B}(\mathcal{H}):\,\Phi(XX^*)=\Phi(X)\Phi(X)^*,\ \Phi(X^*X)=\Phi(X)^*\Phi(X)\}; \tag{2.13}$$

see [34, Lemma 3.9] for a proof.

The *fixed point set* $\mathcal{F}_\Phi$ of a linear map $\Phi:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H})$ is defined as

$$\mathcal{F}_\Phi:=\{X\in\mathcal{B}(\mathcal{H}):\,\Phi(X)=X\}.$$

The same proof as that of, e.g., [13, Lemma 3.4] or [40, Theorem 1 (i)] yields the following:

Lemma 2.6. Let $\Phi:\mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H})$ be a Schwarz contraction. If $\mathcal{F}_{\Phi^*}$ contains an element of $\mathcal{B}(\mathcal{H})_{++}$, then $\mathcal{F}_\Phi$ is a C^*-subalgebra of $\mathcal{M}_\Phi$.

Remark 2.7. In general, $\mathcal{F}_\Phi$ need not be an algebra, and there is no inclusion between $\mathcal{F}_\Phi$ and $\mathcal{M}_\Phi$ in either direction. We give some examples illustrating these in Appendix B and Example 4.5.

3 The standard and the maximal f-divergences

3.1 Introduction to f-divergences

Given two probability density functions (or, more generally, positive functions) ϱ,σ on a finite set $\mathcal{X}$, their f-divergence $S_f(\varrho\|\sigma)$, corresponding to a convex function $f:(0,+\infty)\to\mathbb{R}$, was defined by Csiszár [18] as

$$S_f(\varrho\|\sigma):=\sum_{x\in\mathcal{X}}\sigma(x)f\left(\frac{\varrho(x)}{\sigma(x)}\right). \tag{3.1}$$

(For simplicity, in this section we assume that both ϱ and σ are strictly positive, whether they denote functions or operators.) Most divergence measures used in classical information theory can be written in this form; for instance, $f(t):=t\log t$ yields the relative entropy (Kullback-Leibler divergence), $f_\alpha(t):=\operatorname{sgn}(\alpha-1)t^\alpha$, $\alpha\in(0,+\infty)\setminus\{1\}$, correspond to the Rényi divergences, and $f(t):=|t-1|$ gives the variational distance. All f-divergences are easily seen to be jointly convex in their variables, and monotone non-increasing under the joint action of a stochastic map on their arguments. Moreover, when f is strictly convex, a stochastic map preserves the f-divergence of ϱ and σ if and only if it is reversible on $\{\varrho,\sigma\}$, i.e., there exists a stochastic map Ψ such that $\Psi(\Phi(\varrho))=\varrho$ and $\Psi(\Phi(\sigma))=\sigma$ (see, e.g., [34, Proposition A.3]).

To motivate the definition of the different quantum f-divergences, let us recall the GNS representation theorem, that says that for every positive linear functional σ on a C^*-algebra $\mathcal{A}$, there exists a Hilbert space $\mathcal{H}_\sigma$, a vector $\Omega_\sigma\in\mathcal{H}$, and a representation π_σ of $\mathcal{A}$ on $\mathcal{H}$ such that $\sigma(a)=\langle\Omega_\sigma,\pi_\sigma(a)\Omega_\sigma\rangle$ for all $a\in\mathcal{A}$. In the classical case described above, ϱ and σ define positive linear functionals on the commutative C^*-algebra $\mathbb{C}^{\mathcal{X}}$, which we denote by the same symbols, and GNS representations can be given by choosing $\mathcal{H}=l^2(\mathcal{X})$ (with respect to the counting measure), $\Omega_\varrho=(\sqrt{\varrho(x)})_{x\in\mathcal{X}}$, $\Omega_\sigma=(\sqrt{\sigma(x)})_{x\in\mathcal{X}}$, and $\pi(a):=M_a:\ b\mapsto ab$ (with pointwise multiplication) for any $a,b\in\mathbb{C}^{\mathcal{X}}$. Then the operator $S:=M_{\varrho^{1/2}\sigma^{-1/2}}$ changes the representing vector of σ to that of ϱ, i.e., $S\Omega_\sigma=\Omega_\varrho$, and we have

$$S_f(\varrho\|\sigma)=\left\langle\Omega_\sigma,f(\Delta_{\varrho/\sigma})\Omega_\sigma\right\rangle,$$

where $\Delta_{\varrho/\sigma}:=SS^*=S^*S=M_{\varrho/\sigma}$ is the Radon-Nikodym derivative. This reformulation of (3.1) will be useful to extend the notion of f-divergences to the quantum setting.

In the general finite-dimensional case, when $\mathcal{A}\subset\mathcal{B}(\mathcal{H})$ for some finite-dimensional Hilbert space $\mathcal{H}$, positive linear functionals can be identified with positive elements of $\mathcal{A}$ through $\varrho(a)=\operatorname{Tr}D_\varrho a$, where D_ϱ is the density operator of ϱ. For the rest, we will use the same notation ϱ also for its density operator. Given two positive operators $\varrho,\sigma\in\mathcal{A}$ (we assume again for simplicity that they are both invertible), the GNS representations can be given by choosing $\mathcal{H}:=(\mathcal{A},\langle.,.\rangle_{\mathrm{HS}})$, $\Omega_\varrho:=\varrho^{1/2}$, $\Omega_\sigma:=\sigma^{1/2}$, and $\pi(a):=L_a:\ b\mapsto ab$, $a,b\in\mathcal{A}$. The question is now how to define the Radon-Nikodym derivative, i.e., the non-commutative analogues of the operators S and $\Delta_{\varrho/\sigma}$. One option is to choose $S:=L_{\varrho^{1/2}}R_{\sigma^{-1/2}}$, so that $\Delta_{\varrho/\sigma}:=SS^*=S^*S=L_\varrho R_{\sigma^{-1}}$ becomes the *relative modular operator*. The corresponding quantum f-divergence is

$$S_f(\varrho\|\sigma):=\operatorname{Tr}\sigma^{1/2}f\left(L_\varrho R_{\sigma^{-1}}\right)\sigma^{1/2}=\left\langle I,P_f\left(L_\varrho,R_\sigma\right)I\right\rangle_{\mathrm{HS}}, \tag{3.2}$$

that was defined and investigated by Petz (in a more general form) under the name quasi-entropy [62, 63]. Note that the choice $S:=L_{\sigma^{-1/2}}R_{\varrho^{1/2}}$ results in the same expression. Petz' analysis was extended in [34], and we give further extensions in Section 3.2 below.

Another option is to choose $S:=R_{\sigma^{-1/2}\varrho^{1/2}}$, and $\Delta_{\varrho/\sigma}:=SS^*=R_{\sigma^{-1/2}\varrho\sigma^{-1/2}}$ (the so-called *commutant Radon-Nikodym derivative*), resulting in the f-divergence

$$\widehat{S}_f(\varrho\|\sigma):=\operatorname{Tr}\sigma^{1/2}f\left(\sigma^{-1/2}\varrho\sigma^{-1/2}\right)\sigma^{1/2}=\left\langle I,P_f(\varrho,\sigma)I\right\rangle_{\mathrm{HS}}. \tag{3.3}$$

A special case of this, corresponding to the function $f(t):=t\log t$, has been studied by Belavkin and Staszewski [9] as a quantum extension of the Kullback-Leibler divergence. The above general form was introduced in [68]. Matsumoto [50] showed that this f-divergence is maximal among the monotone quantum f-divergences, and analyzed the preservation of this f-divergence by quantum operations. We will review and extend some of his results in Sections 3.3 and 4. Note that the definitions $S:=L_{\varrho^{1/2}\sigma^{-1/2}}$, $\Delta_{\varrho/\sigma}:=S^*S$; $S:=R_{\varrho^{1/2}\sigma^{-1/2}}$, $\Delta_{\varrho/\sigma}:=S^*S$; and $S:=L_{\sigma^{-1/2}\varrho^{1/2}}$, $\Delta_{\varrho/\sigma}:=SS^*$ all result in the same f-divergence (although with the latter two $S\Omega_\sigma=\Omega_\varrho$ does not hold).

Another natural definition would be to choose $S:=R_{\sigma^{-1/2}\varrho^{1/2}}$ and $\Delta_{\varrho/\sigma}:=S^*S$, leading to the f-divergence

$$\widetilde{S}_f(\varrho\|\sigma):=\operatorname{Tr}\sigma^{1/2}f\left(\varrho^{1/2}\sigma^{-1}\varrho^{1/2}\right)\sigma^{1/2}. \tag{3.4}$$

In general, however, $\widetilde{S}_f$, unlike the other two versions S_f and $\widehat{S}_f$ above, is not monotone under CPTP maps, nor it is jointly convex in its arguments, as we show in Appendix C. Thus, $\widetilde{S}_f$ is not a proper quantum divergence for general operator convex functions f, and hence we don't consider this version further in the paper.

A different and more operational approach is to define quantum f-divergences directly from classical ones. There seems to be two natural ways to do so, namely, to consider the *maximal f-divergence*, introduced by Matsumoto [50] as

$$S_f^{\max}(\varrho\|\sigma) := \inf\{S_f(p\|q) : p, q \in \mathcal{B}(\mathcal{K})_+ \text{ are commuting, } \dim\mathcal{K} < +\infty, \text{ and} \\ \Phi(p) = \varrho,\ \Phi(q) = \sigma \text{ for some CPTP map } \Phi : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})\} \tag{3.5}$$

(denoted by $D_f^{\max}$ in [50]) and the *measured* (or *minimal*) *f-divergence*

$$S_f^{\min}(\varrho\|\sigma) := S_f^{\text{meas}}(\varrho\|\sigma) := \sup\{S_f(\Phi(\varrho)\|\Phi(\sigma)) : \Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K}) \text{ is CPTP,} \\ \dim\mathcal{K} < +\infty, \text{ and } \operatorname{ran}\Phi \text{ is commutative}\}. \tag{3.6}$$

For a given (convex) function $f : (0, +\infty) \to \mathbb{R}$, we say that a functional S_f^q is a quantum f-divergence if S_f^q assigns a number in $(-\infty, +\infty]$ to any pair $(\varrho, \sigma) \in \mathcal{B}(\mathcal{H})_+ \times \mathcal{B}(\mathcal{H})_+$ for any finite-dimensional Hilbert space, such that if ϱ and σ commute then $S_f^q(\varrho\|\sigma) = S_f(\{\varrho(x)\}_{x\in\mathcal{X}}\|\{\sigma(x)\}_{x\in\mathcal{X}})$, where $\{\varrho(x)\}_{x\in\mathcal{X}}$ and $\{\sigma(x)\}_{x\in\mathcal{X}}$ are the diagonal elements of ϱ and σ in an orthonormal basis in which both of them are diagonal. We say that S_f^q is monotone if it is monotone non-increasing under the action of CPTP maps on both arguments of S_f^q. It is clear from the above definitions that

$$S_f^{\min}(\varrho\|\sigma) \le S_f^q(\varrho\|\sigma) \le S_f^{\max}(\varrho\|\sigma). \tag{3.7}$$

for any monotone quantum f-divergence S_f^q, which explains the names "maximal" and "minimal" for the definitions in (3.5) and (3.6).

Matsumoto has shown that $S_f^{\max}(\varrho\|\sigma) = \widehat{S}_f(\varrho\|\sigma)$ for operator convex function f on $[0, +\infty)$, and for ϱ, σ such that $\varrho^0 \le \sigma^0$. For $S_f^{\text{meas}}(\varrho\|\sigma)$, no explicit general formula is known. We will analyze the relation of the f-divergences $\widehat{S}_f = S_f^{\max}$, S_f, and S_f^{meas} in Section 4.

3.2 Standard f-divergences

Petz originally introduced his quasi-entropies [62, 63] by a more general formula than (3.2), as

$$S_f^K(\varrho\|\sigma) := \langle K\sigma^{1/2}, f(L_\varrho R_{\sigma^{-1}})(K\sigma^{1/2})\rangle_{\text{HS}} = \operatorname{Tr}\sigma^{1/2}K^* f\left(L_\varrho R_{\sigma^{-1}}\right)(K\sigma^{1/2}),$$

with K an arbitrary operator, and σ invertible. He proved the monotonicity

$$S_f^K(\Phi(\varrho)\|\Phi(\sigma)) \le S_f^{\Phi^*(K)}(\varrho\|\sigma)$$

of these quantities under the joint action of the dual of unital Schwarz contractions for operator monotone decreasing f on $[0, +\infty)$ with $f(0) \le 0$, and under the restriction onto a subalgebra for operator convex f. His definition and results were extended in the $K = I$ case in [34], in particular, for general positive operators ϱ, σ.

Below we give some further extensions, by only requiring the function f to be defined on $(0, +\infty)$ (as opposed to $[0, +\infty)$ in [34]), while allowing the operators ϱ and σ to have arbitrary supports. Recall our convention stated in the first paragraph of Section 2.2, that $f : (0, +\infty) \to \mathbb{R}$ is a continuous function such that the limits $f(0^+) := \lim_{x\searrow 0} f(x)$ and $f'(+\infty) := \lim_{x\to+\infty} \frac{f(x)}{x}$ exist and their non-negative linear combinations make sense.

Definition 3.1. For $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ let $\varrho = \sum_{a \in \mathrm{spec}(\varrho)} a P_a$ and $\sigma = \sum_{b \in \mathrm{spec}(\sigma)} b Q_b$ be the spectral decompositions. When $\varrho, \sigma > 0$, we have

$$f(L_\varrho R_{\sigma^{-1}}) = \sum_{a \in \mathrm{spec}(\varrho)} \sum_{b \in \mathrm{spec}(\sigma)} f(ab^{-1}) L_{P_a} R_{Q_b},$$

and we define the (standard) *f-divergence* of ϱ and σ as

$$S_f(\varrho\|\sigma) := \langle \sigma^{1/2}, f(L_\varrho R_{\sigma^{-1}}) \sigma^{1/2} \rangle_{\mathrm{HS}} = \mathrm{Tr}\, \sigma^{1/2} f(L_\varrho R_{\sigma^{-1}})(\sigma^{1/2}). \tag{3.8}$$

We extend $S_f(\varrho\|\sigma)$ to general $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ as

$$S_f(\varrho\|\sigma) := \lim_{\varepsilon \searrow 0} S_f(\varrho + \varepsilon I \| \sigma + \varepsilon I). \tag{3.9}$$

Proposition 3.2. For every $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ the limit in (3.9) exists, and we have

$$S_f(\varrho\|\sigma) = \sum_{a,b} P_f(a,b)\, \mathrm{Tr}\, P_a Q_b \tag{3.10}$$

$$= \sum_{a,b} P_f(a\, \mathrm{Tr}\, P_a Q_b, b\, \mathrm{Tr}\, P_a Q_b) \tag{3.11}$$

$$= \sum_{a>0} \sum_{b>0} b f(ab^{-1})\, \mathrm{Tr}\, P_a Q_b + f(0^+)\, \mathrm{Tr}(I - \varrho^0)\sigma + f'(+\infty)\, \mathrm{Tr}\, \varrho(I - \sigma^0) \tag{3.12}$$

with the convention $(+\infty)0 = 0$. In particular, (3.9) coincides with (3.8) for invertible ϱ, σ.

Proof. Since $\varrho + \varepsilon I = \sum_a (a + \varepsilon) P_a$ and $\sigma + \varepsilon I = \sum_b (b + \varepsilon) Q_b$, one has

$$f(L_{\varrho+\varepsilon I} R_{(\sigma+\varepsilon I)^{-1}}) = \sum_{a,b} f((a+\varepsilon)(b+\varepsilon)^{-1}) L_{P_a} R_{Q_b}$$

so that

$$S_f(\varrho + \varepsilon I \| \sigma + \varepsilon I) = \sum_{a,b} (b+\varepsilon) f((a+\varepsilon)(b+\varepsilon)^{-1})\, \mathrm{Tr}\, P_a Q_b.$$

Using (2.5), one finds that

$$\begin{aligned} &\lim_{\varepsilon \searrow 0} S_f(\varrho + \varepsilon I \| \sigma + \varepsilon I) \\ &\quad = \sum_{a,b} P_f(a,b)\, \mathrm{Tr}\, P_a Q_b \\ &\quad = \sum_{a,b>0} b f(ab^{-1})\, \mathrm{Tr}\, P_a Q_b + \sum_{b>0} b f(0^+)\, \mathrm{Tr}\, P_0 Q_b + \sum_{a>0} a f'(+\infty)\, \mathrm{Tr}\, P_a Q_0 \\ &\quad = \sum_{a,b>0} b f(ab^{-1})\, \mathrm{Tr}\, P_a Q_b + f(0^+)\, \mathrm{Tr}(I - \varrho^0)\sigma + f'(+\infty)\, \mathrm{Tr}\, \varrho(I - \sigma^0), \end{aligned}$$

giving (3.10) and (3.12). The equality of (3.10) and (3.11) is trivial. ∎

Remark 3.3. Note that the expression in (3.11) is the classical f-divergence [18] of the functions $p(a,b) := a\, \mathrm{Tr}\, P_a Q_b$ and $q(a,b) := b\, \mathrm{Tr}\, P_a Q_b$, defined on $(\mathrm{spec}\, \varrho) \times (\mathrm{spec}\, \sigma)$ (see [34] and [59] for further details).

Corollary 3.4. $S_f(\varrho\|\sigma) = +\infty$ if and only if one of the following conditions holds:

(i) $f(0^+) = +\infty$ and $\sigma^0 \not\leq \varrho^0$;

(ii) $f'(+\infty) = +\infty$ and $\varrho^0 \not\leq \sigma^0$.

In all other cases, $S_f(\varrho\|\sigma)$ is a finite number.

Example 3.5. The most relevant examples for applications are given by

$$f_\alpha(x) := s(\alpha)x^\alpha \quad \text{for} \quad \alpha \in (0, +\infty), \qquad \text{and} \qquad \eta(x) := x\log x, \qquad x \geq 0,$$

where $s(\alpha) := -1$ for $0 < \alpha < 1$ and $s(\alpha) := 1$ for $\alpha \geq 1$. They give rise to

$$S_{f_\alpha}(\varrho\|\sigma) = \begin{cases} s(\alpha)\operatorname{Tr}\varrho^\alpha\sigma^{1-\alpha}, & \alpha \in (0,1] \text{ or } \varrho^0 \leq \sigma^0, \\ +\infty, & \text{otherwise,} \end{cases}$$

$$S(\varrho\|\sigma) := S_\eta(\varrho\|\sigma) = \begin{cases} \operatorname{Tr}\varrho(\log\varrho - \log\sigma), & \varrho^0 \leq \sigma^0, \\ +\infty, & \text{otherwise,} \end{cases} \tag{3.13}$$

where $S(\varrho\|\sigma)$ is the *Umegaki relative entropy* [71]; see (1.1). The quantities S_{f_α} define the standard *Rényi divergences* as

$$D_\alpha(\varrho\|\sigma) := \frac{1}{\alpha-1}\log\bigl(s(\alpha)S_{f_\alpha}(\varrho\|\sigma)\bigr) - \frac{1}{\alpha-1}\log\operatorname{Tr}\varrho, \qquad \alpha \in (0,+\infty)\setminus\{1\}; \tag{3.14}$$

see (1.2). It is easy to see (by simply computing its second derivative) that $\alpha \mapsto \log\left(s(\alpha)S_{f_\alpha}(\varrho\|\sigma)\right)$ is convex, and hence $\alpha \mapsto D_\alpha(\varrho\|\sigma)$ is increasing for any fixed ϱ, σ; moreover,

$$\lim_{\alpha\to1} D_\alpha(\varrho\|\sigma) = \sup_{\alpha\in(0,1)} D_\alpha(\varrho\|\sigma) = \frac{1}{\operatorname{Tr}\varrho} S(\varrho\|\sigma). \tag{3.15}$$

(Although the function f_α is operator convex on $[0,\infty)$ only for $0 < \alpha \leq 2$, we shall use S_{f_α} for all $\alpha > 0$. See also Example 4.5 below.)

Remark 3.6. In [34], we assumed that f is defined on $[0,+\infty)$, and we defined $S_f(\varrho\|\sigma)$ first for an invertible σ as in (3.8), and extended to non-invertible σ as $S_f(\varrho\|\sigma) := \lim_{\varepsilon\searrow0} S_f(\varrho\|\sigma+\varepsilon I)$, which is slightly different from the above (3.9). However, when $f(0^+) < +\infty$ so that f can be extended to a continuous function on $[0,+\infty)$, we see by expression (3.12) that the present definition is the same as that in [34, Definition 2.1]. The extension of $S_f(\varrho\|\sigma)$ to functions f without the assumption $f(0^+) < +\infty$ is relevant, for instance, to the following symmetry property.

Proposition 3.7. Let $\widetilde{f}$ be the transpose of f. Then for every $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$,

$$S_{\widetilde{f}}(\varrho\|\sigma) = S_f(\sigma\|\varrho).$$

Proof. The assertion follows immediately from expression (3.12) together with (2.6), since $b\widetilde{f}(ab^{-1}) = af(ba^{-1})$ for $a, b > 0$. □

The next proposition shows that the continuity property that is incorporated in definition (3.9) can be extended to the case where the perturbation is not a constant multiple of the identity, but an arbitrary positive operator. This becomes important, for instance, when one studies the behavior of the f-divergences under the action of stochastic maps, in which case one might need to evaluate expressions like

$$\lim_{\varepsilon\searrow0} S_f\left(\Phi(\varrho+\varepsilon I)\|\Phi(\sigma+\varepsilon I)\right) = \lim_{\varepsilon\searrow0} S_f\left(\Phi(\varrho)+\varepsilon\Phi(I)\|\Phi(\sigma)+\varepsilon\Phi(I)\right),$$

which does not reduce to (3.9) unless Φ is unital.

Proposition 3.8. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$.

(i) Assume that both $f(0^+)$ and $f'(+\infty)$ are finite. Then

$$S_f(\varrho\|\sigma) = \lim_{n\to\infty} S_f(\varrho_n\|\sigma_n)$$

for any choice of sequences $\varrho_n, \sigma_n \in \mathcal{B}(\mathcal{H})_+$ such that $\varrho_n \to \varrho, \sigma_n \to 0$ as $n \to +\infty$.

(ii) Let f be an operator convex function on $(0, +\infty)$ (with no restriction on $f(0^+)$ and $f'(+\infty)$). Then

$$S_f(\varrho\|\sigma) = \lim_{n\to\infty} S_f(\varrho + L_n\|\sigma + L_n)$$

for any choice of a sequence $L_n \in \mathcal{B}(\mathcal{H})_+$ such that $\varrho + L_n, \sigma + L_n > 0$ for every n, and $L_n \to 0$ as $n \to +\infty$.

We give the proof of the above proposition, and further observations about the continuity properties of the standard f-divergences, in Appendix D. We remark that in the proof of (ii) of the above proposition, we will use the joint convexity property given in Proposition 3.10 below.

Remark 3.9. Note that (i) of the above proposition can be reformulated as follows: When f is a continuous function on $(0, +\infty)$ such that both $f(0^+)$ and $f'(+\infty)$ are finite, then

$$(\varrho, \sigma) \mapsto S_f(\varrho\|\sigma) \quad \text{is continuous on} \quad \mathcal{B}(\mathcal{H})_+ \times \mathcal{B}(\mathcal{H})_+.$$

The most important properties of f-divergences are their joint convexity and monotonicity under stochastic maps when f is operator convex. These properties follow immediately from the results of [63, 34], even though our definition of f-divergences in this paper is slightly more general than in [63, 34].

Proposition 3.10. Let $f : (0, +\infty) \to \mathbb{R}$ be operator convex. $S_f(\varrho\|\sigma)$ is jointly convex in $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, i.e., for every $\varrho_i, \sigma_i \in \mathcal{B}(\mathcal{H})_+$ and $\lambda_i \geq 0$ for $1 \leq i \leq k$,

$$S_f\left(\sum_{i=1}^k \lambda_i \varrho_i \middle\| \sum_{i=1}^k \lambda_i \sigma_i\right) \leq \sum_{i=1}^k \lambda_i S_f(\varrho_i\|\sigma_i). \tag{3.16}$$

Proof. Immediate from [34, Corollary 4.7] and definition (3.9). □

Remark 3.11. It is clear from (3.12) that the f-divergences have the homogeneity property

$$S_f(\lambda\varrho\|\lambda\sigma) = \lambda S_f(\varrho\|\sigma), \qquad \lambda \geq 0, \quad \varrho, \sigma \in \mathcal{B}(\mathcal{H})_+.$$

Hence, (3.16) is equivalent to the joint subadditivity

$$S_f\left(\sum_{i=1}^k \varrho_i \middle\| \sum_{i=1}^k \sigma_i\right) \leq \sum_{i=1}^k S_f(\varrho_i\|\sigma_i).$$

In particular, it is not necessary that the λ_i's sum up to 1 in (3.16).

The monotonicity property of f-divergences, first shown by Petz [63] in a somewhat restricted setting, was later extended in various ways, e.g., in [48, 70, 34]. The following is an easy adaptation of [34, Theorem 4.3] to the present setting.

Proposition 3.12. Let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a trace-preserving linear map such that the adjoint Φ^* is a Schwarz contraction (see Section 2.5). Then for every $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, and every operator convex function $f : (0, +\infty) \to \mathbb{R}$,

$$S_f(\Phi(\varrho)\|\Phi(\sigma)) \le S_f(\varrho\|\sigma). \tag{3.17}$$

Proof. For $\varepsilon > 0$ let $f_\varepsilon(x) := f(x+\varepsilon)$, $x \ge 0$. By [34, Theorem 4.3] one has

$$S_{f_\varepsilon}(\Phi(\varrho)\|\Phi(\sigma)) \le S_{f_\varepsilon}(\varrho\|\sigma).$$

Thanks to expression (3.12) it is straightforward to see that

$$\lim_{\varepsilon\searrow 0} S_{f_\varepsilon}(\varrho\|\sigma) = S_f(\varrho\|\sigma),$$

and similarly $\lim_{\varepsilon\searrow 0} S_{f_\varepsilon}(\Phi(\varrho)\|\Phi(\sigma)) = S_f(\Phi(\varrho)\|\Phi(\sigma))$, so the assertion follows. ☐

Remark 3.13. As observed in [48] (more explicitly, in [70, Appendix A] and [37, Proposition E.2]), it is known that for a general continuous function f on $(0, +\infty)$, the f-divergence S_f has the joint convexity property in Proposition 3.10 if and only if it has the monotonicity property under CPTP maps. Indeed, this fact holds true for different types of quantum divergences; for example, the proof of the monotonicity under CPTP maps for $D_{\alpha,z}$ given in (1.4) can be reduced to that of the joint convexity/concavity of $(\varrho, \sigma) \mapsto \operatorname{Tr}(\sigma^{\frac{1-\alpha}{2z}}\varrho^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}})^z$ (see [24, 6]).

Remark 3.14. It is not known whether in Proposition 3.12, the assumption that Φ^* is a Schwarz contraction can be weakened to simply requiring that Φ is positive. A non-trivial example is when $f(x) := f_2(x) := x^2$, giving the f-divergence $S_{f_2}(\varrho\|\sigma) = \operatorname{Tr}\varrho^2\sigma^{-1}$. Monotonicity of this f-divergence under trace-preserving positive maps is a consequence of a stronger operator inequality (see, e.g., [34, Lemma 3.5]). Alternatively, this follows from the more general statement in Corollary 3.31, by noting that $S_{f_2} = \widehat{S}_{f_2}$ (see Example 4.2). More importantly, it has been pointed out recently in [55] that Beigi's proof for the monotonicity of the sandwiched Rényi divergences [8] yields that the Umegaki relative entropy (3.13) is monotone under trace-preserving positive maps.

As with any inequality, it is natural to ask when (3.17) holds with equality. This problem was first addressed by Petz, who considered it in the more general von Neumann algebraic framework [65]. When translated to our finite-dimensional setting, his result, given in [65, Theorem 3], says that for a 2-positive and trace-preserving $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$, and $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_{++}$,

$$S_{f_{1/2}}(\Phi(\varrho)\|\Phi(\sigma)) = S_{f_{1/2}}(\varrho\|\sigma) \iff \Phi^*_\sigma(\Phi(\varrho)) = \varrho, \tag{3.18}$$

where $f_{1/2}(x) := -x^{1/2}$ with the corresponding f-divergence $S_{f_{1/2}}(\varrho\|\sigma) = -\operatorname{Tr}\varrho^{1/2}\sigma^{1/2}$, and Φ^*_σ is the adjoint of the map $\Phi_\sigma : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ defined by

$$\Phi_\sigma(X) = \Phi(\sigma)^{-1/2}\Phi\left(\sigma^{1/2}X\sigma^{1/2}\right)\Phi(\sigma)^{-1/2}, \qquad X \in \mathcal{B}(\mathcal{H}). \tag{3.19}$$

More explicitly, $\Phi^*_\sigma : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ is given as

$$\Phi^*_\sigma(Y) := \sigma^{1/2}\Phi^*\left(\Phi(\sigma)^{-1/2}Y\Phi(\sigma)^{-1/2}\right)\sigma^{1/2}, \qquad Y \in \mathcal{B}(\mathcal{K}). \tag{3.20}$$

Since it is easy to check that $\Phi_\sigma^*(\Phi(\sigma)) = \sigma$, the second condition in (3.18) yields the reversibility of Φ in the sense defined below, while reversibility implies the first condition in (3.18) by a double application of the monotonicity inequality (3.17).

By comparing (iii) of [65, Theorem 3] with (i) of [67, Theorem 3.1], one sees that the conditions in (3.18) are further equivalent to the preservation of the Umegaki relative entropy

$$S(\Phi(\varrho)\|\Phi(\sigma)) = S(\varrho\|\sigma).$$

Moreover, it was stated in [43, Theorem 2] (albeit with an incorrect formulation and without a proof) that (3.18) is also equivalent to the preservation of the f_α-divergences for $0 < \alpha < 1$, where $f_\alpha(x) := x^\alpha$.

Remark 3.15. The notation of [65, 42, 43] corresponds to ours as

$$\phi(\cdot) = \operatorname{Tr}\varrho(\cdot), \qquad \omega(\cdot) = \operatorname{Tr}\sigma(\cdot), \qquad \alpha = \Phi^*, \qquad \alpha_\omega^* = \Phi_\sigma,$$

where the first expressions are always from [65], and the second expressions are our notations. We remark that (v) and (vi) of [65, Theorem 3] are incorrectly stated as $\phi \circ \alpha_\omega^* = \phi$ and $\omega \circ \alpha_\phi^* = \omega$, respectively; they should be $\phi \circ \alpha \circ \alpha_\omega^* = \phi$ and $\omega \circ \alpha \circ \alpha_\phi^* = \omega$. This correction was given, e.g., in [42, Theorem 3].

Definition 3.16. Let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a trace-preserving positive linear map and $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$. We say that Φ is *reversible* on the pair ϱ, σ if there exists a trace-preserving positive linear map $\Psi : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ such that

$$\Psi(\Phi(\varrho)) = \varrho, \qquad \Psi(\Phi(\sigma)) = \sigma.$$

Remark 3.17. (1) Note that we only assume positivity of the reverse map Ψ in the above definition, irrespective of the type of positivity of the map Φ. The reason for this becomes clear from (i) $\Longleftrightarrow$ (ii) $\Longleftrightarrow$ (iii) in Theorem 3.18, where we see that the reversibility condition for Φ on the pair ϱ, σ is independent of the choice of the type of positivity for the reverse map; the reversibility conditions with a simply positive reverse map and with a completely positive one are equivalent.

(2) Note that the right-hand side of (3.18) states reversibility with the reverse map Φ_σ^*, except that Φ_σ^* is not necessarily trace-preserving on the whole $\mathcal{B}(\mathcal{K})$. However, its restriction to $\Phi(\sigma)^0\mathcal{B}(\mathcal{K})\Phi(\sigma)^0 = \mathcal{B}(\Phi(\sigma)^0\mathcal{K})$ is trace-preserving, since Φ_σ is unital as a map from $\mathcal{B}(\mathcal{H})$ to $\mathcal{B}(\Phi(\sigma)^0\mathcal{K})$, and it is easy to extend $\Phi_\sigma^*|_{\Phi(\sigma)^0\mathcal{B}(\mathcal{K})\Phi(\sigma)^0}$ to a trace-preserving map on $\mathcal{B}(\mathcal{K})$. We will benefit from this observation in the proof of (ii) $\Longrightarrow$ (iii) of Theorem 3.18.

(3) It is easy to see that if Φ is n-positive for some $n \in \mathbb{N}$ then so is Φ_σ^*. However, if Φ^* is a Schwarz contraction, that need not imply that Φ_σ is a Schwarz contraction, as was pointed out in [40, Proposition 2].

A systematic study of the relation between reversibility and the preservation of f-divergences was carried out in [34], complemented later in [40] with some further results. We summarize these results and give some slight extensions and modifications in the following theorem.

Theorem 3.18. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ be such that $\varrho^0 \le \sigma^0$, and let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a 2-positive trace-preserving linear map. Then the following (i)–(ix) are equivalent:

(i) Φ is reversible on $\{\varrho, \sigma\}$ in the sense of Definition 3.16, i.e., there exists a trace-preserving positive map $\Psi : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ such that $\Psi(\Phi(\varrho)) = \varrho$, $\Psi(\Phi(\sigma)) = \sigma$.

(ii) There exists a trace-preserving map $\Psi : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ such that Ψ^* satisfies the Schwarz inequality and $\Psi(\Phi(\varrho)) = \varrho$, $\Psi(\Phi(\sigma)) = \sigma$.

(iii) There exist CPTP maps $\widetilde{\Phi} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ and $\widetilde{\Psi} : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ such that $\widetilde{\Phi}(\varrho) = \Phi(\varrho)$, $\widetilde{\Phi}(\sigma) = \Phi(\sigma)$ and $\widetilde{\Psi}(\Phi(\varrho)) = \varrho$, $\widetilde{\Psi}(\Phi(\sigma)) = \sigma$.

(iv) $S_f(\Phi(\varrho)\|\Phi(\sigma)) = S_f(\varrho\|\sigma)$ for some operator convex function f on $(0, +\infty)$ such that $f(0^+) < +\infty$ and

$$|\operatorname{supp}\mu_f| \ge \big|\operatorname{spec}\big(L_\varrho R_{\sigma^{-1}}\big) \cup \operatorname{spec}\big(L_{\Phi(\varrho)} R_{\Phi(\sigma)^{-1}}\big)\big|, \tag{3.21}$$

where μ_f is the measure from the integral representation given in (2.3).

(v) $S_f(\Phi(\varrho)\|\Phi(\sigma)) = S_f(\varrho\|\sigma)$ for all operator convex functions f on $[0, +\infty)$.

(vi) $\sigma^0\Phi^*(\Phi(\sigma)^{-z}\Phi(\varrho)^{2z}\Phi(\sigma)^{-z})\sigma^0 = \sigma^{-z}\varrho^{2z}\sigma^{-z}$ for all $z \in \mathbb{C}$.

(vii) $\sigma^0\Phi^*(\Phi(\sigma)^{-1/2}\Phi(\varrho)\Phi(\sigma)^{-1/2})\sigma^0 = \sigma^{-1/2}\varrho\sigma^{-1/2}$.

(viii) $\Phi_\sigma^*(\Phi(\varrho)) = \varrho$ (and also $\Phi_\sigma^*(\Phi(\sigma)) = \sigma$ automatically).

(ix) $\sigma^{-1/2}\varrho\sigma^{-1/2} \in \mathcal{F}_{\Phi^*\circ\Phi_\sigma}$, the set of fixed points of $\Phi^* \circ \Phi_\sigma$.

Moreover, when we assume in addition that ϱ, σ are density operators with invertible σ, the above (i)–(ix) are also equivalent to

(x) $\big\langle \Phi(\varrho - \sigma), \Omega^\kappa_{\Phi(\sigma)}(\Phi(\varrho - \sigma))\big\rangle_{\mathrm{HS}} = \langle \varrho - \sigma, \Omega^\kappa_\sigma(\varrho - \sigma)\rangle_{\mathrm{HS}}$ for some operator decreasing function $\kappa : (0, +\infty) \to (0, +\infty)$ such that

$$|\operatorname{supp}\nu_\kappa| \ge \big|\operatorname{spec}(L_\sigma R_{\sigma^{-1}}) \cup \operatorname{spec}\big(L_{\Phi(\sigma)} R_{\Phi(\sigma)^{-1}}\big)\big|,$$

where Ω^κ_σ is given in (2.11) and ν_κ is the measure from the integral expression in (2.10).

Proof. The equivalence of (ii), (iv), (v), and (viii) is in [34, Theorem 5.1], and (iii) $\Longrightarrow$ (ii) $\Longrightarrow$ (i) is trivial. By Remark 3.14, (i) yields that

$$S(\varrho\|\sigma) = S(\Psi(\Phi(\varrho))\|\Psi(\Phi(\varrho))) \le S(\Phi(\varrho)\|\Phi(\sigma)) \le S(\varrho\|\sigma)$$

for $S = S_\eta$ with $\eta(x) := x \log x$. Since

$$x \log x = \int_{(0,+\infty)} \left(\frac{x}{1+s} - \frac{x}{x+s}\right) ds,$$

we see that μ_f is the Lebesgue measure on $(0, +\infty)$, and hence (i) $\Longrightarrow$ (iv) follows.

Next assume that (ii) holds, and consider the maps $\Phi_0 : \mathcal{B}(\sigma^0\mathcal{H}) = \sigma^0\mathcal{B}(\mathcal{H})\sigma^0 \to \mathcal{B}(\Phi(\sigma)^0\mathcal{K}) = \Phi(\sigma)^0\mathcal{B}(\mathcal{K})\Phi(\sigma)^0$ and $\Psi_0 : \mathcal{B}(\Phi(\sigma)^0\mathcal{K}) \to \mathcal{B}(\sigma^0\mathcal{H})$ given by

$$\Phi_0 := \Phi|_{\sigma^0\mathcal{B}(\mathcal{H})\sigma^0}, \qquad \Psi_0(Y) := \sigma^0\Psi(Y)\sigma^0, \quad Y \in \Phi(\sigma)^0\mathcal{B}(\mathcal{K})\Phi(\sigma)^0.$$

Then it is easy to see that $(\Phi_0)^*$ and $(\Phi_0)_\sigma$ are unital 2-positive maps, and hence Schwarz contractions, and $(\Psi_0)^*$ is a Schwarz contraction; moreover, (ii) is satisfied for $(\Phi_0, \varrho, \sigma, \Psi_0)$ in place of $(\Phi, \varrho, \sigma, \Psi)$. Hence we can use [40, Theorem 4] to conclude that there exist CPTP maps $\widetilde{\Phi}_0 : \mathcal{B}(\sigma^0\mathcal{K}) \to \mathcal{B}(\Phi(\sigma)^0\mathcal{K})$ and $\widetilde{\Psi}_0 : \mathcal{B}(\Phi(\sigma)^0\mathcal{K}) \to \mathcal{B}(\sigma^0\mathcal{K})$ such that $\widetilde{\Phi}_0(\varrho) = \Phi(\varrho)$, $\widetilde{\Phi}_0(\sigma) = \Phi(\sigma)$ and $\widetilde{\Psi}_0(\Phi_0(\varrho)) = \varrho$, $\widetilde{\Psi}_0(\Phi_0(\sigma)) = \sigma$. Define CPTP maps $\widetilde{\Phi} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ and $\widetilde{\Psi} : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ by

$$\widetilde{\Phi}(X) := \widetilde{\Phi}_0(\sigma^0 X \sigma^0) + |\psi_\mathcal{K}\rangle\langle\psi_\mathcal{K}| \cdot \operatorname{Tr}(I - \sigma^0)X, \qquad X \in \mathcal{B}(\mathcal{H}),$$

$$\widetilde{\Psi}(Y) := \widetilde{\Psi}_0(\Phi(\sigma)^0 Y \Phi(\sigma)^0) + |\psi_{\mathcal{H}}\rangle\langle\psi_{\mathcal{H}}| \cdot \mathrm{Tr}(I - \Phi(\sigma)^0)Y, \qquad Y \in \mathcal{B}(\mathcal{K}),$$

where $\psi_{\mathcal{H}} \in \mathcal{H}$, $\psi_{\mathcal{K}} \in \mathcal{K}$ are unit vectors. Then (iii) holds for $\widetilde{\Phi}$ and $\widetilde{\Psi}$.

It was shown in [34, Theorem 5.1] that (iv) implies

$$\sigma^0 \Phi^* \left(\Phi(\sigma)^{-z}\Phi(\varrho)^z\right) = \sigma^{-z}\varrho^z, \qquad z \in \mathbb{C}, \tag{3.22}$$

which is condition (vi) of [34, Theorem 5.1]. The proof of (vi) $\Longrightarrow$ (x) in p. 719 of [34] shows that this implies

$$\sigma^0 \Phi^* \left(\Phi(\sigma)^{-z}\Phi(\varrho)^z Y\right)\sigma^0 = \sigma^{-z}\varrho^z \Phi^*(Y)\sigma^0$$

for any $Y \in \mathcal{B}(\mathcal{K})$ and any $z \in \mathbb{C}$. Hence we get (vi) by choosing $Y := \Phi(\varrho)^z\Phi(\sigma)^{-z}$ and using

$$\Phi^* \left(\Phi(\varrho)^z\Phi(\sigma)^{-z}\right)\sigma^0 = \varrho^z\sigma^{-z}, \qquad z \in \mathbb{C},$$

which follows by taking the adjoint of both sides in (3.22). The implication (vi) $\Longrightarrow$ (vii) is trivial. Even when Φ is only assumed to be positive, the equivalence (vii) $\Longleftrightarrow$ (viii) is a matter of straightforward computation. Thus, it has been shown that (i)–(viii) are all equivalent.

It is clear that (ix) implies (vii), and it is easily verified by using Theorem 3.19 that (viii) implies (ix). Finally, under the restriction of ϱ, σ to density operators, the equivalence (ii) $\Longleftrightarrow$ (x) was given in [40, Proposition 4]. $\square$

Note that when σ is invertible, the equivalences (vii) $\Longleftrightarrow$ (viii) $\Longleftrightarrow$ (ix) hold even when Φ is only assumed to be positive.

Assume that $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ is 2-positive and trace-preserving and $\sigma \in \mathcal{B}(\mathcal{H})_+$. By the above theorem we have

$$\begin{aligned}
&\left\{\varrho \in \mathcal{B}(\mathcal{H})_+ : \varrho^0 \le \sigma^0 \text{ and } S_f(\Phi(\varrho)\|\Phi(\sigma)) = S_f(\varrho\|\sigma) \text{ for all operator convex } f : (0,+\infty) \to \mathbb{R}\right\} \\
&\quad = \left\{\varrho \in \mathcal{B}(\mathcal{H})_+ : \varrho^0 \le \sigma^0 \text{ and } \Phi \text{ is reversible on } \{\varrho, \sigma\}\right\} \\
&\quad = \mathcal{F}_{\Phi_\sigma^* \circ \Phi}.
\end{aligned}$$

In the above proof, we have used the following characterization of $\mathcal{F}_{\Phi_\sigma^* \circ \Phi}$, due to [34, 42, 51, 54]:

Theorem 3.19. Let $\Phi : \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{H}_2)$ be a 2-positive trace-preserving map, let $\sigma_1 := \sigma \in \mathcal{B}(\mathcal{H}_1)_+ \setminus \{0\}$, and $\sigma_2 := \Phi(\sigma)$. Then there exist decompositions $\operatorname{supp}\sigma_m = \bigoplus_{k=1}^r \mathcal{H}_{m,k,L} \otimes \mathcal{H}_{m,k,R}$, $m = 1, 2$, invertible density operators ω_k on $\mathcal{H}_{1,k,R}$, unitaries $U_k : \mathcal{H}_{1,k,L} \to \mathcal{H}_{2,k,L}$, and 2-positive trace-preserving maps $\eta_k : \mathcal{B}(\mathcal{H}_{1,k,R}) \to \mathcal{B}(\mathcal{H}_{2,k,R})$ such that ω_k is invertible on $\mathcal{H}_{1,k,R}$, $\eta_k(\omega_k)$ is invertible on $\mathcal{H}_{2,k,R}$, and

$$\mathcal{F}_{\Phi^* \circ \Phi_\sigma} = \bigoplus_{k=1}^r \mathcal{B}(\mathcal{H}_{1,k,L}) \otimes I_{1,k,R}, \tag{3.23}$$

$$\mathcal{F}_{\Phi_\sigma \circ \Phi^*} = \bigoplus_{k=1}^r \mathcal{B}(\mathcal{H}_{2,k,L}) \otimes I_{2,k,R}, \tag{3.24}$$

$$(\mathcal{F}_{\Phi_\sigma^* \circ \Phi})_+ = \bigoplus_{k=1}^r \mathcal{B}(\mathcal{H}_{1,k,L})_+ \otimes \omega_k, \tag{3.25}$$

$$\Phi(\varrho_{1,k,L} \otimes \varrho_{1,k,R}) = U_k \varrho_{1,k,L} U_k^* \otimes \eta_k(\varrho_{1,k,R}), \tag{3.26}$$

$$\sigma^0 \Phi^*(\varrho_{2,k,L} \otimes \varrho_{2,k,R})\sigma^0 = U_k^* \varrho_{2,k,L} U_k \otimes \eta_k^*(\varrho_{2,k,R}), \tag{3.27}$$

for all $\varrho_{m,k,L} \in \mathcal{B}(\mathcal{H}_{m,k,L})$, $\varrho_{m,k,R} \in \mathcal{B}(\mathcal{H}_{m,k,R})$.

Remark 3.20. Note that the reversibility conditions (i)–(iii) in Theorem 3.18 are symmetric in ϱ and σ, while the rest of the equivalent characterizations of reversibility are not. To understand this, one should first note that deriving reversibility from the preservation of some f-divergence S_f (i.e., the implication (iv)$\Longrightarrow$(i)) may only be possible if $S_f(\varrho\|\sigma) < +\infty$, and the assumptions $\varrho^0 \le \sigma^0$ and $f(0^+) < +\infty$ guarantee this (see Corollary 3.4). If we assumed instead that $\sigma^0 \le \varrho^0$ and $f'(+\infty) < +\infty$ then (iv)$\Longrightarrow$(i) would still hold; the proof of this can be reduced to the one with the original conditions, by using Proposition 3.7 and noting that $|\operatorname{supp}\mu_{\widetilde{f}}| = |\operatorname{supp}\mu_f|$. Of course, in this case ϱ and σ have to be interchanged in points (vi)–(x).

There are two more ways to guarantee that $S_f(\varrho\|\sigma) < +\infty$. One is to assume that $\varrho^0 = \sigma^0$; it is easy to see that in this case we have the implication (iv)$\Longrightarrow$(i) even if we do not assume that $f(0^+) < +\infty$ or $f'(+\infty) < +\infty$; one only has to note that in this case $\operatorname{supp}\mu_f$ in (iv) has to be replaced with $(\operatorname{supp}\lambda)\cap(0,+\infty)$, with λ from (2.2). On the other hand, we do not know whether (i) follows from (iv) if we assume that both $f(0^+) < +\infty$ and $f'(+\infty) < +\infty$, but we do not require any relation between the supports of ϱ and σ.

3.3 Maximal f-divergences

In this section we consider in detail the quantum f-divergence introduced in (3.3). This version of f-divergences was formerly treated in [68], and more recently it was studied in much detail by Matsumoto [50]. While Matsumoto's definition, referred to as the *maximal f-divergence*, is rather different from that given here, it was shown in [50, Lemma 4 and Theorem 5] that the two definitions coincide when $\varrho^0 \le \sigma^0$. Since our starting point here is the operator perspective function, we will use the notation $\widehat{S}_f$ for this family of f-divegences, as in (3.3), instead of the more operationally motivated notation $S_f^{\max}$ in (3.5).

In this section we will always assume that f is operator convex on $(0,+\infty)$. This is primarily to make sense of definition (3.29); see Remark 3.23.

Definition 3.21. For invertible $\varrho,\sigma \in \mathcal{B}(\mathcal{H})_+$ define

$$\begin{aligned}\widehat{S}_f(\varrho\|\sigma) &:= \operatorname{Tr} P_f(\varrho,\sigma)\\ &= \operatorname{Tr}\sigma f(\sigma^{-1/2}\varrho\sigma^{-1/2}) = \langle \sigma^{1/2}, f(\sigma^{-1/2}\varrho\sigma^{-1/2})\sigma^{1/2}\rangle_{\mathrm{HS}}.\end{aligned} \tag{3.28}$$

For general $\varrho,\sigma \in \mathcal{B}(\mathcal{H})_+$ let

$$\widehat{S}_f(\varrho\|\sigma) := \lim_{\varepsilon\searrow 0}\widehat{S}_f(\varrho+\varepsilon I\|\sigma+\varepsilon I). \tag{3.29}$$

Proposition 3.22.

(1) For every $\varrho,\sigma \in \mathcal{B}(\mathcal{H})_+$ the limit in (3.29) exists in $(-\infty,+\infty]$, and it is equal to (3.28) for invertible ϱ,σ.

(2) $\widehat{S}_f(\varrho\|\sigma)$ is jointly convex in $\varrho,\sigma \in \mathcal{B}(\mathcal{H})_+$.

(3) For every $\varrho,\sigma \in \mathcal{B}(\mathcal{H})_+$,

$$\widehat{S}_{\widetilde{f}}(\varrho\|\sigma) = \widehat{S}_f(\sigma\|\varrho).$$

Proof. The joint convexity of $(\varrho,\sigma) \mapsto \widehat{S}_f(\varrho\|\sigma)$ on $\mathcal{B}(\mathcal{H})_{++} \times \mathcal{B}(\mathcal{H})_{++}$ follows from that of the perspective function P_f given in Lemma 2.2 (1). In particular, for every $\varrho,\sigma \in \mathcal{B}(\mathcal{H})_+$ the real function $t \mapsto \widehat{S}_f(\varrho+tI\|\sigma+tI)$ is convex on $(0,+\infty)$, which implies the existence of the limit in (3.29), and that it is in $(-\infty, +\infty]$. The last claim of (1) for invertible ϱ, σ is obvious, and (2) is immediate from definition (3.29) and joint convexity on $\mathcal{B}(\mathcal{H})_{++} \times \mathcal{B}(\mathcal{H})_{++}$. For (3), applying Lemma 2.1 to $\varrho_\varepsilon := \varrho + \varepsilon I$, $\sigma_\varepsilon := \sigma + \varepsilon I$, $\varepsilon > 0$, taking the trace, and then the limit as $\varepsilon \searrow 0$, we get the assertion by (3.29). □

Remark 3.23. By Proposition A.1 note that the operator convexity of f is a necessary and sufficient condition for the joint convexity property of $\widehat{S}_f$ as stated in (2) above. Although the details are not given here, we know that the joint convexity of S_f (equivalent to the monotonicity under CPTP maps, see Remark 3.11) implies the operator convexity of f, whenever f is symmetric (i.e., $f = \widetilde{f}$) or both $f(0^+)$ and $f'(+\infty)$ are finite. However, it is still open whether this is true for a general function f on $(0, +\infty)$.

Since $\widehat{S}_f$ arises as the trace of the operator perspective function P_f, properties of the former can easily follow from those of the latter. From this point, it is natural to study the properties of P_f in further detail. Below, we investigate to what extent the formula $\widehat{S}_f(\varrho, \sigma) = \operatorname{Tr} P_f(\varrho, \sigma)$ can be extended to not necessarily invertible ϱ and σ. For this, we have to investigate whether the perspective function can be extended to not necessarily invertible operators. Note that this is not always possible in a natural way, as the following trivial example shows:

Example 3.24. Let e_1, e_2 be the canonical basis of $\mathbb{C}^2$, and $\varrho := |e_1\rangle\langle e_1|$, $\sigma := |e_2\rangle\langle e_2|$.

(1) Let $f(x) := x^2$, which is operator convex with $f(0) = 0$ and $f'(+\infty) = +\infty$. Then $\lim_{\varepsilon \searrow 0} \langle e_1, P_f(\varrho + \varepsilon I, \sigma + \varepsilon I)e_1\rangle = \lim_{\varepsilon \searrow 0}(1 + \varepsilon)^2/\varepsilon = +\infty$, and hence $\varepsilon \mapsto P_f(\varrho + \varepsilon I, \sigma + \varepsilon I)$ does not have a limit as $\varepsilon \searrow 0$.

(2) Let $f(x) := 1/x$, which is operator convex with $f'(+\infty) = 0$ and $f(0^+) = +\infty$. Then $\lim_{\varepsilon \searrow 0} \langle e_2, P_f(\varrho + \varepsilon I, \sigma + \varepsilon I)e_2\rangle = \lim_{\varepsilon \searrow 0}(1 + \varepsilon)^2/\varepsilon = +\infty$, and hence $\varepsilon \mapsto P_f(\varrho + \varepsilon I, \sigma + \varepsilon I)$ does not have a limit as $\varepsilon \searrow 0$.

Proposition 3.25. Let $\varrho, \sigma, \varrho_n, \sigma_n \in \mathcal{B}(\mathcal{H})_+$, $n \in \mathbb{N}$, be such that $\lim_n \varrho_n = \varrho$ and $\lim_n \sigma_n = \sigma$. In the cases below, the limit $\lim_{n\to\infty} P_f(\varrho_n, \sigma_n)$ exists, independently of the choice of ϱ_n, σ_n, and it coincides with $P_f(\varrho, \sigma)$ when both ϱ and σ are invertible.

(i) If $f(0^+) < +\infty$, $f'(+\infty) < +\infty$, $\varrho \le \varrho_n$ and $\sigma \le \sigma_n$, then

$$\lim_{n\to\infty} P_f(\varrho_n, \sigma_n) = f(0)\sigma + f'(+\infty)\varrho - \sigma\, \tau_{h_f}\, \varrho,$$

where a non-negative operator monotone function h_f on $[0, +\infty)$ is given by $h_f(x) := \int_{(0,+\infty)} x(1 + s)(x + s)^{-1}\, d\nu(s)$, $x \ge 0$, with ν the representing measure from (2.4).

(ii) If $f(0^+) < +\infty$ and $\sigma > 0$, then

$$\lim_{n\to\infty} P_f(\varrho_n, \sigma_n) = \sigma^{1/2} f\left(\sigma^{-1/2}\varrho\sigma^{-1/2}\right)\sigma^{1/2}. \tag{3.30}$$

(iii) If $f'(+\infty) < +\infty$ and $\varrho > 0$, then

$$\lim_{n\to\infty} P_f(\varrho_n, \sigma_n) = \varrho^{1/2} \widetilde{f}\left(\varrho^{-1/2}\sigma\varrho^{-1/2}\right)\varrho^{1/2},$$

where $\widetilde{f}(x) := x f(x^{-1})$ is the transpose of f.

Proof. (i) By (2.4), $f(x) = f(0)+f'(+\infty)x-h_f(x)$, $x \in (0,+\infty)$, where h_f is a non-negative operator monotone function, and hence the assertion is immediate from Lemma 2.3.

(ii) By the assumption, f extends to a continuous function on $[0,+\infty)$, and thus (3.30) follows from the continuity of functional calculus.

(iii) By Lemma 2.1, we have $P_f(\varrho_n,\sigma_n) = P_{\widetilde{f}}(\sigma_n,\varrho_n) = \varrho_n^{1/2}\widetilde{f}\left(\varrho_n^{-1/2}\sigma_n\varrho_n^{-1/2}\right)\varrho_n^{1/2}$ for every $n \in \mathbb{N}$. Since $f'(+\infty) = \widetilde{f}(0^+)$, the assumption implies that $\widetilde{f}$ extends to a continuous function on $[0,+\infty)$, and hence the assertion follows as in (ii). □

For applications, the assumptions $\sigma > 0$ in (ii) and $\varrho > 0$ in (iii) are too restrictive. However, we have the following:

Proposition 3.26. Let $\varrho,\sigma \in \mathcal{B}(\mathcal{H})_+$, and for every $n \in \mathbb{N}$, let $K_n \geq 0$ be such that $\varrho + K_n > 0$, $\sigma + K_n > 0$, and $K_n \to 0$.

(i) If $f(0^+) < +\infty$ and $\varrho^0 \leq \sigma^0$, then

$$\lim_{n\to\infty} P_f(\varrho + K_n,\sigma + K_n) = \sigma^{1/2} f\left(\sigma^{-1/2}\varrho\sigma^{-1/2}\right)\sigma^{1/2}. \tag{3.31}$$

(ii) If $f'(+\infty) < +\infty$ and $\sigma^0 \leq \varrho^0$, then

$$\lim_{n\to\infty} P_f(\varrho + K_n,\sigma + K_n) = \varrho^{1/2} \widetilde{f}\left(\varrho^{-1/2}\sigma\varrho^{-1/2}\right)\varrho^{1/2}. \tag{3.32}$$

(iii) If $\varrho^0 = \sigma^0$ then both (3.31) and (3.32) hold.

Since the proof of the above proposition is rather lengthy, we defer it to Appendix E. Now, we can extend the definition of P_f to not necessarily invertible operators in the following way:

Definition 3.27. Let $\varrho,\sigma \in \mathcal{B}(\mathcal{H})_+$, and $f : (0,+\infty) \to \mathbb{R}$ be an operator convex function such that at least one of the following conditions is satisfied:

(i) $\varrho^0 = \sigma^0$,

(ii) $f(0^+) < +\infty$ and $f'(+\infty) < +\infty$,

(iii) $f(0^+) < +\infty$ and $\varrho^0 \leq \sigma^0$,

(iv) $f'(+\infty) < +\infty$ and $\sigma^0 \leq \varrho^0$.

Then, we define $P_f(\varrho,\sigma)$ as

$$P_f(\varrho,\sigma) := \lim_{n\to\infty} P_f(\varrho + K_n,\sigma + K_n),$$

where $K_n \in \mathcal{B}(\mathcal{H})_+$ is any sequence such that $\varrho + K_n, \sigma + K_n > 0$ for every n and $K_n \to 0$.

Corollary 3.28. If any of the conditions in Definition 3.27 holds, then we have

$$\widehat{S}_f(\varrho\|\sigma) = \operatorname{Tr} P_f(\varrho,\sigma).$$

In complete analogy with Corollary 3.4, we have the following:

Proposition 3.29. $\widehat{S}_f(\varrho\|\sigma) = +\infty$ if and only if one of the following conditions holds:

(i) $f(0^+) = +\infty$ and $\sigma^0 \nleq \varrho^0$;

(ii) $f'(+\infty) = +\infty$ and $\varrho^0 \not\leq \sigma^0$.

In all other cases, $\widehat{S}_f(\varrho\|\sigma)$ is a finite number.

Proof. Assume that $f'(+\infty) = +\infty$ and $\varrho^0 \not\leq \sigma^0$, so that there exists a unit vector ψ such that $\sigma^0\psi = 0$ and $\langle\psi, \varrho\psi\rangle > 0$. For all $\varepsilon > 0$,

$$\begin{aligned}
&\mathrm{Tr}(\sigma+\varepsilon I)^{1/2} f\left((\sigma+\varepsilon I)^{-1/2}(\varrho+\varepsilon I)(\sigma+\varepsilon I)^{-1/2}\right)(\sigma+\varepsilon I)^{1/2} \\
&\quad\geq \left\langle\psi, (\sigma+\varepsilon I)^{1/2} f\left((\sigma+\varepsilon I)^{-1/2}(\varrho+\varepsilon I)(\sigma+\varepsilon I)^{-1/2}\right)(\sigma+\varepsilon I)^{1/2}\psi\right\rangle \\
&\quad= \varepsilon\left\langle\psi, f\left((\sigma+\varepsilon I)^{-1/2}(\varrho+\varepsilon I)(\sigma+\varepsilon I)^{-1/2}\right)\psi\right\rangle \\
&\quad\geq \varepsilon f\left(\left\langle\psi, (\sigma+\varepsilon I)^{-1/2}(\varrho+\varepsilon I)(\sigma+\varepsilon I)^{-1/2}\psi\right\rangle\right) \\
&\quad= \varepsilon f\left(\varepsilon^{-1}\langle\psi, (\varrho+\varepsilon I)\psi\rangle\right) = \varepsilon f\left(\varepsilon^{-1}\langle\psi, \varrho\psi\rangle + 1\right) \\
&\quad= \frac{f\left(\varepsilon^{-1}\langle\psi, \varrho\psi\rangle + 1\right)}{\varepsilon^{-1}\langle\psi, \varrho\psi\rangle + 1}\left(\langle\psi, \varrho\psi\rangle + \varepsilon\right),
\end{aligned}$$

where the second inequality is due to Jensen's inequality. Since the last term converges to $f'(+\infty)\langle\psi, \varrho\psi\rangle = +\infty$ as $\varepsilon \searrow 0$, $\widehat{S}_f(\varrho, \sigma) = +\infty$. When $f(0^+) = +\infty$ and $\sigma^0 \not\leq \varrho^0$, the previous result combined with Proposition 3.22 (3) yields immediately that $\widehat{S}_f(\varrho, \sigma) = +\infty$.

Finiteness of $\widehat{S}_f(\varrho, \sigma)$ in all other cases is immediate from Propositions 3.25 and 3.26. ☐

Proposition 3.30. Let $f : (0, +\infty) \to \mathbb{R}$ be operator convex, and $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ be such that at least one of the conditions in Definition 3.27 holds. Then, for any positive linear map $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$, we have

$$P_f(\Phi(\varrho), \Phi(\sigma)) \leq \Phi\left(P_f(\varrho, \sigma)\right). \tag{3.33}$$

Proof. The proof below is essentially the same as that of [36, Proposition 2.5] (cf. also [50, Lemma 3]). By considering Φ as a map into $\Phi(I)^0\mathcal{B}(\mathcal{K})\Phi(I)^0 = \mathcal{B}(\Phi(I)^0\mathcal{K})$, we can assume without loss of generality that $\Phi(I)^0 = I$. Let $\varrho_n := \varrho + n^{-1}I$ and $\sigma_n := \sigma + n^{-1}I$. Define $\Phi_{\sigma_n} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ by $\Phi_{\sigma_n}(X) := \Phi(\sigma_n)^{-1/2}\Phi(\sigma_n^{1/2}X\sigma_n^{1/2})\Phi(\sigma_n)^{-1/2}$, as in (3.19). Then Φ_{σ_n} is a unital positive map, and Lemma 2.4 yields

$$f(\Phi_{\sigma_n}(\sigma_n^{-1/2}\varrho_n\sigma_n^{-1/2})) \leq \Phi_{\sigma_n}(f(\sigma_n^{-1/2}\varrho_n\sigma_n^{-1/2})),$$

which means that

$$\Phi(\sigma_n)^{1/2} f(\Phi(\sigma_n)^{-1/2}\Phi(\varrho_n)\Phi(\sigma_n)^{-1/2})\Phi(\sigma_n)^{1/2} \leq \Phi(\sigma_n^{1/2} f(\sigma_n^{-1/2}\varrho_n\sigma_n^{-1/2})\sigma_n^{1/2}),$$

i.e., $P_f(\Phi(\varrho_n), \Phi(\sigma_n)) \leq \Phi(P_f(\varrho_n, \sigma_n))$. By now using Propositions 3.25, 3.26 and Definition 3.27, taking the limit $n \to \infty$ gives (3.33). ☐

Now, the monotonicity of $\widehat{S}_f$ follows immediately:

Corollary 3.31. Let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a trace-preserving positive linear map. Then for every $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$,

$$\widehat{S}_f(\Phi(\varrho)\|\Phi(\sigma)) \leq \widehat{S}_f(\varrho\|\sigma). \tag{3.34}$$

Proof. If any of the conditions in Definition 3.27 is satisfied, then (3.34) is immediate from (3.33). Otherwise $\widehat{S}_f(\varrho, \sigma) = +\infty$, according to Proposition 3.29, and thus the assertion is trivial. ☐

Remark 3.32. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ with $\varrho^0 \le \sigma^0$. For any function $\varphi : [0, \infty) \to \mathbb{R}$, one can define $P_\varphi(\varrho, \sigma) := \sigma^{1/2}\varphi(\sigma^{-1/2}\varrho\sigma^{-1/2})\sigma^{1/2}$ simply via functional calculus. When f is operator convex with $f(0^+) < +\infty$, this definition is consistent with case (iii) of Definition 3.27 due to (3.31). When $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ is a positive linear map, one can also define $P_f(\Phi(\varrho), \Phi(\sigma))$ in the same way since $\Phi(\varrho)^0 \le \Phi(\sigma)^0$. If the map Φ_σ defined in (3.19) is considered as a map from $\mathcal{B}(\sigma^0\mathcal{H})$ to $\mathcal{B}(\Phi(\sigma)^0\mathcal{K})$, then it is unital and positive, so one can apply Lemma 2.4 to have

$$f(\Phi_\sigma(\sigma^{-1/2}\varrho\sigma^{-1/2})) \le \Phi_\sigma(f(\sigma^{-1/2}\varrho\sigma^{-1/2})),$$

which means (3.33). Thus, Proposition 3.30, if restricted to this situation, follows in a simpler way without the convergence argument.

Remark 3.33. When $h : (0, +\infty) \to \mathbb{R}$ is non-negative and operator monotone, Proposition 3.30 applied to $f := -h$ shows that for any positive linear map $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ and for every $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$,

$$\Phi(\varrho \, \tau_h \, \sigma) \le \Phi(\varrho) \, \tau_h \, \Phi(\sigma). \tag{3.35}$$

This inequality is essentially due to Ando [2], where it was proved only for the geometric and the harmonic means in a similar way to the proof of Proposition 3.30. We will use this observation in the proof of (f) $\Longrightarrow$ (a) in Theorem 3.34 below.

By Corollary 3.31 it is obvious that if Φ is reversible on $\{\varrho, \sigma\}$ (see Definition 3.16), then

$$\widehat{S}_f(\Phi(\varrho)\|\Phi(\sigma)) = \widehat{S}_f(\varrho\|\sigma)$$

for all operator convex functions f on $(0, +\infty)$. The next theorem presents several equivalent conditions for the equality case of $\widehat{S}_f$ under Φ. We note that the implication (a) $\Longrightarrow$ (d) was shown in [50, Lemma 12] under an additional assumption on the support of μ_f, analogous to (3.21). Here we stress that assumption (3.21) on f is essential in (iv) of Theorem 3.18 (see, e.g., [40, Example 1]), while f in (a) of Theorem 3.34 can be an arbitrary non-linear operator convex function. The equivalence (d) $\Longleftrightarrow$ (h) was also pointed out in [50, Section 9.1]. Moreover, we note that a variant of (a) $\Longrightarrow$ (d) in the case where $\varrho^0 \not\le \sigma^0$ was given in [50, Lemma 12].

Theorem 3.34. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ be such that $\varrho^0 \le \sigma^0$, and let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a positive trace-preserving linear map. Then the following are equivalent:

(a) $\widehat{S}_f(\Phi(\varrho)\|\Phi(\sigma)) = \widehat{S}_f(\varrho\|\sigma)$ for some non-linear operator convex function f on $[0, +\infty)$.

(b) $\widehat{S}_f(\Phi(\varrho)\|\Phi(\sigma)) = \widehat{S}_f(\varrho\|\sigma)$ for all operator convex functions f on $[0, +\infty)$.

(c) $\operatorname{Tr} \Phi(\varrho)^2\Phi(\sigma)^{-1} = \operatorname{Tr} \varrho^2\sigma^{-1}$.

(d) $P_\varphi(\Phi(\varrho), \Phi(\sigma)) = \Phi\left(P_\varphi(\varrho, \sigma)\right)$ for all functions φ on $[0, +\infty)$.

(e) $\Phi(\sigma) \, \tau \, \Phi(\varrho) = \Phi(\sigma \, \tau \, \varrho)$ for all operator connections τ.

(f) $\Phi(\sigma) \, \tau \, \Phi(\varrho) = \Phi(\sigma \, \tau \, \varrho)$ for some non-linear operator connection τ.

(g) $\Phi(\varrho\sigma^{-1}\varrho) = \Phi(\varrho)\Phi(\sigma)^{-1}\Phi(\varrho)$.

(h) $\Phi_\sigma([\varrho/\sigma]^2) = (\Phi_\sigma([\varrho/\sigma]))^2, \quad \text{where} \quad [\varrho/\sigma] := \sigma^{-1/2}\varrho\sigma^{-1/2}$.

If we further assume that Φ is 2-positive, then the above are also equivalent to

(i) $\sigma^{-1/2}\varrho\sigma^{-1/2} \in \mathcal{M}_{\Phi_\sigma}$.

Proof. We shall prove

$$(\mathrm{c}) \Longleftrightarrow (\mathrm{g}) \Longleftrightarrow (\mathrm{h}) \implies (\mathrm{d}) \Longrightarrow (\mathrm{b}) \Longrightarrow (\mathrm{a}) \implies (\mathrm{c}) \quad \text{and} \quad (\mathrm{d}) \Longrightarrow (\mathrm{e}) \Longrightarrow (\mathrm{f}) \implies (\mathrm{a}). \tag{3.36}$$

First, note that $P_\varphi(\varrho,\sigma)$ and $P_\varphi(\Phi(\varrho),\Phi(\sigma))$ are defined in the sense of Remark 3.32, and $P_h(\varrho,\sigma) = \sigma\,\tau_h\,\varrho$ when h is a non-negative operator monotone function on $[0,\infty)$ with the corresponding operator connection τ_h. Hence (d) $\Longrightarrow$ (b) is obvious by Corollary 3.28, and the implications (b) $\Longrightarrow$ (a) and (d) $\Longrightarrow$ (e) $\Longrightarrow$ (f) are trivial. We also remark (although not necessary for the rest of the proof) that (b) $\Longrightarrow$ (c) $\Longrightarrow$ (a) is obvious by applying equality in (b) to the quadratic function.

(c) $\Longleftrightarrow$ (g) is easy since $\Phi(\varrho)\Phi(\sigma)^{-1}\Phi(\varrho) \le \Phi(\varrho\sigma^{-1}\varrho)$ (see, e.g., [12, Proposition 2.7.3] and [34, Lemma 3.5]).

(g) $\Longleftrightarrow$ (h) follows immediately from

$$\begin{aligned}
\Phi_\sigma\big((\sigma^{-1/2}\varrho\sigma^{-1/2})^2\big) &= \Phi(\sigma)^{-1/2}\Phi(\varrho\sigma^{-1}\varrho)\Phi(\sigma)^{-1/2}, \\
\big(\Phi_\sigma(\sigma^{-1/2}\varrho\sigma^{-1/2})\big)^2 &= \Phi(\sigma)^{-1/2}\Phi(\varrho)\Phi(\sigma)^{-1}\Phi(\varrho)\Phi(\sigma)^{-1/2}.
\end{aligned}$$

(h) $\Longrightarrow$ (d). By considering Φ_σ as a map from $\mathcal{B}(\sigma^0\mathcal{H})$ to $\mathcal{B}(\Phi(\sigma)^0\mathcal{K})$, we can assume that Φ_σ is unital. Let $\widetilde{\Phi}_\sigma$ be the restriction of Φ_σ onto the commutative algebra generated by $[\varrho/\sigma] = \sigma^{-1/2}\varrho\sigma^{-1/2}$. By (h), $\sigma^{-1/2}\varrho\sigma^{-1/2}$ is in the multiplicative domain of $\widetilde{\Phi}_\sigma$ (see (2.12) and (2.13)). Thus,

$$\begin{aligned}
\varphi\left(\Phi_\sigma\left(\sigma^{-1/2}\varrho\sigma^{-1/2}\right)\right) &= \varphi\left(\widetilde{\Phi}_\sigma\left(\sigma^{-1/2}\varrho\sigma^{-1/2}\right)\right) \\
&= \widetilde{\Phi}_\sigma\left(\varphi\left(\sigma^{-1/2}\varrho\sigma^{-1/2}\right)\right) = \Phi_\sigma\left(\varphi\left(\sigma^{-1/2}\varrho\sigma^{-1/2}\right)\right),
\end{aligned}$$

where the second equality is due to Lemma 2.5. The equality of the first and the last terms above is exactly (d).

(a) $\Longrightarrow$ (c). For $s \in (0,+\infty)$ set

$$f_s(x) := -\frac{x}{x+s}, \qquad x \in [0,+\infty), \tag{3.37}$$

which is an operator convex function on $[0,+\infty)$. From the integral expression (2.3) of f one has

$$\widehat{S}_f(\varrho\|\sigma) = f(0)\operatorname{Tr}\sigma + a\operatorname{Tr}\varrho + b\operatorname{Tr}\varrho^2\sigma^{-1} + \int_{(0,+\infty)} \left(\frac{\operatorname{Tr}\varrho}{1+s} + \widehat{S}_{f_s}(\varrho\|\sigma)\right) d\mu_f(s) \tag{3.38}$$

and similarly

$$\begin{aligned}
\widehat{S}_f(\Phi(\varrho)\|\Phi(\sigma)) &= f(0)\operatorname{Tr}\Phi(\sigma) + a\operatorname{Tr}\Phi(\varrho) + b\operatorname{Tr}\Phi(\varrho)^2\Phi(\sigma)^{-1} \\
&\quad + \int_{(0,+\infty)} \left(\frac{\operatorname{Tr}\Phi(\varrho)}{1+s} + \widehat{S}_{f_s}(\Phi(\varrho)\|\Phi(\sigma))\right) d\mu_f(s) \\
&= f(0)\operatorname{Tr}\sigma + a\operatorname{Tr}\varrho + b\operatorname{Tr}\Phi(\varrho)^2\Phi(\sigma)^{-1} \\
&\quad + \int_{(0,+\infty)} \left(\frac{\operatorname{Tr}\varrho}{1+s} + \widehat{S}_{f_s}(\Phi(\varrho)\|\Phi(\sigma))\right) d\mu_f(s).
\end{aligned} \tag{3.39}$$

By comparing (3.38) and (3.39) together with the monotonicity property of Corollary 3.31, one must have

$$\operatorname{Tr}\Phi(\varrho)^2\Phi(\sigma)^{-1} = \operatorname{Tr}\varrho^2\sigma^{-1} \quad \text{if } b > 0,$$
$$\widehat{S}_{f_s}(\Phi(\varrho)\|\Phi(\sigma)) = \widehat{S}_{f_s}(\varrho\|\sigma) \quad \text{for all } s \in \operatorname{supp}\mu.$$

Since f is non-linear, if follows that $b > 0$ or $\operatorname{supp}\mu_f$ is not empty. So it suffices to prove that (c) holds if $\widehat{S}_{f_s}(\Phi(\varrho)\|\Phi(\sigma)) = \widehat{S}_{f_s}(\varrho\|\sigma)$ for some $s \in (0, +\infty)$. Since $f_s(x) = -1 + s(x+s)^{-1}$, the assumption implies that

$$\operatorname{Tr}\Phi(\sigma)^{1/2}\big[\Phi(\sigma)^{-1/2}\Phi(\varrho)\Phi(\sigma)^{-1/2} + sI\big]^{-1}\Phi(\sigma)^{1/2} = \operatorname{Tr}\sigma^{1/2}\big[\sigma^{-1/2}\varrho\sigma^{-1/2} + sI\big]^{-1}\sigma^{1/2}.$$

By noting that $\sigma^{-1/2}\varrho\sigma^{-1/2} + sI = \sigma^{-1/2}(\varrho + s\sigma)\sigma^{-1/2} + s(I - \sigma^0)$, the above can be rephrased as

$$\operatorname{Tr}\Phi(\sigma)^2\Phi(\varrho + s\sigma)^{-1} = \operatorname{Tr}\sigma^2(\varrho + s\sigma)^{-1}.$$

As we have already proved (c) $\Longleftrightarrow$ (h) $\Longrightarrow$ (b), we can apply (c) $\Longrightarrow$ (b) to σ and $\varrho + s\sigma$ (in place of ϱ, σ) and $f(x) = (x + \varepsilon)^{-1}$ for any $\varepsilon > 0$. We then find that

$$\begin{aligned}\operatorname{Tr}\Phi(\varrho + s\sigma)^{1/2}&\big[\Phi(\varrho + s\sigma)^{-1/2}\Phi(\sigma)\Phi(\varrho + s\sigma)^{-1/2} + \varepsilon I\big]^{-1}\Phi(\varrho + s\sigma)^{1/2}\\ &= \operatorname{Tr}(\varrho + s\sigma)^{1/2}\big[(\varrho + s\sigma)^{-1/2}\sigma(\varrho + s\sigma)^{-1/2} + \varepsilon I\big]^{-1}(\varrho + s\sigma)^{1/2}.\end{aligned}$$

Letting $\varepsilon \searrow 0$ yields

$$\operatorname{Tr}\Phi(\varrho + s\sigma)^2\Phi(\sigma)^{-1} = \operatorname{Tr}(\varrho + s\sigma)^2\sigma^{-1}$$

so that

$$\operatorname{Tr}\Phi(\varrho)^2\Phi(\sigma)^{-1} + 2s\operatorname{Tr}\Phi(\varrho) + s^2\operatorname{Tr}\Phi(\sigma) = \operatorname{Tr}\varrho^2\sigma^{-1} + 2s\operatorname{Tr}\varrho + s^2\operatorname{Tr}\sigma.$$

Therefore, $\operatorname{Tr}\Phi(\varrho)^2\Phi(\sigma)^{-1} = \operatorname{Tr}\varrho^2\sigma^{-1}$.

(f) $\Longrightarrow$ (a). Assume (f) for $\tau = \tau_h$ with a non-negative operator monotone function h. From the integral expression (2.9) one writes

$$\Phi(\sigma\,\tau_h\,\varrho) = a\Phi(\varrho) + b\Phi(\sigma) + \int_{(0,+\infty)} \Phi(\sigma\,\tau_{h_s}\,\varrho)\,d\nu_h(s), \tag{3.40}$$

$$\Phi(\sigma)\,\tau_h\,\Phi(\varrho) = a\Phi(\varrho) + b\Phi(\sigma) + \int_{(0,+\infty)} \Phi(\sigma)\,\tau_{h_s}\,\Phi(\varrho)\,d\nu_h(s). \tag{3.41}$$

Comparing (3.40) and (3.41) implies by means of (3.35) that

$$\Phi(\sigma)\,\tau_{h_s}\,\Phi(\varrho) = \Phi(\sigma\,\tau_{h_s}\,\varrho) \quad \text{for all } s \in \operatorname{supp}\nu_h.$$

Since $h_s(x) = -(1 + s)f_s(x)$ with f_s given in (3.37), one finds that

$$\operatorname{Tr}\big(\sigma\,\tau_{h_s}\,\varrho\big) = -(1 + s)\widehat{S}_{f_s}(\varrho\|\sigma).$$

Therefore, the above equality means that

$$\widehat{S}_{f_s}(\Phi(\varrho)\|\Phi(\sigma)) = \widehat{S}_{f_s}(\varrho\|\sigma) \quad \text{for } s \in \operatorname{supp}\nu_h.$$

Hence (a) follows since τ_h is non-linear so that $\operatorname{supp}\nu_h$ is not empty.

(i) $\Longleftrightarrow$ (h). As before, by considering Φ_σ as a map from $\mathcal{B}(\sigma^0\mathcal{H})$ to $\mathcal{B}(\Phi(\sigma)^0\mathcal{K})$, we can assume that Φ_σ is unital. If Φ is 2-positive then so is Φ_σ. Hence, (i) is equivalent to (h), according to (2.12) and (2.13). □

Remark 3.35. Note that (c) gives a particularly easy-to-verify criterion for the rest of the points in Theorem 3.34 to hold.

4 Comparison of different f-divergences

In this section we compare the quantum f-divergences $\widehat{S}_f$, S_f, and S_f^{meas}. In particular, in Section 4.1, we extend and strengthen Matsumoto's inequality $S_f(\varrho\|\sigma) \le \widehat{S}_f(\varrho\|\sigma)$, that was proved in [50] for the case where f is operator convex on $[0,+\infty)$ and $\varrho^0 \le \sigma^0$. In Section 4.2, we compare the preservation of S_f and $\widehat{S}_f$ in Theorems 3.18 and 3.34. Finally, in Section 4.3, we discuss the measured f-divergence.

4.1 The relation of S_f and $\widehat{S}_f$

It is easy to verify that if $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ are commuting, then $S_f(\varrho\|\sigma) = \widehat{S}_f(\varrho\|\sigma)$ for every f. The main result of this section, given in Theorem 4.3, is that the converse is also true in the sense that $S_f(\varrho\|\sigma) = \widehat{S}_f(\varrho\|\sigma)$ for some *fixed* operator convex function f implies the commutativity of ϱ and σ, provided that f satisfies some technical condition.

In general, one has

$$S_f(\varrho\|\sigma) \le \widehat{S}_f(\varrho\|\sigma) \tag{4.1}$$

for any operator convex function f on $(0,+\infty)$. By Proposition 3.12, this is a special case of a more general statement proved by Matsumoto [50], given in (3.7) (although he only considered operator convex functions on $[0,+\infty)$). The proof for the general case (i.e., without the assumption $f(0^+) < +\infty$) goes the same way, using Matsumoto's construction of the "minimal reverse test"; we give it in detail below as a preparation for the proof of the stronger inequality given in Theorem 4.3.

Proposition 4.1. For every $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, and every operator convex function $f : (0,+\infty) \to \mathbb{R}$,

$$S_f(\varrho\|\sigma) \le \widehat{S}_f(\varrho\|\sigma).$$

Proof. By definitions (3.9) and (3.29) one may assume that $\varrho, \sigma > 0$. Choose the spectral decomposition of $\sigma^{-1/2}\varrho\sigma^{-1/2}$ as

$$\sigma^{-1/2}\varrho\sigma^{-1/2} = \sum_{i=1}^{k} \lambda_i P_i,$$

where the P_i are orthogonal projections with $\sum_{i=1}^k P_i = I$. For every $i = 1, \dots, k$, let δ_i denote the indicator function of the singleton $\{i\}$ in the commutative algebra $\mathbb{C}^k$, and define a trace-preserving positive linear map Φ from $\mathbb{C}^k$ to $\mathcal{B}(\mathcal{H})$ by

$$\Phi\left(\sum_{i=1}^k x_i\delta_i\right) := \sum_{i=1}^k x_i \frac{\sigma^{1/2}P_i\sigma^{1/2}}{\operatorname{Tr}\sigma P_i},$$

and $\mathbf{a}, \mathbf{b} \in \mathbb{C}^k$ by

$$\mathbf{a} := \sum_{i=1}^k (\lambda_i \operatorname{Tr}\sigma P_i)\delta_i, \qquad \mathbf{b} := \sum_{i=1}^k (\operatorname{Tr}\sigma P_i)\delta_i.$$

Then Φ is CPTP, and

$$\Phi(\mathbf{a}) = \sum_{i=1}^k \lambda_i\sigma^{1/2}P_i\sigma^{1/2} = \varrho, \qquad \Phi(\mathbf{b}) = \sum_{i=1}^k \sigma^{1/2}P_i\sigma^{1/2} = \sigma.$$

Therefore, by the monotonicity property of S_f (Proposition 3.12) one has

$$S_f(\varrho\|\sigma) \le S_f(\mathbf{a}\|\mathbf{b}) = \sum_{i=1}^k (\mathrm{Tr}\,\sigma P_i) f\big((\lambda_i \,\mathrm{Tr}\,\sigma P_i)(\mathrm{Tr}\,\sigma P_i)^{-1}\big)$$
$$= \sum_{i=1}^k (\mathrm{Tr}\,\sigma P_i) f(\lambda_i) = \mathrm{Tr}\,\sigma f(\sigma^{-1/2}\varrho\sigma^{-1/2}) = \widehat{S}_f(\varrho\|\sigma),$$

which is the required inequality. □

It is easy to see that S_f is actually equal to $\widehat{S}_f$ when f is a polynomial of degree two:

Example 4.2. (Quadratic function) For the quadratic function $f_2(x) := x^2$ and for $\varrho, \sigma > 0$,

$$S_{f_2}(\varrho\|\sigma) = \mathrm{Tr}\,\varrho^2\sigma^{-1} = \widehat{S}_{f_2}(\varrho\|\sigma).$$

Therefore, when f is of the form $f(x) = ax^2 + bx + c$ with $a \ge 0$, we have $S_f(\varrho\|\sigma) = \widehat{S}_f(\varrho\|\sigma)$ for all $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$.

Theorem 4.3. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ satisfy $\varrho^0 \le \sigma^0$ and $\varrho\sigma \ne \sigma\varrho$. Then

$$S_f(\varrho\|\sigma) < \widehat{S}_f(\varrho\|\sigma) \tag{4.2}$$

for any operator convex function f on $[0, +\infty)$ such that

$$|\,\mathrm{supp}\,\mu_f| \ge \Big|\mathrm{spec}(\sigma^{-1/2}\varrho\sigma^{-1/2}) \cup \mathrm{spec}\,(L_\varrho R_{\sigma^{-1}})\Big|. \tag{4.3}$$

Proof. The proof is based on the minimal reverse test [50] as in the proof of Proposition 4.1. Write the spectral decomposition of $\sigma^{-1/2}\varrho\sigma^{-1/2}$ as

$$\sigma^{-1/2}\varrho\sigma^{-1/2} = \sum_{i=1}^k \lambda_i P_i, \qquad \lambda_1 > \lambda_2 > \cdots > \lambda_k,$$

and define the trace-preserving positive map $\Phi : \mathbb{C}^k \to \mathcal{B}(\mathcal{H})$ and $\mathbf{a}, \mathbf{b} \in \mathbb{C}^k$ as in the proof of Proposition 4.1. Then $\Phi(\mathbf{a}) = \varrho$, $\Phi(\mathbf{b}) = \sigma$ and $S_f(\varrho\|\sigma) \le S_f(\mathbf{a}\|\mathbf{b}) = \widehat{S}_f(\varrho\|\sigma)$. Now, assume that $S_f(\varrho\|\sigma) = \widehat{S}_f(\varrho\|\sigma)$ and prove that ϱ and σ must be commuting. Since $S_f(\varrho\|\sigma) = S_f(\mathbf{a}\|\mathbf{b})$ and (3.21) is satisfied, it follows from Theorem 3.18 that

$$\mathbf{a}\mathbf{b}^{-1} \in \mathcal{F}_{\Phi^*\circ\Phi_{\mathbf{b}}}. \tag{4.4}$$

Since

$$\Phi_{\mathbf{b}}\left(\sum_{i=1}^k x_i\delta_i\right) = \sigma^{-1/2}\Phi\left(\sum_{i=1}^k (\mathrm{Tr}\,\sigma P_i)x_i\delta_i\right)\sigma^{-1/2}$$
$$= \sigma^{-1/2}\left(\sum_{i=1}^k x_i\sigma^{1/2}P_i\sigma^{1/2}\right)\sigma^{-1/2} = \sum_{i=1}^k x_i P_i \tag{4.5}$$

and $\mathbf{a}\mathbf{b}^{-1} = \sum_{i=1}^k \lambda_i\delta_i$, we have $\Phi_{\mathbf{b}}(\mathbf{a}\mathbf{b}^{-1}) = \sum_{i=1}^k \lambda_i P_i = \sigma^{-1/2}\varrho\sigma^{-1/2}$. Moreover, since

$$\Big\langle X, \Phi\Big(\sum_i x_i\delta_i\Big)\Big\rangle_{\mathrm{HS}} = \mathrm{Tr}\left(X^* \sum_i x_i \,\frac{\sigma^{1/2}P_i\sigma^{1/2}}{\mathrm{Tr}\,\sigma P_i}\right) = \sum_i \overline{\left(\frac{\mathrm{Tr}\,X\sigma^{1/2}P_i\sigma^{1/2}}{\mathrm{Tr}\,\sigma P_i}\right)}\, x_i,$$

we have

$$\Phi^*(X) = \sum_{i=1}^k \frac{\operatorname{Tr} X\sigma^{1/2}P_i\sigma^{1/2}}{\operatorname{Tr}\sigma P_i}\,\delta_i$$

with the convention $0/0 = 0$. Therefore,

$$\Phi^* \circ \Phi_{\mathbf{b}}(\mathbf{ab}^{-1}) = \sum_{i=1}^k \frac{\operatorname{Tr}\sigma^{-1/2}\varrho\sigma^{-1/2}\sigma^{1/2}P_i\sigma^{1/2}}{\operatorname{Tr}\sigma P_i}\,\delta_i = \sum_{i=1}^k \frac{\operatorname{Tr}\varrho P_i}{\operatorname{Tr}\sigma P_i}\,\delta_i$$

so that (4.4) yields

$$\sum_{i=1}^k \lambda_i\delta_i = \sum_{i=1}^k \frac{\operatorname{Tr}\varrho P_i}{\operatorname{Tr}\sigma P_i}\,\delta_i.$$

Since $\varrho = \sum_{j=1}^k \lambda_j\sigma^{1/2}P_j\sigma^{1/2}$, this implies that

$$\lambda_i = \frac{\operatorname{Tr}\varrho P_i}{\operatorname{Tr}\sigma P_i} = \sum_{j=1}^k \lambda_j\pi_j^i, \qquad 1 \le i \le k,$$

where

$$\pi_j^i := \frac{\operatorname{Tr}\sigma^{1/2}P_j\sigma^{1/2}P_i}{\operatorname{Tr}\sigma P_i}, \qquad 1 \le i, j \le k.$$

Note that $\pi_j^i \ge 0$ and $\sum_{j=1}^k \pi_j^i = 1$ for all i. Since $\lambda_1 > \lambda_2 > \cdots$, by taking $i = 1$ we obtain $\pi_j^1 = 0$ for all $j \ne 1$, and hence $\pi_1^i = 0$ for all $i \ne 1$, too, since $\operatorname{Tr}\sigma^{1/2}P_j\sigma^{1/2}P_i = \operatorname{Tr}\sigma^{1/2}P_i\sigma^{1/2}P_j$. Using the same argument for $i = 2, 3, \dots$, we obtain $\pi_j^i = 0$, i.e., $\operatorname{Tr}\sigma^{1/2}P_j\sigma^{1/2}P_i = 0$ for $i \ne j$, so that $P_i\sigma^{1/2}P_j = 0$, $i \ne j$. This yields that $\sigma^{1/2}$ commutes with $\sigma^{-1/2}\varrho\sigma^{-1/2}$, hence $\varrho\sigma^{1/2} = \sigma^{1/2}\varrho$, so that $\varrho\sigma = \sigma\varrho$. □

Example 4.4. (Log function) Consider $\eta(x) := x\log x$ as in Example 3.5. For every $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ with $\varrho^0 \le \sigma^0$ we have

$$\widehat{S}_\eta(\varrho\|\sigma) = \operatorname{Tr}\sigma^{1/2}\varrho\sigma^{-1/2}\log(\sigma^{-1/2}\varrho\sigma^{-1/2}) = \operatorname{Tr}\varrho\log(\varrho^{1/2}\sigma^{-1}\varrho^{1/2}),$$

which is the *Belavkin-Staszewski relative entropy* $S_{\mathrm{BS}}(\varrho\|\sigma)$ introduced in [9]. Proposition 4.1 gives the inequality $S(\varrho\|\sigma) \le S_{\mathrm{BS}}(\varrho\|\sigma)$, which was first proved in [36]. By Theorem 4.3 we further have $S(\varrho\|\sigma) < S_{\mathrm{BS}}(\varrho\|\sigma)$ whenever $\varrho^0 \le \sigma^0$ and $\varrho\sigma \ne \sigma\varrho$.

Example 4.5. (Power functions) Consider f_α, given in Example 3.5, for $\alpha \in (0, 2]$. For $\varrho, \sigma > 0$ we have

$$\widehat{S}_{f_\alpha}(\varrho\|\sigma) = s(\alpha)\operatorname{Tr}\sigma^{1/2}(\sigma^{-1/2}\varrho\sigma^{-1/2})^\alpha\sigma^{1/2}.$$

When $0 < \alpha \le 1$, this is rewritten as

$$\widehat{S}_{f_\alpha}(\varrho\|\sigma) = -\operatorname{Tr}\sigma\,\#_\alpha\,\varrho,$$

where $\#_\alpha$ denotes the weighted geometric mean corresponding to x^α. Proposition 4.1 gives the inequality $\operatorname{Tr}\sigma\,\#_\alpha\,\varrho \le \operatorname{Tr}\varrho^\alpha\sigma^{1-\alpha}$ for $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, which is also a consequence of the well-known log-majorization [3]. When $1 \le \alpha \le 2$ and $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ with $\varrho^0 \le \sigma^0$, by Proposition 4.1 we also have

$$\operatorname{Tr}\varrho^\alpha\sigma^{1-\alpha} \le \operatorname{Tr}\sigma^{1/2}(\sigma^{-1/2}\varrho\sigma^{-1/2})^\alpha\sigma^{1/2},$$

which seems a novel trace inequality in matrix theory. Furthermore, Theorem 4.3 implies that if $\varrho^0 \le \sigma^0$ and $\varrho\sigma \ne \sigma\varrho$, then

$$\operatorname{Tr} \varrho \#_\alpha \sigma < \operatorname{Tr} \varrho^{1-\alpha}\sigma^\alpha \quad \text{for } \alpha \in (0,1), \tag{4.6}$$

$$\operatorname{Tr} \varrho^\alpha\sigma^{1-\alpha} < \operatorname{Tr} \sigma^{1/2}(\sigma^{-1/2}\varrho\sigma^{-1/2})^\alpha\sigma^{1/2} \quad \text{for } \alpha \in (1,2). \tag{4.7}$$

Note that more refined results than (4.6) are found in [31].

Remark 4.6. Further to the above example, it is worth mentioning that if $\varrho^0 \le \sigma^0$ and $\varrho\sigma \ne \sigma\varrho$, then the strict inequality in (4.8) holds in the opposite direction for $\alpha \in (2,+\infty)$. Indeed, by elaborating the method in [3], one can prove the following log-majorization results (for the definition and basics of log-majorization, see [3]):

(a) $\sigma^{1/2}(\sigma^{-1/2}\varrho\sigma^{-1/2})^\alpha\sigma^{1/2} \prec_{\log} (\sigma^{\frac{1-\alpha}{2z}}\varrho^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}})^z$ if $0 < \alpha \le 1$ and $z > 0$,

(b) $(\sigma^{\frac{1-\alpha}{2z}}\varrho^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}})^z \prec_{\log} \sigma^{1/2}(\sigma^{-1/2}\varrho\sigma^{-1/2})^\alpha\sigma^{1/2}$ if $\alpha \ge 1$ and $z \ge \max\{\alpha/2, \alpha-1\}$,

(c) $\sigma^{1/2}(\sigma^{-1/2}\varrho\sigma^{-1/2})^\alpha\sigma^{1/2} \prec_{\log} (\sigma^{\frac{1-\alpha}{2z}}\varrho^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}})^z$ if $\alpha \ge 1$ and $0 < z \le \min\{\alpha/2, \alpha-1\}$.

In particular, when $z = 1$, (a) and (b) imply the inequalities in (4.7) and (4.8), respectively, and (c) implies the opposite inequality of (4.8), where the strict inequality when $\alpha \in (0,+\infty)\setminus\{1,2\}$ can be shown by using [31, Theorem 2.1]. Note that $\operatorname{Tr}(\sigma^{\frac{1-\alpha}{2z}}\varrho^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}})^z$ is the main component of the α-z-Rényi divergence in (1.4).

It is natural to ask whether the support condition (4.3) in Theorem 4.3 is necessary. The following proposition shows that, at least when $\dim\mathcal{H} = 2$, the condition (4.3) is not needed, and $\operatorname{supp}\mu_f \ne \emptyset$ is sufficient to guarantee the strict inequality in (4.2) for any non-commuting pair (ϱ,σ). Note that this condition cannot be further weakened, as $\operatorname{supp}\mu_f = \emptyset$ means that f is a polynomial of degree at most two, in which case $S_f = \widehat{S}_f$, according to Example 4.2.

Proposition 4.7. Let f be an operator convex function on $[0,+\infty)$ that is not a polynomial, i.e., $\operatorname{supp}\mu_f \ne \emptyset$. Then for any non-commuting $\varrho, \gamma \in \mathcal{B}(\mathbb{C}^2)_+$ with $\varrho^0 \le \gamma^0$,

$$S_f(\varrho\|\gamma) < \widehat{S}_f(\varrho\|\gamma).$$

Proof. We sketch the proof here. We may restrict to 2×2 density matrices. In the well-known Bloch sphere description, a qubit density matrix is written as $\frac{1}{2}(I + \mathbf{w}\cdot\sigma)$, where $\mathbf{w}\cdot\sigma := w_1\sigma_1 + w_2\sigma_2 + w_3\sigma_3$ for $\mathbf{w} = (w_1, w_2, w_3) \in \mathbb{R}^3$ with $|\mathbf{w}| := \bigl(w_1^2 + w_2^2 + w_3^2\bigr)^{1/2} \le 1$ and Pauli matrices $\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ and $\sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$. Let $\varrho = \frac{1}{2}(I + \mathbf{w}\cdot\sigma)$ and $\gamma = \frac{1}{2}(I + \mathbf{x}\cdot\sigma)$ with $\mathbf{w}, \mathbf{x} \in \mathbb{R}^3$, and assume that $\varrho, \gamma > 0$, equivalently $|\mathbf{w}|, |\mathbf{x}| < 1$. Set $\mathbf{y} := \mathbf{w} - \mathbf{x}$, $\mathbf{u} := \mathbf{w} - s\mathbf{x}$ and $\mathbf{v} := \mathbf{w} + s\mathbf{x}$. Thanks to the integral expression (2.2), to prove Proposition 4.7, it is enough to show that if $\varrho\gamma \ne \gamma\varrho$ then

$$S_{g_s}(\varrho\|\gamma) < \widehat{S}_{g_s}(\varrho\|\gamma), \tag{4.8}$$

where $g_s(x) := (x-1)^2/(x+s)$ with $s \in (0,+\infty)$; here note that $s = 0$ is excluded due to $f(0^+) < +\infty$. Since

$$S_{g_s}(\varrho\|\gamma) = \operatorname{Tr}(\varrho - \gamma)\,\frac{1}{L_\varrho + sR_\gamma}(\varrho - \gamma),$$

we have by [38, Lemma B.5]

$$S_{g_s}(\varrho\|\gamma) = (1+s)\Big\langle \mathbf{y}, \big[\big\{(1+s)^2 - |\mathbf{u}|^2\big\}I + |\mathbf{u}\rangle\langle\mathbf{u}| - |\mathbf{v}\rangle\langle\mathbf{v}|\big]^{-1}\mathbf{y}\Big\rangle. \tag{4.9}$$

On the other hand, by using [38, (B2)], we have

$$\begin{aligned}\widehat{S}_{g_s}(\varrho\|\gamma) &= \operatorname{Tr}\gamma^{-1}(\varrho-\gamma)\gamma(\varrho+s\gamma)^{-1}(\varrho-\gamma)\\ &= \frac{1}{2(1-|\mathbf{x}|^2)\big[(1+s)^2-|\mathbf{v}|^2\big]}\operatorname{Tr}(I-\mathbf{x}\cdot\sigma)(\mathbf{y}\cdot\sigma)(I+\mathbf{x}\cdot\sigma)[(1+s)I-\mathbf{v}\cdot\sigma](\mathbf{y}\cdot\sigma).\end{aligned}$$

A bit tedious computation using [38, (B1)] gives

$$\operatorname{Tr}(I-\mathbf{x}\cdot\sigma)(\mathbf{y}\cdot\sigma)(I+\mathbf{x}\cdot\sigma)[(1+s)I-\mathbf{v}\cdot\sigma](\mathbf{y}\cdot\sigma) = 2(1+s)|\mathbf{y}|^2(1-|\mathbf{x}|^2)$$

and hence

$$\widehat{S}_{g_s}(\varrho\|\gamma) = \frac{1+s}{(1+s)^2-|\mathbf{v}|^2}\,|\mathbf{y}|^2. \tag{4.10}$$

Here, note that $\varrho\gamma \ne \gamma\varrho$ if and only if $\mathbf{w},\mathbf{x}$ are linearly independent, equivalently so are $\mathbf{u},\mathbf{v}$. When this holds, an elementary but again tedious computation with (4.9) and (4.10) shows that (4.8) is equivalent to

$$|\mathbf{u}|^2 + |\mathbf{v}|^2 - 2\left(\frac{1-s}{1+s}\right)\mathbf{u}\cdot\mathbf{v} < 4s.$$

Since $\mathbf{u}-\mathbf{v} = -2s\mathbf{x}$ and $\mathbf{u}\cdot\mathbf{v} = |\mathbf{w}|^2 - s^2|\mathbf{x}|^2$, the above left-hand side is $\frac{4s}{1+s}(|\mathbf{w}|^2+s|\mathbf{x}|^2) < 4s$ since $|\mathbf{w}|,|\mathbf{x}| < 1$. When $\varrho \not> 0$ and $\gamma > 0$, the computation is similar with $|\mathbf{w}| = 1$ and $|\mathbf{x}| < 1$. ☐

4.2 The relation of the preservation conditions

In this section we compare the implications of the preservation of the two f-divergences, S_f and $\widehat{S}_f$, by a quantum operation; that is, we compare Theorem 3.18 and Theorem 3.34. As it turns out, the preservation of S_f is in general strictly stronger than the preservation of $\widehat{S}_f$, i.e., in general the preservation of $\widehat{S}_f$ does not imply the reversibility of the quantum operation as in Definition 3.16.

This can be seen in various ways. In [34, Remark 5.4], an example from [44] was used to show states ϱ,σ and a CPTP map Φ such that Φ is not reversible on $\{\varrho,\sigma\}$, but $S_{f_2}(\Phi(\varrho)\|\Phi(\sigma)) = S_{f_2}(\varrho\|\sigma)$ holds for $f_2(x) = x^2$. By Example 4.2 and (c) of Theorem 3.34, this latter condition implies that $\widehat{S}_f(\Phi(\varrho)\|\Phi(\sigma)) = \widehat{S}_f(\varrho\|\sigma)$ for every operator convex function f on $(0,+\infty)$; yet reversibility does not hold. The example from [44] is rather involved; below we give a much simpler one, in Example 4.8.

Another way to see the above statement is to consider Matsumoto's minimal reverse test $(\Phi,\mathbf{a},\mathbf{b})$ as in the proof of Proposition 4.1. Then

$$\widehat{S}_f(\Phi(\mathbf{a})\|\Phi(\mathbf{b})) = \widehat{S}_f(\varrho\|\sigma) = S_f(\mathbf{a}\|\mathbf{b}) = \widehat{S}_f(\mathbf{a}\|\mathbf{b})$$

for any operator convex function f on $(0,+\infty)$, and thus all of (a)–(h) in Theorem 3.34 hold. However, if f satisfies the support condition (4.3) and $\varrho^0 \le \sigma^0$ and $\varrho\sigma \ne \sigma\varrho$, then by Theorem 4.3 we have

$$S_f(\Phi(\mathbf{a})\|\Phi(\mathbf{b})) = S_f(\varrho\|\sigma) < \widehat{S}_f(\varrho\|\sigma) = S_f(\mathbf{a}\|\mathbf{b}),$$

and hence none of (i)–(ix) in Theorem 3.18 hold. Note that while the argument in the previous paragraph was based on a very specific example, using the function f_2, the argument in this paragraph shows that, in general, preservation of $\widehat{S}_f$ does not imply reversibility for any function that satisfies the support condition (4.3).

Yet another approach is given in Example 4.8 below, where we directly compare (vii) of Theorem 3.18 and (g) of Theorem 3.34. Note that the map used in [34, Remark 5.4] is not unital, and neither is the map Φ in the minimal reverse test unless ϱ, σ are commuting and $k = \dim \mathcal{H}$ (i.e., all P_i are rank one). Hence, Example 4.8 with a unital qutrit channel gives a further non-trivial insight into the difference of the preservation of the two f-divergences.

On the other hand, the points of Theorems 3.18 and 3.34 become equivalent when some further conditions are imposed on (Φ, ϱ, σ). This happens, for instance, in the qubit case when Φ is unital, as shown in Proposition 4.10, or in the case where $\Phi(\varrho)$ and $\Phi(\sigma)$ commute, given in Proposition 4.11 below.

Example 4.8. Let $\mathcal{H} = \mathbb{C}^3$ and P be the orthogonal projection onto $\mathbb{C}^2 \oplus 0$. Let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be the pinching

$$\Phi(X) := PXP + (I - P)X(I - P),$$

which is a unital qutrit channel. Let $\varrho := |\psi\rangle\langle\psi|$ with $\psi \in \operatorname{ran} P$, and $\sigma := b_1|x_1\rangle\langle x_1| + b_2|x_2\rangle\langle x_2| + |x_3\rangle\langle x_3|$ with $b_1, b_2 > 0$, where $\{x_1, x_2, x_3\}$ is an orthonormal basis in $\mathbb{C}^3$. It is easy to verify that

$$\begin{aligned} &\Phi^*(\Phi(\sigma)^{-1/2}\Phi(\varrho)\Phi(\sigma)^{-1/2}) = \sigma^{-1/2}\varrho\sigma^{-1/2} && (4.11)\\ &\qquad\Longleftrightarrow\quad |(P\sigma P)^{-1/2}\psi\rangle\langle(P\sigma P)^{-1/2}\psi| = |\sigma^{-1/2}\psi\rangle\langle\sigma^{-1/2}\psi|, \quad \text{and} && (4.12)\\ &\Phi(\varrho\sigma^{-1}\varrho) = \Phi(\varrho)\Phi(\sigma)^{-1}\Phi(\varrho) && (4.13)\\ &\qquad\Longleftrightarrow\quad \langle\psi, \sigma^{-1}\psi\rangle = \langle\psi, (P\sigma P)^{-1}\psi\rangle, && (4.14) \end{aligned}$$

where (4.11) is (vii) of Theorem 3.18, and (4.13) is (g) of Theorem 3.34. Hence, in order to find an example where the equivalent points of of Theorem 3.34 hold, but those of Theorem 3.18 do not, we have to set the parameters above so that

- $\sigma^{-1/2}\psi$ and $(P\sigma P)^{-1/2}\psi$ are linearly independent (i.e., (4.12) fails), and (4.15)
- $\|\sigma^{-1/2}\psi\| = \|(P\sigma P)^{-1/2}\psi\|$ (i.e., (4.14) holds). (4.16)

In order to achieve this, let us choose

$$\psi := \begin{bmatrix}1\\1\\0\end{bmatrix}, \quad x_1 := \frac{1}{\sqrt{3}}\begin{bmatrix}1\\1\\1\end{bmatrix}, \quad x_2 := \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\-1\end{bmatrix}, \quad x_3 := \frac{1}{\sqrt{6}}\begin{bmatrix}1\\-2\\1\end{bmatrix}.$$

It is straightforward to compute

$$\sigma^{-1/2}\psi = b_1^{-1/2}\langle x_1, \psi\rangle x_1 + b_2^{-1/2}\langle x_2, \psi\rangle x_2 + \langle x_3, \psi\rangle x_3 = \begin{bmatrix}\frac{2}{3}b_1^{-1/2} + \frac{1}{2}b_2^{-1/2} - \frac{1}{6}\\ \frac{2}{3}b_1^{-1/2} + \frac{1}{3}\\ \frac{2}{3}b_1^{-1/2} - \frac{1}{2}b_2^{-1/2} - \frac{1}{6}\end{bmatrix},$$

and

$$\|\sigma^{-1/2}\psi\|^2 = \frac{4}{3}b_1^{-1} + \frac{1}{2}b_2^{-1} + \frac{1}{6}. \tag{4.17}$$

On the other hand, we have

$$P\sigma P = b_1|Px_1\rangle\langle Px_1| + b_2|Px_2\rangle\langle Px_2| + |Px_3\rangle\langle Px_3| = \begin{bmatrix} \frac{2b_1+3b_2+1}{6} & \frac{b_1-1}{3} & 0 \\ \frac{b_1-1}{3} & \frac{b_1+2}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

and

$$(P\sigma P)^{-1} = \frac{6}{b_1b_2 + 3b_1 + 2b_2} \begin{bmatrix} \frac{b_1+2}{3} & -\frac{b_1-1}{3} & 0 \\ -\frac{b_1-1}{3} & \frac{2b_1+3b_2+1}{6} & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

so that

$$\|(P\sigma P)^{-1/2}\psi\|^2 = \frac{3(b_2+3)}{b_1b_2 + 3b_1 + 2b_2}. \tag{4.18}$$

We find that (4.17) and (4.18) are equal, for instance, when $b_1 = 1/3$ and $b_2 = 3/11$, in which case the third coordinate of $\sigma^{-1/2}\psi$ is non-zero. Therefore, when $\sigma = \frac{1}{3}|x_1\rangle\langle x_1| + \frac{3}{11}|x_2\rangle\langle x_2| + |x_3\rangle\langle x_3|$, we see that both (4.15) and (4.16) are satisfied, as required.

This shows that $\widehat{S}_f(\Phi(\varrho)\|\Phi(\sigma)) = \widehat{S}_f(\varrho\|\sigma)$ for any operator convex f on $[0, +\infty)$, while $S_f(\Phi(\varrho)\|\Phi(\sigma)) < S_f(\varrho\|\sigma)$ for any operator convex f such that $|\operatorname{supp}\mu_f| \geq 7$. In particular, Φ is not reversible on $\{\varrho, \sigma\}$, while (a)–(h) of Theorem 3.34 hold.

Remark 4.9. Since in the above example $\Phi^* \circ \Phi_\sigma = \Phi_\sigma$, comparing this with (ix) of Theorem 3.18 and (h) of Theorem 3.34 shows that Φ_σ is an example of a unital channel $\Psi : \mathcal{B}(\mathbb{C}^3) \to \mathcal{B}(\mathbb{C}^3)$ such that

$$\mathbb{C}I \subsetneqq \mathcal{F}_\Psi \subsetneqq \mathcal{M}_\Psi \subsetneqq \mathcal{B}(\mathbb{C}^3);$$

cf. also Appendix B.

The next proposition shows that Example 4.8 has minimal dimension among *unital* channels for which the points of Theorems 3.18 and 3.34 are inequivalent, though we have a *non-unital* qubit channel showing the difference (see the discussion before Example 4.8).

Proposition 4.10. All the points of Theorems 3.18 and 3.34 are equivalent to each other for any unital qubit channel $\Phi : \mathcal{B}(\mathbb{C}^2) \to \mathcal{B}(\mathbb{C}^2)$.

Proof. Let Φ be a unital qubit channel, and let $\varrho, \gamma \in \mathcal{B}(\mathbb{C}^2)_+$ with $\gamma > 0$. Assume that the equivalent statements of Theorem 3.34 hold for Φ and ϱ, γ, and we prove that Φ is reversible on $\{\varrho, \gamma\}$. By considering $(\varrho + \gamma)/\operatorname{Tr}(\varrho + \gamma)$ and $\gamma/\operatorname{Tr}\gamma$ in place of ϱ and γ, respectively, it suffices to assume that ϱ and γ are invertible density matrices, so we write $\varrho = \frac{1}{2}(I + \mathbf{w} \cdot \sigma)$ and $\gamma = \frac{1}{2}(I + \mathbf{x} \cdot \sigma)$ with $|\mathbf{w}|, |\mathbf{x}| < 1$, and let $\mathbf{y}$ and $\mathbf{v}$ be as in the proof of Proposition 4.7. We may also assume that $\varrho \neq \gamma$, i.e., $\mathbf{w} \neq \mathbf{x}$. In the Bloch sphere description, recall that Φ acts on density matrices as follows:

$$\Phi : \frac{1}{2}(I + \mathbf{z} \cdot \sigma) \longmapsto \frac{1}{2}(I + T\mathbf{z} \cdot \sigma), \qquad \mathbf{z} \in \mathbb{R}^3,\ |\mathbf{z}| \leq 1,$$

where T is a 3×3 real matrix with the operator norm $\|T\|_\infty \leq 1$. Consider $g_s(x) := (x-1)^2/(x+s)$, $s \in [0, +\infty)$, as given in the proof of Proposition 4.7. By assumption we have the equality $\widehat{S}_{g_s}(\varrho\|\gamma) = \widehat{S}_{g_s}(\Phi(\varrho)\|\Phi(\sigma))$, which means by (4.10) that

$$\frac{1+s}{(1+s)^2 - |\mathbf{v}|^2}\,|\mathbf{y}|^2 = \frac{1+s}{(1+s)^2 - |T\mathbf{v}|^2}\,|T\mathbf{y}|^2.$$

Since $\|T\|_\infty \le 1$, this forces $|T\mathbf{v}| = |\mathbf{v}|$ and $|T\mathbf{y}| = |\mathbf{y}|$, which are equivalent to $T^*T\mathbf{v} = \mathbf{v}$ and $T^*T\mathbf{y} = \mathbf{y}$. Hence $T^*T\mathbf{w} = \mathbf{w}$ and $T^*T\mathbf{x} = \mathbf{x}$. Now, recall [38, (17) and (22)] that the so-called Bogoliubov-Kubo-Mori monotone Riemannian metric on invertible density matrices is $\langle X, \Omega_\gamma^{\mathrm{BKM}}(Y)\rangle_{\mathrm{HS}} = \operatorname{Tr} X\Omega_\gamma^{\mathrm{BKM}}(Y)$ for $X, Y \in \mathcal{B}(\mathbb{C}^2)^0_{\mathrm{sa}}$, where $\Omega_\gamma^{\mathrm{BKM}} = \Omega_\gamma^\kappa$ with $\kappa(x) := (\log x)/(x-1)$ in (2.11) is given as

$$\Omega_\gamma^{\mathrm{BKM}}(Y) := \frac{1}{2}\int_0^\infty \frac{1}{2\gamma + sI}\, Y\, \frac{1}{2\gamma + sI}\, ds. \tag{4.19}$$

Thanks to [38, (B21)] we have

$$\begin{aligned} &\frac{1}{2}\operatorname{Tr}(\mathbf{y}\cdot\sigma)\frac{1}{(1+s)I + \mathbf{x}\cdot\sigma}(\mathbf{y}\cdot\sigma)\frac{1}{(1+s)I + \mathbf{x}\cdot\sigma} \\ &\qquad = \frac{|\mathbf{y}|^2}{\big[(1+s)^2 - |\mathbf{x}|^2\big]^2}\big[(1+s)^2 + |\mathbf{x}|^2\cos 2\theta\big], \end{aligned}$$

where θ is the angle between $\mathbf{x}$ and $\mathbf{y}$. Since $|T\mathbf{x}| = |\mathbf{x}|$, $|T\mathbf{y}| = |\mathbf{y}|$ and

$$(T\mathbf{x})\cdot(T\mathbf{y}) = \mathbf{x}\cdot(T^*T\mathbf{y}) = \mathbf{x}\cdot\mathbf{y},$$

it follows that the angle between $T\mathbf{x}$ and $T\mathbf{y}$ coincides with θ. Therefore,

$$\begin{aligned} &\frac{1}{2}\operatorname{Tr}((T\mathbf{y})\cdot\sigma)\frac{1}{(1+s)I + (T\mathbf{x})\cdot\sigma}((T\mathbf{y})\cdot\sigma)\frac{1}{(1+s)I + (T\mathbf{x})\cdot\sigma} \\ &\qquad = \frac{1}{2}\operatorname{Tr}(\mathbf{y}\cdot\sigma)\frac{1}{(1+s)I + \mathbf{x}\cdot\sigma}(\mathbf{y}\cdot\sigma)\frac{1}{(1+s)I + \mathbf{x}\cdot\sigma}. \end{aligned}$$

Integrate the above for $s \in (0, +\infty)$, and apply (4.19) to obtain

$$\big\langle \Phi(\mathbf{y}\cdot\sigma), \Omega_{\Phi(\gamma)}^{\mathrm{BKM}}(\Phi(\mathbf{y}\cdot\sigma))\big\rangle_{\mathrm{HS}} = \big\langle \mathbf{y}\cdot\sigma, \Omega_\gamma^{\mathrm{BKM}}(\mathbf{y}\cdot\sigma)\big\rangle_{\mathrm{HS}}.$$

Since

$$\frac{\log x}{x-1} = \int_{(0,+\infty)} \frac{1}{(x+s)(1+s)}\, ds,$$

it follows that (x) of Theorem 3.18 holds with $\operatorname{supp}\nu_\kappa = (0, +\infty)$, so that Φ is reversible on $\{\varrho, \gamma\}$. □

Proposition 4.11. Let ϱ, σ, and Φ be as in Theorem 3.34. If $\Phi(\varrho)$ commutes with $\Phi(\sigma)$, then the points of Theorem 3.34 imply those of Theorem 3.18.

Proof. By Propositions 3.12 and 4.1, we have

$$S_f(\Phi(\varrho)\|\Phi(\sigma)) \le S_f(\varrho\|\sigma) \le \widehat{S}_f(\varrho\|\sigma) \tag{4.20}$$

for all operator convex functions f on $[0, +\infty)$. Assume now (b) of Theorem 3.34. Since $\Phi(\varrho)$ and $\Phi(\sigma)$ commute, we then have

$$S_f(\Phi(\varrho)\|\Phi(\sigma)) = \widehat{S}_f(\Phi(\varrho)\|\Phi(\sigma)) = \widehat{S}_f(\varrho\|\sigma)$$

for all operator convex functions f on $[0, +\infty)$, from which, when combined with (4.20), we get that $S_f(\Phi(\varrho)\|\Phi(\sigma)) = S_f(\varrho\|\sigma)$ for all operator convex functions f on $[0, +\infty)$, i.e., all the points of Theorem 3.34 hold. □

By Theorems 3.18, 3.34, and Proposition 4.11 we have

Corollary 4.12. Let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a 2-positive trace-preserving map. If $\Phi(\varrho)$ commutes with $\Phi(\sigma)$ for all $\varrho \in \mathcal{B}(\mathcal{H})$ (in particular, if Φ is a quantum-classical channel, i.e., the range of Φ is commutative), then $\mathcal{F}_{\Phi^*\circ\Phi_\sigma} = \mathcal{M}_{\Phi_\sigma}$.

In particular, if Φ is a unital channel (trace-preserving) and $\sigma = I$ (so $\Phi(\sigma) = I$), then $\mathcal{F}_{\Phi^*\circ\Phi} = \mathcal{M}_\Phi$ holds. This is contained in [16, Theorem 11], where the fixed point algebra $\mathcal{F}_{\Phi^*\circ\Phi}$ was denoted by $UCC(\Phi)$ and called the UCC algebra (*unitarily correctable* codes). The unitality of the channel Φ seems essential in [16].

Another special case is when Φ is a (trace-preserving) conditional expectation onto a subalgebra of $\mathcal{B}(\mathcal{H})$ and $\Phi(\sigma) = \sigma$. In this case, $\Phi_\sigma = \Phi$ and Φ^* is the inclusion map of the subalgebra into $\mathcal{B}(\mathcal{H})$, hence $\Phi^* \circ \Phi_\sigma = \Phi_\sigma = \Phi$. Moreover, we have $\mathcal{F}_\Phi = \mathcal{M}_\Phi$ by the above corollary since $\Phi(I) = I$, which is also easily verified directly, and therefore the points of Theorem 3.1 imply those of Theorem 3.16.

4.3 Measured f-divergence

A measurement $\mathcal{M}$ on $\mathcal{H}$ is given by $(M_x)_{x\in\mathcal{X}}$, where $\mathcal{X}$ is a finite set (the set of possible outcomes), $M_x \in \mathcal{B}(\mathcal{H})_+$ for all $x \in \mathcal{X}$, and $\sum_{x\in\mathcal{X}} M_x = I$. The measurement $\mathcal{M}$ is then a CPTP map from $\mathcal{B}(\mathcal{H})$ to $\mathbb{C}^{\mathcal{X}}$, given by $\mathcal{M}(A) := \sum_{x\in\mathcal{X}}(\mathrm{Tr}\, AM_x)\delta_x$, where δ_x is the indicator function of the singleton $\{x\}$. We will use the same notation for this CPTP map and the collection of operators $(M_x)_{x\in\mathcal{X}}$. We will denote the set of all measurements on $\mathcal{H}$ with outcomes in $\mathcal{X}$ by $\mathrm{POVM}(\mathcal{H}|\mathcal{X})$.

We say that the measurement is projective if all the M_x are projections, and it is a von Neumann measurement if all the M_x are rank 1 projections. We will use the notation

$$|\mathcal{M}| := |\mathcal{X}|.$$

It is easy to see that with definition (3.6), we have

$$S_f^{\mathrm{meas}}(\varrho\|\sigma) = \sup\{S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma)) : \mathcal{M} \text{ measurement on } \mathcal{H}\}. \tag{4.21}$$

Here we use the classical f-divergence

$$S_f(p,q) := \sum_{x\in\mathcal{X}} P_f(p(x), q(x)), \qquad p, q \in [0, +\infty)^{\mathcal{X}},$$

that reduces to (3.1) when both p and q are strictly positive. We can introduce two variants of the measured f-divergences, by restricting the measurements to projective and von Neumann measurements, respectively:

$$S_f^{\mathrm{pr}}(\varrho\|\sigma) := \sup\{S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma)) : \mathcal{M} \text{ projective measurement on } \mathcal{H}\}, \tag{4.22}$$

$$S_f^{\mathrm{vN}}(\varrho\|\sigma) := \sup\{S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma)) : \mathcal{M} \text{ rank 1 projective measurement on } \mathcal{H}\}. \tag{4.23}$$

Obviously,

$$S_f^{\mathrm{vN}}(\varrho\|\sigma) \le S_f^{\mathrm{pr}}(\varrho\|\sigma) \le S_f^{\mathrm{meas}}(\varrho\|\sigma) \tag{4.24}$$

for any ϱ, σ and any f.

Lemma 4.13. For any $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, and any convex function $f : (0, +\infty) \to \mathbb{R}$,

$$S_f^{\mathrm{vN}}(\varrho\|\sigma) = S_f^{\mathrm{pr}}(\varrho\|\sigma).$$

Proof. By (4.24), we only have to prove $S_f^{\mathrm{vN}}(\varrho\|\sigma) \geq S_f^{\mathrm{pr}}(\varrho\|\sigma)$. To this end, let $\mathcal{M}$ be a projective measurement, given by the measurement operators P_x, $x \in \mathcal{X}$. Each P_x can be decomposed as $P_x = \sum_{i=1}^{k_x} |e_{x,i}\rangle\langle e_{x,i}|$, where $\{e_{x,i}\}_{i=1}^{k_x}$ is an ONB in $\operatorname{ran} P_x$. By the generalized log-sum inequality (i.e., the joint convexity of the classical perspective function), for every $\varepsilon > 0$ we have

$$\sum_{i=1}^{k_x} (\operatorname{Tr} |e_{x,i}\rangle\langle e_{x,i}|\sigma + \varepsilon) f\left(\frac{\operatorname{Tr} |e_{x,i}\rangle\langle e_{x,i}|\varrho + \varepsilon}{\operatorname{Tr} |e_{x,i}\rangle\langle e_{x,i}|\sigma + \varepsilon}\right) \geq (\operatorname{Tr} P_x\sigma + k_x\varepsilon) f\left(\frac{\operatorname{Tr} P_x\varrho + k_x\varepsilon}{\operatorname{Tr} P_x\sigma + k_x\varepsilon}\right).$$

Summing over x, and taking the limit $\varepsilon \searrow 0$ yields

$$S_f\left(\{\operatorname{Tr} |e_{x,i}\rangle\langle e_{x,i}|\varrho\}_{x,i} \| \{\operatorname{Tr} |e_{x,i}\rangle\langle e_{x,i}|\sigma\}_{x,i}\right) \geq S_f\left(\{\operatorname{Tr} P_x\varrho\}_x \| \{\operatorname{Tr} P_x\sigma\}_x\right),$$

from which the assertion follows immediately. ☐

Due to Lemma 4.13, we will only use the notation S_f^{pr} for the rest, with the understanding that the supremum in (4.22) is achieved at a von Neumann measurement (see Proposition 4.17 below).

When f is operator convex, the inequalities in (4.24) can be continued as

$$S_f^{\mathrm{pr}}(\varrho\|\sigma) \leq S_f^{\mathrm{meas}}(\varrho\|\sigma) \leq S_f(\varrho\|\sigma) \tag{4.25}$$

for any ϱ, σ, according to Proposition 3.12. It is an interesting open question whether the first inequality holds as an equality for a general operator convex function f and every ϱ, σ. This has been shown very recently in [10] to be true for

$$f(x) = f_\alpha(x) = s(\alpha)x^\alpha \quad \text{for} \quad \alpha \in (0, +\infty), \qquad \text{and} \qquad f(x) = \eta(x) = x\log x, \tag{4.26}$$

(cf. Example 3.5); we will give some further insight into this result after Theorem 4.18.

On the other hand, equality in the second inequality in (4.25) turns out to be very restrictive; indeed, under some mild technical conditions on f, $S_f^{\mathrm{meas}}(\varrho\|\sigma) = S_f(\varrho\|\sigma)$ implies that ϱ and σ commute, in which case all the inequalities in (4.25) hold trivially as equalities. We will show this in Theorem 4.18, by combining a result by Petz [67, Lemma 4.1] with Theorem 3.18. For this, we will show that all the suprema in (4.21)–(4.23) are attained, an interesting fact in itself. These will follow by simple compactness and continuity arguments. For (4.21), we need some preparation first; namely, we show that it is sufficient to consider measurements with at most $(\dim\mathcal{H})^2$ outcomes.

Lemma 4.14. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ and $f : (0, +\infty) \to \mathbb{R}$ be an operator convex function. For any measurement $\mathcal{M} = (M_x)_{x\in\mathcal{X}}$ on $\mathcal{H}$, there exists a measurement $\widetilde{M} = (\widetilde{M}_k)_{k\in\{1,\dots,(\dim\mathcal{H})^2\}}$ such that $S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma)) \leq S_f\left(\widetilde{M}(\varrho)\|\widetilde{\mathcal{M}}(\sigma)\right)$. As a consequence,

$$S_f^{\mathrm{meas}}(\varrho\|\sigma) = \sup\{S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma)) : \mathcal{M} \in \mathrm{POVM}(\mathcal{H}|[d^2])\}, \tag{4.27}$$

where $[d^2] := \{1, \dots, (\dim\mathcal{H})^2\}$.

Proof. $\mathrm{POVM}(\mathcal{H}|\mathcal{X})$ is a compact convex set of the finite-dimensional complex vector space $\mathcal{B}(\mathcal{H})^{\mathcal{X}} := \{A : \mathcal{X} \to \mathcal{B}(\mathcal{H})\}$ (equipped with any norm). Thus, any $\mathcal{M} \in \mathrm{POVM}(\mathcal{H}|\mathcal{X})$ can be decomposed as $\mathcal{M} = \sum_{i\in\mathcal{I}} p_i\mathcal{M}^{(i)}$, where $\mathcal{I}$ is a finite set, p is a probability distribution on $\mathcal{I}$, and all the $\mathcal{M}^{(i)}$ are extremal points of $\mathrm{POVM}(\mathcal{H}|\mathcal{X})$. Using the convexity of S_f (Proposition 3.10), we get that

$$S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma)) \leq \sum_{i\in\mathcal{I}} p_i S_f(\mathcal{M}^{(i)}(\varrho)\|\mathcal{M}^{(i)}(\sigma)) \leq S_f(\mathcal{M}^{(i)}(\varrho)\|\mathcal{M}^{(i)}(\sigma))$$

for some $i \in \mathcal{I}$. Various characterizations of the extremal points of $\mathrm{POVM}(\mathcal{H}|\mathcal{X})$ were given, e.g., in [5, 19, 61]; in particular, it is known that if $\mathcal{M}^{(i)}$ is an extremal point of $\mathrm{POVM}(\mathcal{H}|\mathcal{X})$ then $|\{x \in \mathcal{X} : M_x^{(i)} \neq 0\}| \leq (\dim \mathcal{H})^2$. Since $S_f(\mathcal{M}^{(i)}(\varrho)\|\mathcal{M}^{(i)}(\sigma))$ only depends on the outcome probabilities $(\operatorname{Tr} M_x^{(i)}\varrho)_{x\in\mathcal{X}}$ and $(\operatorname{Tr} M_x^{(i)}\sigma)_{x\in\mathcal{X}}$, we can assume without loss of generality that $\mathcal{M}^{(i)}$ has outcomes in $[d^2]$. From this, the assertion follows. □

Remark 4.15. Note that Lemma 4.14 holds for any convex function f for which S_f is jointly convex. According to Proposition 3.10, operator convexity of f is sufficient for this, and Remark 3.23 shows that it is also likely to be necessary.

Next, we want to show that the supremum in (4.27) is attained. Since $\mathrm{POVM}(\mathcal{H}|\mathcal{X})$ is compact, the assertion would follow if the map $\mathcal{M} \mapsto S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma))$ was continuous. This is not possible in general, since $S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma))$ can be $+\infty$, but with some care, these pathological cases can be treated as well. The following observation about classical f-divergences will be useful in this direction:

Remark 4.16. It is easy to see from the definition (2.5) that P_f is continuous on

$$A_{\gamma_0,\gamma_1} := \{(r\cos\gamma, r\sin\gamma) : r \geq 0, \gamma_0 \leq \gamma \leq \gamma_1\}$$

for any $0 < \gamma_0 < \gamma_1 < \pi/2$. If $f(0^+) < +\infty$ then P_f is continuous also on $A_{\gamma_0,\pi/2}$ for any $0 < \gamma_0 < \pi/2$, and if $f'(+\infty) < +\infty$ then P_f is continuous on A_{0,γ_1} for any $0 < \gamma_1 < \pi/2$. In particular, if $f(0^+)$ and $f'(+\infty)$ are both finite then P_f is continuous on $\mathbb{R}_+ \times \mathbb{R}_+$, where $\mathbb{R}_+ := [0, +\infty)$.

Let $S_{f,\mathcal{X}}$ denote the classical f-divergence on $\mathbb{R}_+^{\mathcal{X}} \times \mathbb{R}_+^{\mathcal{X}} \equiv (\mathbb{R}_+ \times \mathbb{R}_+)^{\mathcal{X}}$. By the above, we have

$$S_{f,\mathcal{X}} \ \text{ is continuous on } \begin{cases} A^{\mathcal{X}}_{\gamma_0,\gamma_1}, & \text{for any } \ 0 < \gamma_0 < \gamma_1 < \pi/2, \\ A^{\mathcal{X}}_{\gamma_0,\pi/2}, & \text{for any } \ 0 < \gamma_0 < \pi/2, \ \text{ if } \ f(0^+) < +\infty, \\ A^{\mathcal{X}}_{0,\gamma_1}, & \text{for any } \ 0 < \gamma_1 < \pi/2, \ \text{ if } \ f'(+\infty) < +\infty. \end{cases}$$

Proposition 4.17. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ and $f : (0, +\infty) \to \mathbb{R}$ be a convex function. Then the suprema in (4.22) and (4.23) are attained. If f is also operator convex then the suprema in (4.27) and (4.21) are attained as well.

Proof. It is enough to prove the assertions about (4.23) (due to Lemma 4.13) and about (4.27). We start by proving the latter.

Note that for any $\mathcal{M} \in \mathrm{POVM}(\mathcal{H}|[d^2])$,

$$S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma)) = \sum_{k=1}^{d^2} P_f(\operatorname{Tr} \varrho M_k, \operatorname{Tr} \sigma M_k) = S_{f,[d^2]}\left((\operatorname{Tr} M_k\varrho)_{k=1}^{d^2}, (\operatorname{Tr} M_k\sigma)_{k=1}^{d^2}\right).$$

For fixed ϱ and σ, the map

$$\mathrm{POVM}(\mathcal{H}|[d^2]) \ni M \mapsto \left((\operatorname{Tr} \varrho M_k)_{k=1}^{d^2}, (\operatorname{Tr} \sigma M_k)_{k=1}^{d^2}\right) \in \mathbb{R}_+^{d^2} \times \mathbb{R}_+^{d^2} \equiv (\mathbb{R}_+ \times \mathbb{R}_+)^{d^2} \quad (4.28)$$

is continuous. Thus, by Remark 4.16, if $f(0^+)$ and $f'(+\infty)$ are both finite then the map $\mathcal{M} \mapsto S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma))$ is continuous on the compact set $\mathrm{POVM}(\mathcal{H}|[d^2])$, and therefore the supremum in (4.27) is attained. Hence, the only thing left is to prove the assertion when $f(0^+)$ and $f'(+\infty)$ are not both finite.

If $f(0^+) = +\infty$ and $\sigma^0 \nleq \varrho^0$ then for the two-outcome measurement $\mathcal{M} = (\varrho^0, I - \varrho^0)$ we have $S_f(\varrho\|\sigma) = +\infty = S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma))$ (see Corollary 3.4), from which it is trivial that the supremum in (4.27) is attained. Similarly, if $f'(+\infty) = +\infty$ and $\varrho^0 \nleq \sigma^0$ then we can choose $\mathcal{M} = (\sigma^0, I - \sigma^0)$ to arrive at the same conclusion.

Hence, for the rest we assume that $\sigma^0 \leq \varrho^0$ when $f(0^+) = +\infty$, and $\varrho^0 \leq \sigma^0$ when $f'(+\infty) = +\infty$. Note that if $\sigma^0 \leq \varrho^0$ then there exists a positive constant $c_1 > 0$ such that $\sigma \leq c_1 \varrho$, and hence for any measurement operator M, $\operatorname{Tr} \sigma M \leq c_1 \operatorname{Tr} \varrho M$. This means that the map in (4.28) maps $\mathrm{POVM}(\mathcal{H}|[d^2])$ into $A^{[d^2]}_{0,\gamma_1}$, where $\gamma_1 := \arctan c_1$. Similarly, if $\varrho^0 \leq \sigma^0$ then there exists a $c_0 > 0$ such that the map in (4.28) maps $\mathrm{POVM}(\mathcal{H}|[d^2])$ into $A^{[d^2]}_{\gamma_0,\pi/2}$, where $\gamma_0 := \arctan c_0$. Hence we see that in the remaining cases, the map in (4.28) maps $\mathrm{POVM}(\mathcal{H}|[d^2])$ into a domain on which $P_{f,[d^2]}$ is continuous, and thus we can use continuity and compactness again to conclude that the supremum in (4.27) is attained.

The proof of the assertion about (4.23) goes almost the same way. Let $d := \dim \mathcal{H}$, and equip $\mathcal{H}^d := \times_{i=1}^d \mathcal{H}$ with the product topology. Let $\mathrm{ONB}(\mathcal{H})$ be the set of all ONB's $(e_i)_{i=1}^d$ of $\mathcal{H}$. Then $\mathrm{ONB}(\mathcal{H})$ is a compact subset of $\mathcal{H}^d$, and

$$\mathrm{ONB}(\mathcal{H}) \ni (e_i)_{i=1}^d \longmapsto \Big((\langle e_i, \varrho e_i \rangle)_{i=1}^d, \langle e_i, \sigma e_i \rangle)_{i=1}^d \Big)$$

is continuous. Repeating the above argument with this map in place of the one in (4.28), and $S_{f,[d]}$ in place of $S_{f,[d^2]}$, yields the assertion. □

Now we are ready to prove the following:

Theorem 4.18. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ be such that $\varrho^0 \leq \sigma^0$. The following are equivalent:

(i) $S_f(\varrho\|\sigma) = S_f^{\mathrm{meas}}(\varrho\|\sigma)$ for some operator convex function f on $[0, +\infty)$ such that

$$|\operatorname{supp} \mu_f| \geq |\operatorname{spec}(L_\varrho R_{\sigma^{-1}})| + (\dim \mathcal{H})^2.$$

(ii) $\varrho\sigma = \sigma\varrho$.

(iii) $S_f(\varrho\|\sigma) = S_f^{\mathrm{pr}}(\varrho\|\sigma)$ for all convex functions $f : (0, +\infty) \to \mathbb{R}$.

(iv) $S_f(\varrho\|\sigma) = S_f^{\mathrm{pr}}(\varrho\|\sigma)$ for a continuous operator convex function f on $[0, +\infty)$ such that

$$|\operatorname{supp} \mu_f| \geq |\operatorname{spec}(L_\varrho R_{\sigma^{-1}})| + \dim \mathcal{H}.$$

Proof. The implications (ii) $\Longrightarrow$ (iii) $\Longrightarrow$ (iv), and (ii) $\Longrightarrow$ (i) are obvious. Assume that (i) or (iv) holds; then, by Proposition 4.17, there exists a measurement $\mathcal{M}$ such that $S_f(\varrho\|\sigma) = S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma))$. Then, by Theorem 3.18, $S_f(\varrho\|\sigma) = S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma))$ for $f(x) := -x^{1/2}$. A straightforward modification of the argument by Petz in [67, Lemma 4.1] (to avoid the assumption $\sigma > 0$) then shows (ii). □

It is a very natural requirement for a quantum divergence to be invariant under isometric embeddings of a system into a larger system. It is easy to see that both quantum f-divergences S_f and $\widehat{S}_f$ have this invariance property, i.e.,

$$S_f(V\varrho V^* \| V\sigma V^*) = S_f(\varrho\|\sigma)$$

for any $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ and any isometry $V : \mathcal{H} \to \mathcal{K}$, and the same holds true for $\widehat{S}_f$. It is easy to see that the same holds also for the measured f-divergence S_f^{meas}. However, it is not clear whether S_f^{pr} has the same invariance property. In fact, the next proposition says that this is equivalent to the equality $S_f^{\mathrm{meas}} = S_f^{\mathrm{pr}}$.

Proposition 4.19. For every $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ and any convex function f on $(0, +\infty)$, we have:

(1) $S_f^{\mathrm{pr}}(V\varrho V^* \| V\sigma V^*) \geq S_f^{\mathrm{pr}}(\varrho\|\sigma)$ for any isometry $V : \mathcal{H} \to \mathcal{K}$.

(2) $S_f^{\mathrm{meas}}(\varrho\|\sigma) = \sup\left\{ S_f^{\mathrm{pr}}(V\varrho V^* \| V\sigma V^*) : V \text{ isometry} \right\}$.

(3) The following (i) and (ii) are equivalent:

 (i) $S_f^{\mathrm{pr}}(V\varrho V^* \| V\sigma V^*) = S_f^{\mathrm{pr}}(\varrho\|\sigma)$ for any isometry V;

 (ii) $S_f^{\mathrm{meas}}(\varrho\|\sigma) = S_f^{\mathrm{pr}}(\varrho\|\sigma)$.

Proof. (1) For every projective measurement $\mathcal{M} = (P_x)_{x\in\mathcal{X}}$ on $\mathcal{H}$ one can define a projective measurement $\mathcal{M}_V = (Q_x)_{x\in\mathcal{X}\cup\{x_0\}}$, $x_0 \notin \mathcal{X}$, on $\mathcal{K}$, by

$$Q_x := VP_xV^* \quad \text{for} \quad x \in \mathcal{X}, \qquad Q_{x_0} := I_{\mathcal{K}} - VV^*.$$

From $\operatorname{Tr} Q_xV\varrho V^* = \operatorname{Tr} P_x\varrho$ and $\operatorname{Tr} Q_{x_0}V\varrho V^* = 0$ as well as the same for $V\sigma V^*$, it follows that $S_f(\mathcal{M}_V(V\varrho V^*)\|\mathcal{M}_V(V\sigma V^*)) = S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma))$, implying (1).

(2) The inequality $\geq$ is obvious since

$$S_f^{\mathrm{meas}}(\varrho\|\sigma) = S_f^{\mathrm{meas}}(V\varrho V^*\|V\sigma V^*) \geq S_f^{\mathrm{pr}}(V\varrho V^*\|V\sigma V^*)$$

for any isometry V. For the converse, for any measurement $\mathcal{M} = (M_x)_{x\in\mathcal{X}}$ on $\mathcal{H}$, by Naimark's dilation theorem, we get an isometry $V : \mathcal{H} \to \mathcal{K}$ and a projective measurement $\overline{\mathcal{M}} = (P_x)_{x\in\mathcal{X}}$ on $\mathcal{K}$ such that $M_x = V^*P_xV$ for all $x \in \mathcal{X}$. Since $\operatorname{Tr} M_x\varrho = \operatorname{Tr} P_xV\varrho V^*$, we have

$$S_f(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma)) = S_f(\overline{\mathcal{M}}(V\varrho V^*)\|\overline{\mathcal{M}}(V\sigma V^*)) \leq S_f^{\mathrm{pr}}(V\varrho V^*\|V\sigma V^*).$$

(3) is immediate from (1) and (2). □

It is easy to see that monotonicity implies invariance under isometries, but not the other way around; an example for the latter is S_{f_α} with $\alpha > 2$, that is invariant under isometries but not monotone [56, Page 5]. We say that a quantum f-divergence S_f^q is *invariant under partial isometries* if

$$S_f^q(V\varrho V^*\|V\sigma V^*) = S_f^q(\varrho\|\sigma)$$

for any $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ and any partial isometry $V : \mathcal{H} \to \mathcal{K}$ such that $\varrho^0, \sigma^0 \leq V^*V$. It is easy to see that any f-divergence S_f is invariant under partial isometries. Proposition 4.19 yields the following:

Corollary 4.20. For a convex function f on $(0, +\infty)$, the following are equivalent:

(i) S_f^{pr} is invariant under partial isometries;

(ii) S_f^{pr} is invariant under isometries;

(iii) $S_f^{\mathrm{pr}} = S_f^{\mathrm{meas}}$;

(iv) S_f^{pr} is monotone under positive trace-preserving maps;

(v) S_f^{pr} is monotone under CPTP maps.

Proof. (i) $\Longrightarrow$ (ii) is trivial, (ii) $\Longrightarrow$ (iii) follows from Proposition 4.19, (iii) $\Longrightarrow$ (iv) is trivial as S_f^{meas} is monotone under positive trace-preserving maps, and (iv) $\Longrightarrow$ (v) is again trivial. Assume now that (v) holds, and let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ and $V : \mathcal{H} \to \mathcal{K}$ be a partial isometry such that $\varrho^0, \sigma^0 \le V^*V$. We use a construction from [72, Section 4.6.3] to prove (i). For fixed states $\tau_{\mathcal{H}} \in \mathcal{B}(\mathcal{H})$, $\tau_{\mathcal{K}} \in \mathcal{B}(\mathcal{K})$, define $\Phi_{\mathcal{H}\to\mathcal{K}}(\cdot) := V(\cdot)V^* + \tau_{\mathcal{K}} \operatorname{Tr}(\cdot)(I - V^*V)$ and $\Phi_{\mathcal{K}\to\mathcal{H}}(\cdot) := V^*(\cdot)V + \tau_{\mathcal{H}} \operatorname{Tr}(\cdot)(I - VV^*)$. Then $\Phi_{\mathcal{H}\to\mathcal{K}}$ and $\Phi_{\mathcal{K}\to\mathcal{H}}$ are CPTP maps such that $\Phi_{\mathcal{H}\to\mathcal{K}}(\varrho) = V\varrho V^*$, $\Phi_{\mathcal{K}\to\mathcal{H}}(V\varrho V^*) = \varrho$, and similarly for σ. The assumed monotonicity of S_f^{pr} then yields $S_f^{\mathrm{pr}}(\varrho\|\sigma) \le S_f^{\mathrm{pr}}(V\varrho V^*\|V\sigma V^*) \le S_f^{\mathrm{pr}}(\varrho\|\sigma)$, proving (i). □

Analogously to the corresponding definitions for f-divergences, one can define the measured versions of the Rényi divergences as

$$D_\alpha^{\mathrm{meas}}(\varrho\|\sigma) := \sup\{D_\alpha(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma)) : \mathcal{M} \text{ measurement on } \mathcal{H}\}, \tag{4.29}$$

$$D_\alpha^{\mathrm{pr}}(\varrho\|\sigma) := \sup\{D_\alpha(\mathcal{M}(\varrho)\|\mathcal{M}(\sigma)) : \mathcal{M} \text{ projective measurement on } \mathcal{H}\} \tag{4.30}$$

for every $\alpha \in (0, +\infty)$, where $D_1(\varrho\|\sigma) := \frac{1}{\operatorname{Tr}\varrho} S(\varrho\|\sigma)$, according to (3.15). For $\alpha \ne 1$, these are simply functions of $S_{f_\alpha}^{\mathrm{meas}}$ and $S_{f_\alpha}^{\mathrm{pr}}$, respectively. Note that D_α is monotone non-increasing under measurements for $\alpha \in (0, 2]$ according to (3.14) and Proposition 3.12. While for $\alpha > 2$, D_α is not monotone under CPTP maps, it is still monotone under measurements, as it has been shown in [27, Section 3.7]. Thus, it is meaningful to take the suprema in the definitions (4.29) and (4.30).

Now we review the results of [10] on the equality $S_f^{\mathrm{pr}} = S_f^{\mathrm{meas}}$ for the functions f_α and η in (4.26). The key ingredients are the following variational expressions, given in [10, Lemma 3]:

$$S_{f_\alpha}^{\mathrm{pr}}(\varrho\|\sigma) = \sup_{\omega \in \mathcal{B}(\mathcal{H})_{++}} \begin{cases} s(\alpha)\alpha \operatorname{Tr} \varrho\omega + s(\alpha)(1-\alpha) \operatorname{Tr} \sigma\omega^{\frac{\alpha}{\alpha-1}}, & \alpha \in (0, 1/2), \\ s(\alpha)\alpha \operatorname{Tr} \varrho\omega^{\frac{\alpha-1}{\alpha}} + s(\alpha)(1-\alpha) \operatorname{Tr} \sigma\omega, & \alpha \in [1/2, +\infty). \end{cases} \tag{4.31}$$

Here, note that the above expressions hold for general $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, though proved in [10] under the assumption $\varrho^0 \le \sigma^0$. In fact, if $\varrho^0 \not\le \sigma^0$, then both sides of (4.31) are $+\infty$ when $\alpha > 1$, and (4.31) when $\alpha \in (0, 1)$ follows by taking $\sup_{\varepsilon>0}$ of both sides of the expression for ϱ and $\sigma + \varepsilon I$, noting that $S_{f_\alpha}^{\mathrm{pr}}(\varrho\|\sigma) = \sup_{\varepsilon>0} S_{f_\alpha}^{\mathrm{pr}}(\varrho\|\sigma + \varepsilon I)$.

The following Proposition 4.21 is the same as Theorems 2 and 4 in [10]; here we provide a proof based on (4.31) and Proposition 4.19 (2), different from the one in [10].

Proposition 4.21. Let $f = f_\alpha$ for $\alpha \in (0, +\infty)$ or $f(x) = \eta(x) = x \log x$. Then $S_f^{\mathrm{meas}} = S_f^{\mathrm{pr}}$, and hence $D_\alpha^{\mathrm{meas}} = D_\alpha^{\mathrm{pr}}$ for every $\alpha \in (0, +\infty)$.

Proof. Assume that $\alpha \in (0, 1/2)$. By (4.31), for any $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ and any isometry $V : \mathcal{H} \to \mathcal{K}$, we have

$$S_{f_\alpha}^{\mathrm{pr}}(V\varrho V^*\|V\sigma V^*) = \sup_{\omega \in \mathcal{B}(\mathcal{H})_{++}} s(\alpha)\alpha \operatorname{Tr} V\varrho V^*\omega + s(\alpha)(1-\alpha) \operatorname{Tr} V\sigma V^*\omega^{\frac{\alpha}{\alpha-1}}.$$

Since $x \mapsto s(\alpha)(1-\alpha)x^{\frac{\alpha}{\alpha-1}}$ is operator concave, we have $s(\alpha)(1-\alpha)V^*\omega^{\frac{\alpha}{\alpha-1}}V \le s(\alpha)(1-\alpha)\,(V^*\omega V)^{\frac{\alpha}{\alpha-1}}$; see, e.g., [32, Theorem 2.5.7]. Moreover, $\omega > 0$ implies $V^*\omega V > 0$, and hence

$$\begin{aligned} S_{f_\alpha}^{\mathrm{pr}}(V\varrho V^*\|V\sigma V^*) &\le \sup_{\omega \in \mathcal{B}(\mathcal{H})_{++}} s(\alpha)\alpha \operatorname{Tr} \varrho\,(V^*\omega V) + s(\alpha)(1-\alpha) \operatorname{Tr} \sigma\,(V^*\omega V)^{\frac{\alpha}{\alpha-1}} \\ &= \sup_{\tilde\omega \in \mathcal{B}(\mathcal{K})_{++}} s(\alpha)\alpha \operatorname{Tr} \varrho\tilde\omega + s(\alpha)(1-\alpha) \operatorname{Tr} \sigma\tilde\omega^{\frac{\alpha}{\alpha-1}} \end{aligned}$$

$$= S_{f_\alpha}^{\mathrm{pr}}(\varrho\|\sigma).$$

Taking now the supremum over all isometries V and using Proposition 4.19 (2), we get the assertion. The proof for $\alpha \ge 1/2$ goes the same way.

Consider now the Rényi divergences D_α defined in Example 3.5. By the above, $S_{f_\alpha}^{\mathrm{pr}} = S_{f_\alpha}^{\mathrm{meas}}$ for all $\alpha \in (0,+\infty)$, and hence $D_\alpha^{\mathrm{pr}} = D_\alpha^{\mathrm{meas}}$ for all $\alpha \in (0,+\infty) \setminus \{1\}$, with the obvious definitions of the latter quantities; see (4.29) and (4.30). Moreover, (3.15) implies

$$\frac{1}{\operatorname{Tr}\varrho} S^{\mathrm{pr}}(\varrho\|\sigma) = \sup_{\alpha\in(0,1)} D_\alpha^{\mathrm{pr}}(\varrho\|\sigma), \qquad \frac{1}{\operatorname{Tr}\varrho} S^{\mathrm{meas}}(\varrho\|\sigma) = \sup_{\alpha\in(0,1)} D_\alpha^{\mathrm{meas}}(\varrho\|\sigma).$$

Combining these yields the assertion for $f = \eta$. □

Remark 4.22. From Propositions 4.19 (3) and 4.21 we also see that $S_{f_\alpha}^{\mathrm{pr}}$ and $S^{\mathrm{pr}} = S_\eta^{\mathrm{pr}}$ are invariant under isometries. If one could prove these invariances directly, that would immediately imply Proposition 4.21, again due to Proposition 4.19 (3).

Remark 4.23. In [10], $S^{\mathrm{pr}} = S^{\mathrm{meas}}$ was proved using a separate variational expression for the projectively measured relative entropy S^{pr}. The same argument as above, using operator concavity and Proposition 4.19 (2), could be applied to that variational formula to obtain $S^{\mathrm{pr}} = S^{\mathrm{meas}}$; however, in the above proof we could proceed in a simpler way, without using the variational formula for S^{pr}.

Consider also the sandwiched Rényi divergences, defined in (1.3). These quantities have been shown to be monotone non-increasing under CPTP maps for $\alpha \ge 1/2$ in [8, 24, 52, 56, 73]; in fact, for $\alpha \ge 1$, they are also monotone under positive trace-preserving maps [8, 55]. By the Araki-Lieb-Thirring inequality [4, 49], we have

$$D_\alpha^*(\varrho\|\sigma) \le D_\alpha(\varrho\|\sigma) \tag{4.32}$$

for any ϱ, σ and $\alpha \in (0,+\infty)$ [73], with equality if and only if ϱ commutes with σ or $\alpha = 1$ [31]. In particular, monotonicity of D_α^* for $\alpha > 2$ and (4.32) give an alternative proof for the non-increasing property of D_α under measurements for $\alpha > 2$. More generally, if $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ is a positive trace-preserving map, and $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ are such that $\Phi(\varrho)$ and $\Phi(\sigma)$ commute, then $D_\alpha(\Phi(\varrho)\|\Phi(\sigma)) \le D_\alpha^*(\varrho\|\sigma) \le D_\alpha(\varrho\|\sigma)$ for any $\alpha \in [1/2,+\infty)$; in particular, $D_\alpha(\Phi(\varrho)\|\Phi(\sigma)) \le D_\alpha(\varrho\|\sigma)$ also for $\alpha > 2$.

It is straightforward from the definition of the measured Rényi divergence that for any fixed ϱ, σ, $n \mapsto D_\alpha^{\mathrm{meas}}(\varrho^{\otimes n}\|\sigma^{\otimes n})$ is superadditive, and hence

$$\overline{D}_\alpha^{\mathrm{meas}}(\varrho\|\sigma) := \sup_{n\in\mathbb{N}} \frac{1}{n} D_\alpha^{\mathrm{meas}}\left(\varrho^{\otimes n}\|\sigma^{\otimes n}\right) = \lim_{n\to\infty} \frac{1}{n} D_\alpha^{\mathrm{meas}}\left(\varrho^{\otimes n}\|\sigma^{\otimes n}\right). \tag{4.33}$$

We call $\overline{D}_\alpha^{\mathrm{meas}}$ the *regularized measured Rényi divergence*. Moreover, for $\alpha \ge 1/2$ we have

$$\overline{D}_\alpha^{\mathrm{meas}}(\varrho\|\sigma) = D_\alpha^*(\varrho\|\sigma); \tag{4.34}$$

see [36] for $\alpha = 1$, [52] for $\alpha > 1$, and [29] for $\alpha \in [1/2, 1)$. For $\alpha \in (0, 1/2)$ this is no longer true, and instead we have $D_\alpha^*(\varrho\|\sigma) \le D_\alpha^{\mathrm{meas}}(\varrho\|\sigma)$, with strict inequality for non-commuting ϱ, σ, as it has been shown very recently in [10, Theorem 7]. However, it is true for any $\alpha \in (0,+\infty)$ and any $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ that there exists a sequence of measurements $\mathcal{M}_n$ on $\mathcal{H}^{\otimes n}$, $n \in \mathbb{N}$, such that

$$D_\alpha^*(\varrho\|\sigma) = \lim_{n\to\infty} \frac{1}{n} D_\alpha\left(\mathcal{M}_n(\varrho^{\otimes n})\|\mathcal{M}_n(\sigma^{\otimes n})\right).$$

Such a measurement can be chosen as a von Neumann measurement in a common eigenbasis of $\sigma^{\otimes n}$ and $\mathcal{P}_{\sigma^{\otimes n}}(\varrho^{\otimes n})$, where $\mathcal{P}_{\sigma^{\otimes n}}$ is the pinching by the spectral projections of $\sigma^{\otimes n}$; see [36] for $\alpha = 1$, [52, Theorem 3.7] for $\alpha > 1$, and Lemma 3 and Corollary 4 in [29] for $\alpha \in (0, 1)$.

The relations of the various quantum Rényi divergences mentioned above can be summarized as follows:

Proposition 4.24. For any $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, we have

$$D^*_\alpha(\varrho\|\sigma) \le D^{\mathrm{pr}}_\alpha(\varrho\|\sigma) = D^{\mathrm{meas}}_\alpha(\varrho\|\sigma) \le \overline{D}^{\mathrm{meas}}_\alpha(\varrho\|\sigma) \le D_\alpha(\varrho\|\sigma), \qquad \alpha \in (0, 1/2), \tag{4.35}$$

$$D^{\mathrm{pr}}_\alpha(\varrho\|\sigma) = D^{\mathrm{meas}}_\alpha(\varrho\|\sigma) \le \overline{D}^{\mathrm{meas}}_\alpha(\varrho\|\sigma) = D^*_\alpha(\varrho\|\sigma) \le D_\alpha(\varrho\|\sigma), \qquad \alpha \in [1/2, +\infty). \tag{4.36}$$

If ϱ and σ commute or $D_\alpha(\varrho\|\sigma) = +\infty$ then all the inequalities above are equalities; otherwise all the inequalities are strict, except the first inequality in (4.36) for $\alpha = 1/2$, the last inequality in (4.36) for $\alpha = 1$, and possibly the last two inequalities in (4.35), of which at least one is strict.

Proof. When ϱ and σ commute or $D_\alpha(\varrho\|\sigma) = +\infty$ then it is straightforward that all the above quantities are equal to each other, and hence for the rest we assume the contrary.

The relations $D^*_\alpha(\varrho\|\sigma) \le D^{\mathrm{pr}}_\alpha(\varrho\|\sigma) = D^{\mathrm{meas}}_\alpha(\varrho\|\sigma)$ for $\alpha \in (0, 1/2)$, with strict inequality for non-commuting ϱ, σ, as well as $D^{\mathrm{pr}}_\alpha(\varrho\|\sigma) = D^{\mathrm{meas}}_\alpha(\varrho\|\sigma)$ for $\alpha \in [1/2, +\infty)$, and the strict inequality $D^{\mathrm{meas}}_\alpha(\varrho\|\sigma) < D^*_\alpha(\varrho\|\sigma)$ for non-commuting ϱ, σ and $\alpha > 1/2$, were proved in [10].

If the last two inequalities in (4.35) are both equalities then we also have $D^{\mathrm{pr}}_\alpha(\varrho\|\sigma) = D_\alpha(\varrho\|\sigma)$, and $\varrho\sigma = \sigma\varrho$ follows by Theorem 4.18 applied to $f_\alpha(t) = -t^\alpha$. Finally, the last inequality in (4.36) and its equality case follow from the Araki-Lieb-Thirring inequality and its equality case, as discussed above. □

Remark 4.25. The case $\alpha = 1/2$ is special in the sense that $D^*_{1/2} = -2\log F$, where F is the fidelity, so that $D^*_{1/2} = D^{\mathrm{meas}}_{1/2}$; see, e.g., [58, Chapter 9].

Remark 4.26. It is an interesting open problem to find a closed expression for $\overline{D}^{\mathrm{meas}}_\alpha(\varrho\|\sigma)$ for $\alpha \in (0, 1/2)$; one possible candidate is $D_\alpha(\varrho\|\sigma)$, based on (4.35). This is related to another question left open in the above proposition, namely whether both of the last two inequalities in (4.35) are strict for non-commuting ϱ and σ.

Remark 4.27. Note that both the standard and the sandwiched Rényi divergences are additive, i.e., $D_\alpha\left(\varrho^{\otimes n}\|\sigma^{\otimes n}\right) = nD_\alpha(\varrho\|\sigma)$, $D^*_\alpha\left(\varrho^{\otimes n}\|\sigma^{\otimes n}\right) = nD^*_\alpha(\varrho\|\sigma)$ for all ϱ, σ, all $n \in \mathbb{N}$, and all $\alpha \in (0, +\infty)$. By Proposition 4.24 and (4.33)–(4.34), we see that the measured Rényi divergences are not additive for $\alpha > 1/2$; more precisely, if $\varrho\sigma \ne \sigma\varrho$ then for every $\alpha > 1/2$ there exists an $n \in \mathbb{N}$ such that $D^{\mathrm{meas}}_\alpha(\varrho^{\otimes n}\|\sigma^{\otimes n}) > nD^{\mathrm{meas}}_\alpha(\varrho\|\sigma)$. It is an open question whether the same holds for $\alpha \in (0, 1/2)$.

We close this section by proving the strict positivity of f-divergences (when properly normalized as $f(1) = 0$) on pairs of quantum states. More precisely, we prove a Pinsker-type inequality for the projectively measured f-divergences. While we don't use it in the rest of the paper, it is interesting in its own right.

The quantum version of the *Pinsker* (or *Pinsker-Csiszár*) *inequality*

$$\frac{1}{2}\|\varrho - \sigma\|_1^2 \le S(\varrho\|\sigma) \tag{4.37}$$

for quantum states ϱ, σ was first shown in [35], where $\|\cdot\|_1$ denotes the trace-norm. The following proposition is not only a generalization to general f-divergences, but it also strengthens (4.37) even in the case of the relative entropy, according to Theorem 4.18.

Proposition 4.28. Let f be an operator convex function on $(0,+\infty)$ with $f(1)=0$. Then for every density operators ϱ,σ on $\mathcal{H}$,

$$\frac{f''(1)}{2}\,\|\varrho-\sigma\|_1^2\le S_f^{\mathrm{pr}}(\varrho\|\sigma),$$

where $S_f^{\mathrm{pr}}(\varrho\|\sigma)$ is given in (4.22). Hence, $\frac{f''(1)}{2}\,\|\varrho-\sigma\|_1^2\le S_f^{q}(\varrho\|\sigma)$ holds for every quantum f-divergence in the sense stated in Section 3.1. Here, $f''(1)>0$ if and only if f is non-linear.

Proof. Let $(e_i)_{i=1}^d$ be an orthonormal basis consisting of eigenvectors of $\varrho-\sigma$, and define $\mathcal{E}(X):=\sum_{i=1}^d\langle e_i,Xe_i\rangle\,|e_i\rangle\langle e_i|$, $X\in\mathcal{B}(\mathcal{H})$. Set $p:=\mathcal{E}(\varrho)=\sum_{i=1}^d p_i|e_i\rangle\langle e_i|$ and $q:=\mathcal{E}(\sigma)=\sum_{i=1}^d q_i|e_i\rangle\langle e_i|$. Since $\varrho-\sigma=\mathcal{E}(\varrho-\sigma)=p-q$ and $S_f(p\|q)\le S_f^{\mathrm{pr}}(\varrho\|\sigma)$, it suffices to show that

$$\frac{f''(1)}{2}\,\|p-q\|_1^2\le S_f(p\|q). \tag{4.38}$$

Although this is known [26, Theorem 3] for a more general class of convex functions f, we have, for operator convex f, the following simple proof based on the integral expression in (2.2). As easily verified, note that

$$f''(1)=2\biggl(c+\int_{[0,+\infty)}\frac{1}{1+s}\,d\lambda(s)\biggr), \tag{4.39}$$

which shows that $f''(1)>0$ if and only if f is non-linear. We may assume by continuity that $p,q>0$, and we have the expression

$$S_f(p\|q)=c\sum_{i=1}^d\frac{(p_i-q_i)^2}{q_i}+\int_{[0,+\infty)}\sum_{i=1}^d\frac{(p_i-q_i)^2}{p_i+sq_i}\,d\lambda(s). \tag{4.40}$$

We estimate

$$\begin{aligned}\sum_{i=1}^d|p_i-q_i|&=\sum_{i=1}^d\frac{|p_i-q_i|}{\sqrt{q_i}}\sqrt{q_i}\le\Biggl(\sum_{i=1}^d\frac{(p_i-q_i)^2}{q_i}\Biggr)^{1/2}\Biggl(\sum_{i=1}^d q_i\Biggr)^{1/2}\\&=\Biggl(\sum_{i=1}^d\frac{(p_i-q_i)^2}{q_i}\Biggr)^{1/2},\end{aligned} \tag{4.41}$$

and for every $s\in[0,+\infty)$,

$$\begin{aligned}\sum_{i=1}^d|p_i-q_i|&=\sum_{i=1}^d\frac{|p_i-q_i|}{\sqrt{p_i+sq_i}}\sqrt{p_i+sq_i}\le\Biggl(\sum_{i=1}^d\frac{(p_i-q_i)^2}{p_i+sq_i}\Biggr)^{1/2}\Biggl(\sum_{i=1}^d(p_i+sq_i)\Biggr)^{1/2}\\&=\Biggl(\sum_{i=1}^d\frac{(p_i-q_i)^2}{p_i+sq_i}\Biggr)^{1/2}(1+s)^{1/2}.\end{aligned} \tag{4.42}$$

Combining (4.39)–(4.42) yields (4.38). □

5 Reversibility via Rényi divergences

The notion of the *α-z-Rényi relative entropy* was first introduced in [39, Section 3.3], and further studied in [6]. It is defined for two positive operators $\varrho,\sigma\in\mathcal{B}(\mathcal{H})_+$ with $\varrho^0\le\sigma^0$ as

$$D_{\alpha,z}(\varrho\|\sigma):=\frac{1}{\alpha-1}\log\mathrm{Tr}\Bigl(\sigma^{\frac{1-\alpha}{2z}}\varrho^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}}\Bigr)^z=\frac{1}{\alpha-1}\log\mathrm{Tr}\Bigl(\varrho^{\frac{\alpha}{2z}}\sigma^{\frac{1-\alpha}{z}}\varrho^{\frac{\alpha}{2z}}\Bigr)^z,$$

for any $\alpha \in \mathbb{R} \setminus \{1\}$ and $z > 0$. Below we restrict to the case $\alpha, z > 0$ with $\alpha \neq 1$. The above definition can be extended to general $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ as

$$D_{\alpha,z}(\varrho\|\sigma) := \lim_{\varepsilon \searrow 0} \frac{1}{\alpha - 1} \log \operatorname{Tr}\Big(\varrho^{\frac{\alpha}{2z}} (\sigma + \varepsilon I)^{\frac{1-\alpha}{z}} \varrho^{\frac{\alpha}{2z}}\Big)^z. \tag{5.1}$$

Lemma 5.1. The limit in (5.1) exists, and is equal to

$$\begin{cases} \frac{1}{\alpha-1} \log \operatorname{Tr}\Big(\varrho^{\frac{\alpha}{2z}} \sigma^{\frac{1-\alpha}{z}} \varrho^{\frac{\alpha}{2z}}\Big)^z, & \alpha \in (0,1) \text{ or } \varrho^0 \leq \sigma^0, \\ +\infty, & \text{otherwise.} \end{cases}$$

Proof. The only slightly non-trivial part of the claim is when $\alpha > 1$ and $\varrho^0 \not\leq \sigma^0$. In this case, there exists a unit vector $\psi \perp \operatorname{supp} \sigma$ such that $\langle \psi, \varrho^0 \psi \rangle > 0$. Note that $(\sigma + \varepsilon I)^{\frac{1-\alpha}{z}} \geq \varepsilon^{\frac{1-\alpha}{z}} |\psi\rangle\langle\psi|$, and thus

$$\begin{aligned} \operatorname{Tr}\Big(\varrho^{\frac{\alpha}{2z}} (\sigma + \varepsilon I)^{\frac{1-\alpha}{z}} \varrho^{\frac{\alpha}{2z}}\Big)^z \geq \varepsilon^{1-\alpha} \operatorname{Tr}\Big(\varrho^{\frac{\alpha}{2z}} |\psi\rangle\langle\psi| \varrho^{\frac{\alpha}{2z}}\Big)^z &= \varepsilon^{1-\alpha} \operatorname{Tr}\Big(|\psi\rangle\langle\psi| \varrho^{\frac{\alpha}{z}} |\psi\rangle\langle\psi|\Big)^z \\ &= \varepsilon^{1-\alpha} \Big\langle \psi, \varrho^{\frac{\alpha}{z}} \psi \Big\rangle^z, \end{aligned}$$

that tends to $+\infty$ as $\varepsilon \searrow 0$. ∎

We also introduce the notation

$$Q_{\alpha,z}(\varrho\|\sigma) := \lim_{\varepsilon \searrow 0} \operatorname{Tr}\Big(\varrho^{\frac{\alpha}{2z}} (\sigma + \varepsilon I)^{\frac{1-\alpha}{z}} \varrho^{\frac{\alpha}{2z}}\Big)^z = \begin{cases} \operatorname{Tr}\Big(\varrho^{\frac{\alpha}{2z}} \sigma^{\frac{1-\alpha}{z}} \varrho^{\frac{\alpha}{2z}}\Big)^z, & \alpha \in (0,1) \text{ or } \varrho^0 \leq \sigma^0, \\ +\infty, & \text{otherwise,} \end{cases}$$

so that

$$D_{\alpha,z}(\varrho\|\sigma) = \frac{1}{\alpha - 1} \log Q_{\alpha,z}(\varrho\|\sigma).$$

The α-z-Rényi relative entropies have the following monotonicity property: For any $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, and any CPTP map $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$,

$$D_{\alpha,z}(\Phi(\varrho)\|\Phi(\sigma)) \leq D_{\alpha,z}(\varrho\|\sigma), \tag{5.2}$$

whenever

(a) $0 < \alpha < 1, \ z \geq \max\{\alpha, 1 - \alpha\}$, or

(b) $1 < \alpha \leq 2, \ z = 1$, or

(c) $1 < \alpha = z$, or

(d) $1 < \alpha \leq 2, \ z = \alpha/2$.

See [33] for the proof of (a), [2] for (b), [8, 24] for (c), and [14] for (d) (cf. also [6, Theorem 1]).

The *sandwiched Rényi divergence* introduced in [56, 73] is

$$D_\alpha^*(\varrho\|\sigma) := \frac{1}{\alpha - 1} \log \operatorname{Tr}\Big(\sigma^{\frac{1-\alpha}{2\alpha}} \varrho \sigma^{\frac{1-\alpha}{2\alpha}}\Big)^\alpha,$$

which is the $z = \alpha$ case of the α-z-Rényi relative entropy. From (5.2) in cases (a) and (c) we have for any $\alpha \in [1/2, +\infty) \setminus \{1\}$

$$D^*_\alpha(\Phi(\varrho)\|\Phi(\sigma)) \le D^*_\alpha(\varrho\|\sigma). \tag{5.3}$$

As presented in (1.3) and (1.4) in the Introduction, the formulas of $D^*_\alpha(\varrho\|\sigma)$ and $D_{\alpha,z}(\varrho\|\sigma)$ are often given with division by $\operatorname{Tr}\varrho$ inside the logarithm. However, the difference between with or without this division is irrelevant to our discussions on the monotonicity inequality and the characterization of its equality case. Thus, we here adopt, for the sake of simplicity, the definitions without the division by $\operatorname{Tr}\varrho$.

In this section, we shall prove monotonicity (5.2) in some special cases of ϱ, σ and Φ, for some ranges of α, z, including values not covered in previous works. Our main result is the characterization of equality in the monotonicity inequality (5.2) in these cases. For the latter, we will consider the following possible characterizations:

(E0) $D^*_\alpha(\Phi(\varrho)\|\Phi(\sigma)) = D^*_\alpha(\varrho\|\sigma)$,

(E1) $D_{\alpha,z}(\Phi(\varrho)\|\Phi(\sigma)) = D_{\alpha,z}(\varrho\|\sigma)$,

(E2) $\Phi^*(\Phi(\varrho)) = \varrho$, $\Phi^*(\Phi(\sigma)) = \sigma$,

(E3) $\Phi^*_\sigma(\Phi(\varrho)) = \varrho$, $\Phi^*_\sigma(\Phi(\sigma)) = \sigma$, (see (3.20) for the map Φ^*_σ),

(E4) $\Phi^*_\varrho(\Phi(\varrho)) = \varrho$, $\Phi^*_\varrho(\Phi(\sigma)) = \sigma$,

(E5) there exists a unitary U such that $\Phi(\varrho) = U\varrho U^*$, $\Phi(\sigma) = U\sigma U^*$.

Theorem 5.2. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, and let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be a bistochastic map. The monotonicity inequality (5.2) holds if at least one of the following conditions is satisfied:

(i) $\alpha \le z \le 1$ and $\sigma \in \mathcal{F}_\Phi$,

(ii) $0 < 1-\alpha \le z \le 1$ and $\varrho \in \mathcal{F}_\Phi$,

(iii) $\alpha \ge z \ge \max\{1, \alpha/2\}$ and $\sigma \in \mathcal{F}_\Phi$,

(iv) $\alpha > 1$, $z \ge \max\{1, \alpha-1\}$, and $\varrho \in \mathcal{F}_\Phi$.

If we also assume that Φ is 2-positive, then we have the following characterizations of equality in the monotonicity inequality:

(1) If (i) holds with $\varrho^0 \le \sigma^0$, then we have (E1) $\Longleftrightarrow$ (E2) $\Longleftrightarrow$ (E3) $\Longleftrightarrow$ (E5).

(2) If (i) holds with $z \ne \alpha$ and $\sigma^0 \le \varrho^0$, then we have (E1) $\Longleftrightarrow$ (E4).

(3) If (ii) holds with $\sigma^0 \le \varrho^0$, then we have (E1) $\Longleftrightarrow$ (E2) $\Longleftrightarrow$ (E4) $\Longleftrightarrow$ (E5).

(4) If (ii) holds with $z \ne 1-\alpha$ and $\varrho^0 \le \sigma^0$, then we have (E1) $\Longleftrightarrow$ (E3).

(5) If (iii) holds with $\varrho^0 \le \sigma^0$, then we have (E1) $\Longleftrightarrow$ (E2) $\Longleftrightarrow$ (E3) $\Longleftrightarrow$ (E5).

(6) If (iv) holds with $z \ne \alpha - 1$ and $\sigma^0 = I$, then we have (E1) $\Longleftrightarrow$ (E3).

Moreover, without the assumption that Φ is 2-positive, we have (E1) $\Longleftrightarrow$ (E2) $\Longleftrightarrow$ (E3) in (1) and (5), and (E1) $\Longleftrightarrow$ (E2) $\Longleftrightarrow$ (E4) in (3).

Before giving the proof of Theorem 5.2, we give some remarks and a corollary.

Remark 5.3. For $\alpha > 1$, unless $\varrho^0 \leq \sigma^0$, we have $D_{\alpha,z}(\varrho\|\sigma) = +\infty$, so that the monotonicity inequality (5.2) holds trivially, while the preservation of $D_{\alpha,z}(\varrho\|\sigma)$ has no implication on reversibility in general. Therefore, in cases (iii) and (iv), reversibility cannot be obtained in general, if instead of the conditions in (5) and (6) above, one assumes $\sigma^0 \leq \varrho^0$ as in (2) or (3).

Remark 5.4. Note that in the cases (2), (4), and (6) in Theorem 5.2, we do not get (E5) in general. For instance, with the notations of Theorem 3.19 where $\mathcal{H}_1 = \mathcal{H}_2 = \bigoplus_{k=1}^r \mathcal{H}_{k,L} \otimes \mathcal{H}_{k,R}$, let ϱ, σ, and Φ be given as

$$\varrho = \bigoplus_k \varrho_k \otimes \omega_k, \qquad \sigma = \bigoplus_k \sigma_k \otimes \omega_k, \qquad \Phi(X_k \otimes Y_k) = U_k X_k U_k^* \otimes \eta_k(Y_k),$$

such that the conditions of (2) are satisfied. Then it is clear that $\Phi_\varrho^*(\Phi(\sigma)) = \sigma$, i.e., (E4) holds. Now, assume that $\sigma_i = 0$ for some i; then the condition $\sigma \in \mathcal{F}_\Phi$ imposes no restriction on η_i. Hence, for this i, we can take ω_i and η_i so that the spectrum of $\eta_i(\omega_i)$ is different from the spectrum of ω_i, while for all $k \neq i$, $\eta_k(\cdot) = V_k \cdot V_k^*$ with some unitaries V_k. Then it is clear that there exists no unitary U such that $\Phi(\varrho) = U\varrho U^*$, i.e., (E5) does not hold.

From the $z = \alpha$ case of the above theorem we have

Corollary 5.5. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, and let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be a bistochastic map. The monotonicity inequality (5.3) holds if one of the following conditions is satisfied:

(i) $\sigma \in \mathcal{F}_\Phi$ (for arbitrary $\alpha \in (0, +\infty) \setminus \{1\}$),

(ii) $1/2 \leq \alpha < 1$ and $\varrho \in \mathcal{F}_\Phi$.

If Φ is 2-positive, then we have the following characterizations of equality in the monotonicity inequality:

(1) If (i) holds with $\varrho^0 \leq \sigma^0$, then we have (E0) $\Longleftrightarrow$ (E2) $\Longleftrightarrow$ (E3) $\Longleftrightarrow$ (E5).

(2) If (ii) holds with $\sigma^0 \leq \varrho^0$, then we have (E0) $\Longleftrightarrow$ (E2) $\Longleftrightarrow$ (E4) $\Longleftrightarrow$ (E5).

(3) If (ii) holds with $\alpha \neq 1/2$ and $\varrho^0 \leq \sigma^0$, then we have (E0) $\Longleftrightarrow$ (E3) $\Longleftrightarrow$ (E5).

Moreover, without the assumption that Φ is 2-positive, we have (E0) $\Longleftrightarrow$ (E2) $\Longleftrightarrow$ (E3) in (1) and (E0) $\Longleftrightarrow$ (E2) $\Longleftrightarrow$ (E4) in (2).

Remark 5.6. (a) Note that the monotonicity in (ii), and in (i) for $\alpha \geq 1/2$ above are special cases of the general monotonicity (5.3) for $\alpha \geq 1/2$, although they are derived in a different way than the known proofs of (5.3). On the other hand, the monotonicity (5.3) does not hold in general for $\alpha \in (0, 1/2)$ (see [10, Section IV]), and hence for this range of α, the monotonicity in (i) does not follow from known monotonicity results.

(b) A special case of the monotonicity in (i) of Corollary 5.5 above is the monotonicity under the pinching by the spectral projections of σ, given in [56, Proposition 14].

(c) Concurrently to our paper, Jenčová [41] proved the characterization "(E0) for some $\alpha > 1 \Longleftrightarrow$ (E3)" when $\varrho^0 \leq \sigma^0$, from which the characterizations in Corollary 5.5 follow easily when $\alpha > 1$.

The case $\alpha = 2$ is special, as reversibility can be obtained easily from the preservation of D_2^*, as has been shown very recently in [41, Lemma 2]. Below we give a different proof.

Proposition 5.7. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ with $\varrho^0 \le \sigma^0$ and $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ be a 2-positive trace-preserving (not necessarily bistochastic) map. Then

$$D_2^*(\Phi(\varrho)\|\Phi(\sigma)) = D_2^*(\varrho\|\sigma) \iff \Phi_\sigma^*(\Phi(\varrho)) = \varrho.$$

Proof. When $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ are density operators with $\sigma > 0$, since

$$\big\langle \varrho - \sigma, L_\sigma^{-1/2} R_\sigma^{-1/2}(\varrho - \sigma)\big\rangle_{\mathrm{HS}} = \mathrm{Tr}(\varrho - \sigma)\sigma^{-1/2}(\varrho - \sigma)\sigma^{-1/2} = \mathrm{Tr}\big(\sigma^{-1/4}\varrho\sigma^{-1/4}\big)^2 - 1,$$

one finds that $D_2^*(\Phi(\varrho)\|\Phi(\sigma)) = D_2^*(\varrho\|\sigma)$ if and only if

$$\big\langle \Phi(\varrho - \sigma), \Omega_{\Phi(\sigma)}^\kappa(\Phi(\varrho - \sigma))\big\rangle_{\mathrm{HS}} = \big\langle \varrho - \sigma, \Omega_\sigma^\kappa(\varrho - \sigma)\big\rangle_{\mathrm{HS}}$$

with $\kappa(x) := x^{-1/2}$. By virtue of (x) of Theorem 3.18, this implies that Φ is reversible on $\{\varrho, \sigma\}$ if and only if $D_2^*(\Phi(\varrho)\|\Phi(\sigma)) = D_2^*(\varrho\|\sigma)$. This result can immediately be extended to general $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ with $\varrho^0 \le \sigma^0$ by normalizing ϱ, σ and restricting Φ to $\sigma^0\mathcal{B}(\mathcal{H})\sigma^0 = \mathcal{B}(\sigma^0\mathcal{H})$. □

Before we give the proof of Theorem 5.2, we need some preparation, given below. For any self-adjoint $X \in \mathcal{B}(\mathcal{H})$, we denote by $\lambda^\downarrow(X) := (\lambda_1^\downarrow(X), \dots, \lambda_d^\downarrow(X))$ the vector of the decreasingly ordered eigenvalues of X, where $d := \dim \mathcal{H}$. The following Lemmas 5.8 and 5.9 are standard; we include their proofs for readers' convenience.

Lemma 5.8. For any $X \in \mathcal{B}(\mathcal{H})_{\mathrm{sa}}$, and any $k \in \{1, \dots, d\}$,

$$\lambda_1^\downarrow(X) + \dots + \lambda_k^\downarrow(X) = \max\{\mathrm{Tr}\, XA : 0 \le A \le I,\ \mathrm{Tr}\, A \le k\}. \tag{5.4}$$

Proof. We have $X = \sum_{i=1}^d \lambda_i^\downarrow(X)|e_i\rangle\langle e_i|$ for some orthonormal basis $\{e_i\}_{i=1}^d$, and hence for any $0 \le A \le I$ such that $\mathrm{Tr}\, A \le k$, we have $\mathrm{Tr}\, XA = \sum_{i=1}^d \lambda_i^\downarrow(X)\,\langle e_i, Ae_i\rangle \le \sum_{i=1}^k \lambda_i^\downarrow(X)$, since $\langle e_i, Ae_i\rangle \le 1$ and $\sum_{i=1}^d \langle e_i, Ae_i\rangle \le k$. The equality in (5.4) is attained by $A := \sum_{i=1}^k |e_i\rangle\langle e_i|$. □

Lemma 5.9. Let $X \in \mathcal{B}(\mathcal{H})_{\mathrm{sa}}$ and $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be a bistochastic map. Then $\lambda^\downarrow(\Phi(X))$ is majorized by $\lambda^\downarrow(X)$, in notation $\lambda^\downarrow(\Phi(X)) \prec \lambda^\downarrow(X)$, i.e., for all $k = 1, \dots, d$,

$$\lambda_1^\downarrow(\Phi(X)) + \dots + \lambda_k^\downarrow(\Phi(X)) \le \lambda_1^\downarrow(X) + \dots + \lambda_k^\downarrow(X),$$

with equality for $k = d$. Hence, there exist permutations $\pi_k \in S_d$ and probability weights $p_k > 0$, $k = 1, \dots, r$, such that all the vectors $\big(\lambda_{\pi_k(i)}^\downarrow(X)\big)_{i=1}^d$ for $k = 1, \dots, r$ are different, and

$$\lambda_i^\downarrow(\Phi(X)) = \sum_{k=1}^r p_k \lambda_{\pi_k(i)}^\downarrow(X), \qquad i = 1, \dots, d. \tag{5.5}$$

Proof. By (5.4),

$$\begin{aligned}
\lambda_1^\downarrow(\Phi(X)) + \dots + \lambda_k^\downarrow(\Phi(X)) &= \max\{\mathrm{Tr}\, \Phi(X)A : 0 \le A \le I,\ \mathrm{Tr}\, A \le k\} \\
&= \max\{\mathrm{Tr}\, X\Phi^*(A) : 0 \le A \le I,\ \mathrm{Tr}\, A \le k\} \\
&\le \sup\{\mathrm{Tr}\, XB : 0 \le B \le I,\ \mathrm{Tr}\, B \le k\} \\
&= \lambda_1^\downarrow(X) + \dots + \lambda_k^\downarrow(X),
\end{aligned}$$

where we used that $0 \le \Phi^*(A) \le \Phi^*(I) = I$, and $\mathrm{Tr}\, \Phi^*(A) = \mathrm{Tr}\, A \le k$. The majorization relation just established yields immediately the second assertion (see, e.g., [32, Theorem 4.1.1] for a proof). □

The following lemma can be considered as an analogue of Lemma 2.4, where operator convexity is relaxed to ordinary convexity, on the expense of replacing the positive semidefinite order with the trace order, and requiring that Φ is also trace-preserving.

Lemma 5.10. Let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be a bistochastic map, $X \in \mathcal{B}(\mathcal{H})_{\mathrm{sa}}$, and let f be a convex function on an interval containing $\operatorname{spec}(X)$. Then

$$\operatorname{Tr} f(\Phi(X)) \leq \operatorname{Tr} f(X).$$

If f is strictly convex, then equality holds if and only if there exists a unitary U such that $\Phi(X) = UXU^*$.

Proof. By (5.5), we have

$$\begin{aligned}\operatorname{Tr} f(\Phi(X)) &= \sum_{i=1}^{d} f\left(\sum_{k=1}^{r} p_k \lambda^{\downarrow}_{\pi_k(i)}(X)\right) \leq \sum_{i=1}^{d}\sum_{k=1}^{r} p_k f\left(\lambda^{\downarrow}_{\pi_k(i)}(X)\right) \qquad (5.6)\\ &= \sum_{k=1}^{r} p_k \sum_{i=1}^{d} f\left(\lambda^{\downarrow}_{\pi_k(i)}(X)\right) = \operatorname{Tr} f(X).\end{aligned}$$

Moreover, if f is strictly convex, then the inequality in (5.6) is strict, unless $r = 1$. Hence, if equality holds in (5.6), then $r = 1$, which means that $\lambda^{\downarrow}_i(\Phi(X)) = \lambda^{\downarrow}_i(X)$, $1 \leq i \leq d$. This implies the existence of a unitary U such that $\Phi(X) = UXU^*$. Conversely, if $\Phi(X) = UXU^*$ for some unitary U then it is obvious that $\operatorname{Tr} f(\Phi(X)) = \operatorname{Tr} f(X)$. □

Lemma 5.11. Let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be a bistochastic map and let $X \in \mathcal{B}(\mathcal{H})_{\mathrm{sa}}$. Then the following are equivalent:

(i) $\operatorname{Tr} f(\Phi(X)) = \operatorname{Tr} f(X)$ for all real functions f on $\operatorname{spec}(X)$.

(ii) $\operatorname{Tr} f(\Phi(X)) = \operatorname{Tr} f(X)$ for some strictly convex or strictly concave f on an interval containing $\operatorname{spec}(X)$.

(iii) $\operatorname{Tr} \Phi(X)^2 = \operatorname{Tr} X^2$.

(iv) $\Phi(X) = UXU^*$ for some unitary U.

(v) $(\Phi^* \circ \Phi)(X) = X$.

Proof. (i) $\Longrightarrow$ (iii) $\Longrightarrow$ (ii) is trivial, (ii) $\Longrightarrow$ (iv) follows from Lemma 5.10, and (iv) $\Longrightarrow$ (i) is obvious. Hence, it is enough to show (iii) $\Longleftrightarrow$ (v). Note that for any $X \in \mathcal{B}(\mathcal{H})_{\mathrm{sa}}$,

$$0 \leq \operatorname{Tr} X^2 - \operatorname{Tr} \Phi(X)^2 = \langle X, X\rangle_{\mathrm{HS}} - \langle \Phi(X), \Phi(X)\rangle_{\mathrm{HS}} = \langle X, (I - (\Phi^* \circ \Phi))X\rangle_{\mathrm{HS}},$$

where the first inequality is due to Lemma 5.10. Note that $\Phi^* \circ \Phi$ is positive semidefinite with respect to the Hilbert-Schmidt inner product, and the above inequality shows that $\Phi^* \circ \Phi \leq I$ $(= I_{\mathcal{B}(\mathcal{H})})$. Hence, $I - (\Phi^* \circ \Phi)$ is positive semidefinite, and thus the above can be written as

$$0 \leq \operatorname{Tr} X^2 - \operatorname{Tr} \Phi(X)^2 = \left\| (I - (\Phi^* \circ \Phi))^{1/2} X \right\|_{\mathrm{HS}}^2.$$

Thus,

$$\operatorname{Tr} X^2 = \operatorname{Tr} \Phi(X)^2 \iff (I - (\Phi^* \circ \Phi))^{1/2} X = 0 \iff X = (\Phi^* \circ \Phi)X.$$

□

Corollary 5.12. For any bistochastic map $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$,

$$\mathcal{F}_\Phi = \mathcal{F}_{\Phi^*}.$$

Proof. We show that $\mathcal{F}_\Phi \subseteq \mathcal{F}_{\Phi^*}$, which implies $\mathcal{F}_\Phi = \mathcal{F}_{\Phi^*}$ since $(\Phi^*)^* = \Phi$. Assume that $X \in \mathcal{F}_\Phi$; then $X_1 := \frac{1}{2}(X + X^*)$ and $X_2 := \frac{1}{2i}(X - X^*)$ are also in $\mathcal{F}_\Phi$, and hence we can assume without loss of generality that $X^* = X \in \mathcal{F}_\Phi$. Then, by (iv)$\Longrightarrow$(v) of Lemma 5.11, we get that $X = (\Phi^* \circ \Phi)(X) = \Phi^*(X)$, i.e., $X \in \mathcal{F}_{\Phi^*}$. □

When Φ is 2-positive, the unitary in (iv) of Lemma 5.11 can be chosen independently of X:

Lemma 5.13. Let $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be a 2-positive bistochastic map. Then there exists a unitary U such that

$$\Phi(X) = UXU^*, \qquad \Phi^*(X) = U^*XU, \qquad X \in \mathcal{F}_{\Phi^*\circ\Phi}.$$

Proof. Note that with the notations of Theorem 3.19, we have $\Phi_I = \Phi$ and $\Phi_I^* = \Phi^*$, and hence $\mathcal{F}_{\Phi_I^*\circ\Phi} = \mathcal{F}_{\Phi^*\circ\Phi_I}$. This in turn yields that $\omega_k = I_{1,k,R}$ for all k in the decomposition (3.25), and unitality of Φ and Φ^* yields $\eta_k(I_{1,k,R}) = I_{2,k,R}$ and $\eta_k^*(I_{2,k,R}) = I_{1,k,R}$ for all k. Defining $U := \bigoplus_k U_k \otimes I_{1,k,R}$ then gives the desired unitary. □

Remark 5.14. The statement of the above lemma may not hold when Φ is only assumed to be positive, as one can easily see by choosing Φ to be the transposition in some orthonormal basis.

Now we are in a position to prove Theorem 5.2.

Proof of Theorem 5.2. The proof is divided into several steps.

(1a) Assume (i) first. Since $0 < \frac{\alpha}{z} \le 1$, we have $\Phi(\varrho^{\frac{\alpha}{z}}) \le \Phi(\varrho)^{\frac{\alpha}{z}}$ due to Lemma 2.4, so that

$$\sigma^{\frac{1-\alpha}{2z}}\Phi(\varrho^{\frac{\alpha}{z}})\sigma^{\frac{1-\alpha}{2z}} \le \sigma^{\frac{1-\alpha}{2z}}\Phi(\varrho)^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}}. \tag{5.7}$$

Hence,

$$\operatorname{Tr}\Big(\sigma^{\frac{1-\alpha}{2z}}\Phi(\varrho^{\frac{\alpha}{z}})\sigma^{\frac{1-\alpha}{2z}}\Big)^z \le \operatorname{Tr}\Big(\sigma^{\frac{1-\alpha}{2z}}\Phi(\varrho)^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}}\Big)^z = \operatorname{Tr}\Big(\Phi(\sigma)^{\frac{1-\alpha}{2z}}\Phi(\varrho)^{\frac{\alpha}{z}}\Phi(\sigma)^{\frac{1-\alpha}{2z}}\Big)^z, \tag{5.8}$$

due to $\sigma \in \mathcal{F}_\Phi$. Using also that Φ is bistochastic, Lemma 2.6 yields that $\sigma^{\frac{1-\alpha}{2z}} \in \mathcal{F}_\Phi \subseteq \mathcal{M}_\Phi$, and hence

$$\sigma^{\frac{1-\alpha}{2z}}\Phi(\varrho^{\frac{\alpha}{z}})\sigma^{\frac{1-\alpha}{2z}} = \Phi\big(\sigma^{\frac{1-\alpha}{2z}}\big)\Phi(\varrho^{\frac{\alpha}{z}})\Phi\big(\sigma^{\frac{1-\alpha}{2z}}\big) = \Phi\big(\sigma^{\frac{1-\alpha}{2z}}\varrho^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}}\big). \tag{5.9}$$

Using Lemma 5.10, and that $x \mapsto x^z$ is concave for $0 < z \le 1$, we get

$$\operatorname{Tr}\big(\sigma^{\frac{1-\alpha}{2z}}\varrho^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}}\big)^z \le \operatorname{Tr}\Big(\Phi\big(\sigma^{\frac{1-\alpha}{2z}}\varrho^{\frac{\alpha}{z}}\sigma^{\frac{1-\alpha}{2z}}\big)\Big)^z. \tag{5.10}$$

Putting together (5.8)–(5.10), we get the desired monotonicity inequality (5.2).

If (5.2) holds with equality (i.e., (E1) holds), we must have equalities in (5.8) and (5.10). In particular, equality in (5.8), together with the strict monotonicity of $X \in \mathcal{B}(\mathcal{H})_+ \mapsto \operatorname{Tr} X^z$, implies that (5.7) holds with equality. Multiplying both sides of (5.7) with $\sigma^{\frac{\alpha-1}{2z}}$ yields

$$\sigma^0\Phi(\varrho^{\frac{\alpha}{z}})\sigma^0 = \sigma^0\Phi(\varrho)^{\frac{\alpha}{z}}\sigma^0. \tag{5.11}$$

(1b) We assume (i) with $\varrho^0 \leq \sigma^0$. If (E1) holds then, by the above, we have (5.11), and using that $\Phi(\varrho)^0 \leq \Phi(\sigma)^0 = \sigma^0$, we get

$$\Phi(\varrho^{\frac{\alpha}{z}}) = \Phi(\varrho)^{\frac{\alpha}{z}}.$$

Since this gives $\operatorname{Tr}\Phi(\varrho)^{\frac{\alpha}{z}} = \operatorname{Tr}\varrho^{\frac{\alpha}{z}}$, it follows from Lemma 5.11 that

$$\Phi^* \circ \Phi(\varrho) = \varrho$$

whenever $\alpha < z$. When $\alpha = z$, since $0 < \alpha < 1$, equality in (5.10) implies by Lemma 5.11 again that

$$\Phi^* \circ \Phi\big(\sigma^{\frac{1-\alpha}{2\alpha}}\varrho\sigma^{\frac{1-\alpha}{2\alpha}}\big) = \sigma^{\frac{1-\alpha}{2\alpha}}\varrho\sigma^{\frac{1-\alpha}{2\alpha}}.$$

Since $\sigma \in \mathcal{F}_\Phi = \mathcal{F}_{\Phi^*}$ by Corollary 5.12, it follows from Lemma 2.6 that $\sigma^{\frac{1-\alpha}{2\alpha}} \in \mathcal{M}_\Phi \cap \mathcal{M}_{\Phi^*}$. Hence we have

$$\sigma^0(\Phi^* \circ \Phi(\varrho))\sigma^0 = \sigma^0\varrho\sigma^0,$$

so that $\Phi^* \circ \Phi(\varrho) = \varrho$ since $(\Phi^* \circ \Phi(\varrho))^0 \leq (\Phi^* \circ \Phi(\sigma))^0 = \sigma^0$. This proves (E2) since $\Phi^*\circ\Phi(\sigma) = \sigma$. In the converse direction, assume that (E2) holds. Then $\Phi^*(\Phi(\sigma)) = \sigma = \Phi(\sigma)$. Applying the above established monotonicity to Φ^* and $\Phi(\varrho), \Phi(\sigma)$ in place of Φ and ϱ, σ, we get

$$D_{\alpha,z}(\varrho\|\sigma) = D_{\alpha,z}(\Phi^*(\Phi(\varrho))\|\Phi^*(\Phi(\sigma))) \leq D_{\alpha,z}(\Phi(\varrho)\|\Phi(\sigma)) \leq D_{\alpha,z}(\varrho\|\sigma),$$

proving the equality in (5.2). Hence (E1) $\Longleftrightarrow$ (E2). Finally, notice that $\sigma^{1/2} \in \mathcal{F}_{\Phi^*} \subseteq \mathcal{M}_{\Phi^*}$ implies

$$\begin{aligned}\Phi^*_\sigma(Y) &= \sigma^{1/2}\Phi^*\left(\Phi(\sigma)^{-1/2}Y\Phi(\sigma)^{-1/2}\right)\sigma^{1/2} = \Phi^*\big(\sigma^{1/2}\big)\Phi^*\left(\sigma^{-1/2}Y\sigma^{-1/2}\right)\Phi^*\big(\sigma^{1/2}\big) \\ &= \Phi^*\left(\sigma^{1/2}\sigma^{-1/2}Y\sigma^{-1/2}\sigma^{1/2}\right) = \Phi^*\left(\sigma^0 Y\sigma^0\right)\end{aligned}$$

for any $Y \in \mathcal{B}(\mathcal{H})$. In particular, if $\varrho^0 \leq \sigma^0$ then $\Phi^*_\sigma(\Phi(\varrho)) = \Phi^*(\Phi(\varrho))$, proving (E2) $\Longleftrightarrow$ (E3).

(1c) In (1) we also assume that Φ is 2-positive; then (E2) implies (E5) by Lemma 5.13. Obviously, (E5) implies (E1), completing the proof of (1).

(2) Assume (i) with $\sigma^0 \leq \varrho^0$ instead of $\varrho^0 \leq \sigma^0$, and $z \neq \alpha$. Assume that (E1) holds; then by the argument in (1a), we have (5.11). Multiplying with $\Phi(\sigma)^{\frac{z-\alpha}{2z}}$ from both sides, and taking the trace, we get

$$\operatorname{Tr}\Phi(\sigma)^{1-\frac{\alpha}{z}}\Phi(\varrho)^{\frac{\alpha}{z}} = \operatorname{Tr}\Phi(\sigma)^{1-\frac{\alpha}{z}}\Phi(\varrho^{\frac{\alpha}{z}}) = \operatorname{Tr}\Phi(\sigma^{1-\frac{\alpha}{z}}\varrho^{\frac{\alpha}{z}}) = \operatorname{Tr}\sigma^{1-\frac{\alpha}{z}}\varrho^{\frac{\alpha}{z}},$$

where we have used again that $\sigma \in \mathcal{F}_\Phi \subseteq \mathcal{M}_\Phi$. This means that the quantum f-divergence S_f is preserved, i.e.,

$$S_f(\Phi(\sigma)\|\Phi(\varrho)) = S_f(\sigma\|\varrho),$$

where $f(x) := -x^{1-\frac{\alpha}{z}}$ with $1 - \frac{\alpha}{z} \in (0, 1)$. Hence, when Φ is 2-positive, by Theorem 3.18 we have (E4). Assume now that (E4) holds, i.e., $\varrho, \sigma \in \mathcal{F}_{\Phi^*_\varrho\circ\Phi}$. Using then Theorem 3.19 (with the role of ϱ and σ interchanged), the decomposition in (3.25) yields immediately (E1).

(3) & (4) Assume now that (ii) holds. Note that for $0 < \alpha < 1$, we have $Q_{\alpha,z}(\varrho\|\sigma) = Q_{1-\alpha,z}(\sigma\|\varrho)$ so that $D_{\alpha,z}(\varrho\|\sigma) = D_{1-\alpha,z}(\sigma\|\varrho)$ for all z. Hence the claim about monotonicity follows from the case (i) already proved in (1a). When the monotonicity inequality holds

with equality, the assertions in (3) and (4) also follow from (1) and (2) proved above, by interchanging ϱ and σ together with changing α to $1-\alpha$.

(5) Next, assume (iii). Since $1 \le \alpha/z \le 2$, the function $x \mapsto x^{\alpha/z}$ is operator convex, and $x \mapsto x^z$ is convex. Thus, the inequalities in (5.7), (5.8), and (5.10) hold in the opposite directions, proving the monotonicity inequality (5.2) as in the proof (1a). When $\varrho^0 \le \sigma^0$, the proof for the equality case goes the same way as in the proofs (1b) and (1c) above, completing the proof of (5).

(6) Finally, assume (iv). Since

$$Q_{\alpha,z}(\varrho\|\sigma) = \lim_{\varepsilon\searrow 0} Q_{\alpha,z}(\varrho\|\sigma+\varepsilon I), \qquad Q_{\alpha,z}(\Phi(\varrho)\|\Phi(\sigma)) = \lim_{\varepsilon\searrow 0} Q_{\alpha,z}(\varrho\|\Phi(\sigma+\varepsilon I)),$$

we may assume that $\sigma^0 = I$, to show the monotonicity inequality (5.2). Since $-1 \le \frac{1-\alpha}{z} < 0$, Lemma 2.4 yields

$$\varrho^{\frac{\alpha}{2z}}\Phi(\sigma)^{\frac{1-\alpha}{z}}\varrho^{\frac{\alpha}{2z}} \le \varrho^{\frac{\alpha}{2z}}\Phi(\sigma^{\frac{1-\alpha}{z}})\varrho^{\frac{\alpha}{2z}}. \tag{5.12}$$

As in the proof (1a), this implies

$$\begin{aligned}\operatorname{Tr}\Bigl(\Phi(\varrho)^{\frac{\alpha}{2z}}\Phi(\sigma)^{\frac{1-\alpha}{z}}\Phi(\varrho)^{\frac{\alpha}{2z}}\Bigr)^z &= \operatorname{Tr}\Bigl(\varrho^{\frac{\alpha}{2z}}\Phi(\sigma)^{\frac{1-\alpha}{z}}\varrho^{\frac{\alpha}{2z}}\Bigr)^z \le \operatorname{Tr}\Bigl(\varrho^{\frac{\alpha}{2z}}\Phi(\sigma^{\frac{1-\alpha}{z}})\varrho^{\frac{\alpha}{2z}}\Bigr)^z \\ &= \operatorname{Tr}\Bigl(\Phi\bigl(\varrho^{\frac{\alpha}{2z}}\sigma^{\frac{1-\alpha}{z}}\varrho^{\frac{\alpha}{2z}}\bigr)\Bigr)^z \le \operatorname{Tr}\bigl(\varrho^{\frac{\alpha}{2z}}\sigma^{\frac{1-\alpha}{z}}\varrho^{\frac{\alpha}{2z}}\bigr)^z,\end{aligned}$$

where the equalities are due to $\varrho \in \mathcal{F}_\Phi \subseteq \mathcal{M}_\Phi$, and the last inequality follows from Lemma 5.10. This proves monotonicity (5.2).

Now, if (5.2) holds with equality, then we have equality in (5.12), and hence,

$$\varrho^0\Phi(\sigma)^{\frac{1-\alpha}{z}}\varrho^0 = \varrho^0\Phi(\sigma^{\frac{1-\alpha}{z}})\varrho^0.$$

Therefore, similarly to the above proof of (2), we have

$$\operatorname{Tr}\Phi(\varrho)^{1-\frac{1-\alpha}{z}}\Phi(\sigma)^{\frac{1-\alpha}{z}} = \operatorname{Tr}\varrho^{1-\frac{1-\alpha}{z}}\sigma^{\frac{1-\alpha}{z}}.$$

Assuming that $z \ne \alpha - 1$, we have $1 - \frac{1-\alpha}{z} \in (1,2)$, and the above equality means that the f-divergence $S_f(\varrho\|\sigma)$, corresponding to $f(t) = t^{1-\frac{1-\alpha}{z}}$, is preserved by Φ. Hence, by Theorem 3.18, we get (E3). The implication (E3) $\Longrightarrow$ (E1) follows by observing that (E3) means $\varrho, \sigma \in \mathcal{F}_{\Phi_\sigma^*\circ\Phi}$, and using the decomposition (3.25) in Theorem 3.19, similarly to the proof of (2) above. □

Remark 5.15. We remark that the exclusion of $z = 1-\alpha$ is essential in the statement (4) of Theorem 5.2. Let $\Phi : \mathcal{B}(\mathbb{C}^2) \to \mathcal{B}(\mathbb{C}^2)$ be the diagonal pinching by regarding $\mathcal{B}(\mathbb{C}^2)$ as the 2×2 matrices. Let $\varrho := \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$, and for $a > b > 0$ and $0 < \theta < \frac{\pi}{2}$, let

$$\sigma := \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} = \begin{bmatrix} a\cos^2\theta + b\sin^2\theta & (a-b)\cos\theta\sin\theta \\ (a-b)\cos\theta\sin\theta & a\sin^2\theta + b\cos^2\theta \end{bmatrix}.$$

Then

$$S(\varrho\|\sigma) = -\operatorname{Tr}\varrho\log\sigma = -(\log a)\cos^2\theta - (\log b)\sin^2\theta$$

while

$$S(\Phi(\varrho)\|\Phi(\sigma)) = -\operatorname{Tr}\varrho\log\Phi(\sigma) = -\log(a\cos^2\theta + b\sin^2\theta) < S(\varrho\|\sigma),$$

and hence Φ is not reversible for ϱ, σ. However, for any $\alpha \in (0,1)$ we have

$$\mathrm{Tr}\big(\sigma^{1/2}\varrho^{\frac{\alpha}{1-\alpha}}\sigma^{1/2}\big)^{1-\alpha} = (a\cos^2\theta + b\sin^2\theta)^{1-\alpha} = \mathrm{Tr}\big(\Phi(\sigma)^{1/2}\Phi(\varrho)^{\frac{\alpha}{1-\alpha}}\Phi(\sigma)^{1/2}\big)^{1-\alpha},$$

so that $D_{\alpha,z}(\Phi(\varrho)\|\Phi(\sigma)) = D_{\alpha,z}(\varrho\|\sigma)$ for $z = 1-\alpha$. In particular when $\alpha = z = 1/2$, since

$$D_{1/2,1/2}(\varrho\|\sigma) = -2\log F(\varrho,\sigma)$$

with the fidelity $F(\varrho,\sigma) := \mathrm{Tr}\,|\varrho^{1/2}\sigma^{1/2}|$, we notice that when $\varrho^0 \le \sigma^0$ and $\varrho \in \mathcal{F}_\Phi$, the equality $F(\Phi(\varrho),\Phi(\sigma)) = F(\varrho,\sigma)$ does not imply the reversibility of Φ on ϱ,σ in general (cf. also [52, Corollary A.9]). But it does so when $\varrho^0 \le \sigma^0$ and $\sigma \in \mathcal{F}_\Phi$, as follows from (1) of Theorem 5.2.

Remark 5.16. The max-relative entropy [20] is defined as the limit of the sandwiched Rényi divergences:

$$D_{\max}(\varrho\|\sigma) := \lim_{\alpha\to+\infty} D_\alpha^*(\varrho\|\sigma) = \inf\{\gamma : \varrho \le e^\gamma\sigma\}.$$

It is known [52, Corollary A.9] that preservation of the max-relative entropy does not imply reversibility. Below we give an example that shows that reversibility does not follow from the preservation of the max-relative entropy even in the very special case where the second state is a fixed point of the map (cf. (1) of Theorem 5.2). Consider 3×3 invertible density matrices $\sigma = \mathrm{diag}(\mu_1,\mu_2,\mu_3)$ and

$$\varrho = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & a & c \\ 0 & \overline{c} & b \end{bmatrix}, \quad \lambda, a, b > 0, \quad c \ne 0, \quad |c|^2 < ab, \quad \lambda + a + b = 1.$$

Let $\Phi : \mathbb{M}_3 \to \mathbb{M}_3$ be the diagonal pinching, i.e., $\Phi(X)$ is the diagonal part of X. Then

$$\mathrm{Tr}\,\Phi(\varrho)^2\Phi(\sigma)^{-1} = \frac{\lambda^2}{\mu_1} + \frac{a^2}{\mu_2} + \frac{b^2}{\mu_3},$$

$$\mathrm{Tr}\,\varrho^2\sigma^{-1} = \frac{\lambda^2}{\mu_1} + \frac{a^2+|c|^2}{\mu_2} + \frac{b^2+|c|^2}{\mu_3},$$

so that

$$\mathrm{Tr}\,\Phi(\varrho)^2\Phi(\sigma)^{-1} < \mathrm{Tr}\,\varrho^2\sigma^{-1}.$$

By Theorem 3.34, this is equivalent to that $\sigma^{-1/2}\varrho\sigma^{-1/2} \notin \mathcal{M}_{\Phi_\sigma}$, and it implies that Φ is not reversible on $\{\varrho,\sigma\}$. On the other hand,

$$\big\|\Phi(\sigma)^{-1/2}\Phi(\varrho)\Phi(\sigma)^{-1/2}\big\|_\infty = \max\left\{\frac{\lambda}{\mu_1}, \frac{a}{\mu_2}, \frac{b}{\mu_3}\right\},$$

$$\begin{aligned}\big\|\sigma^{-1/2}\varrho\sigma^{-1/2}\big\|_\infty &= \max\left\{\frac{\lambda}{\mu_1}, \left\|\begin{bmatrix}\mu_2^{-1/2} & 0 \\ 0 & \mu_3^{-1/2}\end{bmatrix}\begin{bmatrix} a & c \\ \overline{c} & b\end{bmatrix}\begin{bmatrix}\mu_2^{-1/2} & 0 \\ 0 & \mu_3^{-1/2}\end{bmatrix}\right\|_\infty\right\} \\ &= \max\left\{\frac{\lambda}{\mu_1}, \frac{1}{2}\left(\frac{a}{\mu_2} + \frac{b}{\mu_3} + \sqrt{\left(\frac{a}{\mu_2} - \frac{b}{\mu_3}\right)^2 + \frac{4|c|^2}{\mu_2\mu_3}}\right)\right\}.\end{aligned}$$

When the μ_i's are fixed and $\lambda \nearrow 1$ (hence $a, b, |c| \searrow 0$), we have

$$\big\|\Phi(\sigma)^{-1/2}\Phi(\varrho)\Phi(\sigma)^{-1/2}\big\|_\infty = \frac{\lambda}{\mu_1} = \big\|\sigma^{-1/2}\varrho\sigma^{-1/2}\big\|_\infty,$$

which means that $D_{\max}(\Phi(\varrho)\|\Phi(\sigma)) = D_{\max}(\varrho\|\sigma)$.

6 Closing remarks

Remark 6.1. In this paper we treat f-divergences for general positive operators. We note that restricting to density operators would make no essential difference. Indeed, for $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$, $\sigma \neq 0$, write $\varrho = \alpha\varrho_1$ and $\sigma = \beta\sigma_1$, where ϱ_1, σ_1 are density operators and $\alpha = \operatorname{Tr}\varrho$, $\beta = \operatorname{Tr}\sigma > 0$. For any operator convex function f, since

$$S_f(\varrho\|\sigma) = S_{f_1}(\varrho_1\|\sigma_1), \qquad \widehat{S}_f(\varrho\|\sigma) = \widehat{S}_{f_1}(\varrho_1\|\sigma_1)$$

with $f_1(x) := \beta f(\alpha\beta^{-1}x)$, one can easily obtain properties of S_f and $\widehat{S}_f$ for general positive operators from those restricting to density operators.

Remark 6.2. We may treat trace-preserving positive linear maps $\Phi : \mathcal{A}_1 \to \mathcal{A}_2$ between general finite-dimensional C^*-algebras $\mathcal{A}_1$, $\mathcal{A}_2$. When $\mathcal{A}_1 \subseteq \mathcal{B}(\mathcal{H})$ and $\mathcal{A}_2 \subseteq \mathcal{B}(\mathcal{K})$, we can extend Φ to $\widetilde{\Phi} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{K})$ by $\widetilde{\Phi} := \Phi \circ \mathcal{E}_{\mathcal{A}_1}$, where $\mathcal{E}_{\mathcal{A}_1} : \mathcal{B}(\mathcal{H}) \to \mathcal{A}_1$ is the trace-preserving conditional expectation onto $\mathcal{A}_1$. Then $\widetilde{\Phi}^* = \Phi^* \circ \mathcal{E}_{\mathcal{A}_2}$. It is straightforward to reformulate the results of this paper for $\varrho, \sigma \in \mathcal{A}_1$ and $\widetilde{\Phi}$ into those for ϱ, σ and Φ. Thus the generalization to the setting of finite-dimensional C^*-algebras is automatic.

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A Extension of Lemma 2.2

Proposition A.1. Let f be a real function on $(0, +\infty)$. The following conditions are equivalent:

(i) $(A, B) \in \mathcal{B}(\mathcal{H})_{++} \times \mathcal{B}(\mathcal{H})_{++} \mapsto P_f(A, B)$ is jointly operator convex for any finite-dimensional Hilbert space $\mathcal{H}$;

(ii) for every $B \in \mathcal{B}(\mathcal{H})_{++}$, $A \in \mathcal{B}(\mathcal{H})_{++} \mapsto \operatorname{Tr} P_f(A, B)$ is convex for any finite-dimensional Hilbert space $\mathcal{H}$;

(iii) for every $A \in \mathcal{B}(\mathcal{H})_{++}$, $B \in \mathcal{B}(\mathcal{H})_{++} \mapsto \operatorname{Tr} P_f(A, B)$ is convex for any finite-dimensional Hilbert space $\mathcal{H}$;

(iv) f is operator convex on $(0, +\infty)$;

(v) $\widetilde{f}$ is operator convex on $(0, +\infty)$.

Proof. That (i) implies (ii) and (iii) is trivial. Since $\operatorname{Tr} P_f(B^{1/2}AB^{1/2}, B) = \operatorname{Tr} B^{1/2}f(A)B^{1/2}$ for $A, B \in \mathcal{B}(\mathcal{H})_{++}$, we have (ii) $\Longrightarrow$ (iv). The proof of (iv) $\Longrightarrow$ (i) is in [21] or [23]. Apply these to $\widetilde{f}$ and use Lemma 2.1 to prove that (iii) $\Longrightarrow$ (v) $\Longrightarrow$ (i).

Although the equivalence of (iv) and (v) has already been shown, it may be worth giving a different proof based on Kraus' characterization of operator convex functions, see [32, Corollary 2.7.8]. Indeed, since

$$\frac{\widetilde{f}(x) - \widetilde{f}(1)}{x - 1} = -\frac{f(x^{-1}) - f(1)}{x^{-1} - 1} + f(1),$$

the operator convexity of $\widetilde{f}$ follows from that of f and vice versa by Kraus' theorem. □

Proposition A.2. Let h be a real function on $(0, +\infty)$. The following conditions are equivalent

(i) $(A, B) \in \mathcal{B}(\mathcal{H})_{++} \times \mathcal{B}(\mathcal{H})_{++} \mapsto P_h(A, B)$ is jointly operator monotone increasing for any finite-dimensional Hilbert space $\mathcal{H}$;

(ii) $(A, B) \in \mathcal{B}(\mathcal{H})_{++} \times \mathcal{B}(\mathcal{H})_{++} \mapsto \operatorname{Tr} P_h(A, B)$ is jointly monotone increasing for any finite-dimensional Hilbert space $\mathcal{H}$;

(iii) h is non-negative and operator monotone on $(0, +\infty)$;

(iv) h is operator monotone on $(0, +\infty)$ and $\widetilde{h}$ is numerically increasing on $(0, +\infty)$;

(v) $\widetilde{h}$ is non-negative and operator monotone on $(0, +\infty)$;

(vi) $\widetilde{h}$ is operator monotone on $(0, +\infty)$ and h is numerically increasing on $(0, +\infty)$.

To prove the proposition, we give a lemma.

Lemma A.3. Let h be an operator monotone function on $(0, +\infty)$. Then h is non-negative on $(0, +\infty)$ if and only if $\widetilde{h}$ is numerically increasing on $(0, +\infty)$.

Proof. According to [25, Theorem 1.9], h admits the integral representation

$$h(x) = h(1) + \gamma(x - 1) + \int_{[0,+\infty)} \frac{x - 1}{x + s}\, d\mu(s), \qquad x \in (0, +\infty),$$

with a constant $\gamma \geq 0$ and a positive measure μ on $[0, +\infty)$ such that $\int_{[0,+\infty)}(1+s)^{-1}\, d\mu(s) < +\infty$. Note that

$$\frac{d^2}{dx^2}\left(\frac{x - 1}{x + s}\right) = \frac{1 + s}{(x + s)^2} \geq 0.$$

Since $(1-x)/(x+s) \nearrow 1/s$ for $s \geq 0$ (where $1/0 = +\infty$) as $x \searrow 0$, the monotone convergence theorem yields that

$$\lim_{x \searrow 0} \int_{[0,+\infty)} \frac{1 - x}{x + s}\, d\mu(s) = \int_{[0,+\infty)} \frac{1}{s}\, d\mu(s),$$

so that

$$h(0+) = \lim_{x \searrow 0} h(x) = h(1) - \gamma - \int_{[0,+\infty)} \frac{1}{s}\, d\mu(s) \in [-\infty, +\infty).$$

This implies that h is non-negative on $(0, +\infty)$, i.e., $h(0+) \geq 0$ if and only if

$$\int_{[0,+\infty)} s^{-1}\, d\mu(s) < +\infty \quad \text{and} \quad h(1) - \gamma - \int_{[0,+\infty)} \frac{1}{s}\, d\mu(s) \geq 0. \tag{A.1}$$

Moreover, note that

$$\widetilde{h}(x) = xh(x^{-1}) = h(1)x + \gamma(1-x) + \int_{[0,+\infty)} \frac{1-x}{x^{-1}+s}\,d\mu(s).$$

If (A.1) is satisfied, then

$$\widetilde{h}(x) = \gamma + \left(h(1) - \gamma - \int_{[0,+\infty)} \frac{1}{s}\,d\mu(s)\right)x + \int_{[0,+\infty)} \frac{1+s}{s(x^{-1}+s)}\,d\mu(s)$$

is obviously increasing on $(0,+\infty)$.

Conversely, assume that (A.1) is not satisfied. If $\int_{[0,+\infty)} s^{-1}\,d\mu(s) = +\infty$, then

$$\widetilde{h}(x) = h(1)x + \gamma(1-x) - (x-1)\int_{[0,+\infty)} \frac{1}{x^{-1}+s}\,d\mu(s) \longrightarrow -\infty$$

as $x \to +\infty$, so obviously $\widetilde{h}$ is not increasing on $(0,+\infty)$. If $\int_{[0,+\infty)} s^{-1}\,d\mu(s) < +\infty$ but $h(1) - \gamma - \int_{[0,+\infty)} s^{-1}\,d\mu(s) < 0$, then

$$\widetilde{h}(x) = \gamma + \left(h(1) - \gamma - \int_{[0,+\infty)} \frac{1}{x^{-1}+s}\,d\mu(s)\right)x + \int_{[0,+\infty)} \frac{1}{x^{-1}+s}\,d\mu(s)$$

is not increasing on $(0,+\infty)$. □

Proof of Proposition A.2. It is trivial that (i) implies (ii). If (ii) holds, then as in the proof of Proposition A.1, one can see that h and $\widetilde{h}$ are operator monotone on $(0,+\infty)$, so (iv) follows. By Lemma A.3, (iii) $\Longleftrightarrow$ (iv) and (v) $\Longleftrightarrow$ (vi) are obvious. (iii) $\Longleftrightarrow$ (v) is well-known, see, e.g., [32, Corollary 2.5.6]. Although (iii) $\Longrightarrow$ (i) is also well-known in the theory of operator means [46], we give a proof for convenience. Since (iii) $\Longleftrightarrow$ (v), (iii) means that h and $\widetilde{h}$ are operator monotone on $(0,+\infty)$. If $A_1, A_2, B_1, B_2 \in \mathcal{B}(\mathcal{H})_{++}$ are such that $A_1 \le A_2$ and $B_1 \le B_2$, then

$$\begin{aligned} P_h(A_1,B_1) &= B_1^{1/2} h(B_1^{-1/2}A_1B_1^{-1/2})B^{1/2} \le B_1^{1/2} h(B_1^{-1/2}A_2B_1^{-1/2})B^{1/2} \\ &= A_2^{1/2}\widetilde{h}(A_2^{-1/2}B_1A_2^{-1/2})A_2^{1/2} \le A_2^{1/2}\widetilde{h}(A_2^{-1/2}B_2A_2^{-1/2})A_2^{1/2} = P_h(A_2,B_2) \end{aligned}$$

by Lemma 2.1 for the second equality. □

Remark A.4. Note that neither Proposition A.2 nor Lemma A.3 hold when "operator monotone" is replaced with "numerically increasing". Indeed, for $f(t) := t^2 + 1$ we have $f \ge 0$ and f is numerically increasing, but $\widetilde{f}(s) = \frac{1}{s} + s$ is neither increasing nor decreasing, and so P_f is neither increasing nor decreasing in its second variable.

B Examples for $\mathcal{F}_\Phi$ and $\mathcal{M}_\Phi$

Example B.1. Let U be a unitary on $\mathcal{H}$, which determines the bistochastic map $\Phi(\cdot) = U(\cdot)U^*$. Then it is trivial to check that

$$\mathcal{F}_\Phi = \{X \in \mathcal{B}(\mathcal{H}) : UX = XU\} \subseteq \mathcal{B}(\mathcal{H}) = \mathcal{M}_\Phi,$$

and the inclusion is strict unless $U \in \mathbb{C}I$.

Proposition B.2. Let $e_1, \ldots, e_d$ be an orthonormal basis in a Hilbert space $\mathcal{H}$, and let $T \in \mathbb{R}_+^{d\times d}$ be a stochastic matrix, i.e., $\sum_{y=1}^d T_{xy} = 1$, $1 \le x \le d$. Define

$$\Phi(X) := \sum_{x=1}^d |e_x\rangle\langle e_x| \sum_{y=1}^d T_{xy} \langle e_y, X e_y\rangle, \qquad X \in \mathcal{B}(\mathcal{H}).$$

Then Φ is a unital CP map, which is trace-preserving if and only if T is bistochastic, i.e., $\sum_{x=1}^d T_{xy} = 1$, $1 \le y \le d$, as well. If none of the columns of T are zero then

$$\mathcal{M}_\Phi = \big\{X \in \mathcal{B}(\mathcal{H}) : \langle e_x, X e_y\rangle = 0,\ x \ne y,\ \text{and} \\ \langle e_y, X e_y\rangle = \langle e_z, X e_z\rangle \ \text{if } T_{xy}T_{xz} > 0 \text{ for some } x\big\}.$$

In particular, if T has a strictly positive row then $\mathcal{M}_\Phi = \mathbb{C}I$.

Proof. It is clear from the definition that Φ is CPTP. For every $a, b \in \{1, \ldots, d\}$ and $X \in \mathcal{B}(\mathcal{H})$, we have

$$\Phi(X|e_b\rangle\langle e_a|) = \Phi(|Xe_b\rangle\langle e_a|) = \sum_{x=1}^d |e_x\rangle\langle e_x| T_{xa} \langle e_a, X e_b\rangle.$$

Now, if $a \ne b$ then $\Phi(|e_a\rangle\langle e_b|) = 0$, and if $X \in \mathcal{M}_\Phi$, we get

$$\Phi(X|e_b\rangle\langle e_a|) = \Phi(X)\Phi(|e_a\rangle\langle e_b|) = 0.$$

Thus, if the a-th column of T is not zero, then we get $\langle e_a, X e_b\rangle = 0$ for all $b \ne a$. In particular, if none of the columns of T are zero, then all elements in $\mathcal{M}_\Phi$ are diagonal in the basis $\{e_x\}_{x=1}^d$.

Now, let $F \in \mathcal{B}(\mathcal{H})$ be diagonal in the given basis, so that it can be written as $F = \sum_{x=1}^d f(x)|e_x\rangle\langle e_x|$. Then

$$\begin{aligned}\langle e_x, [\Phi(F^*F) - \Phi(F)^*\Phi(F))]\, e_x\rangle &= \sum_y T_{xy}|f(y)|^2 - \sum_{y,z} T_{xy}\overline{f}(y)T_{xz}f(z) \\ &= \sum_y (T_{xy} - T_{xy}^2)|f(y)|^2 - \sum_{y,z\colon y\ne z} T_{xy}\overline{f}(y)T_{xz}f(z).\end{aligned}$$

Note that $T_{xy} - T_{xy}^2 = T_{xy}(1 - T_{xy}) = T_{xy}\sum_{z\colon z\ne y} T_{xz}$, and hence the first term above is

$$\sum_y (T_{xy} - T_{xy}^2)|f(y)|^2 = \sum_{y,z\colon y\ne z} T_{xy}T_{xz}|f(y)|^2 = \frac{1}{2}\sum_{y,z\colon y\ne z} T_{xy}T_{xz}(|f(y)|^2 + |f(z)|^2).$$

The second term can be written as

$$\sum_{y,z\colon y\ne z} T_{xy}\overline{f}(y)T_{xz}f(z) = \frac{1}{2}\sum_{y,z\colon y\ne z} T_{xy}T_{xz}(\overline{f}(y)f(z) + f(y)\overline{f}(z)).$$

Thus,

$$\begin{aligned}\langle e_x, [\Phi(F^*F) - \Phi(F)^*\Phi(F))]\, e_x\rangle &= \frac{1}{2}\sum_{y,z\colon y\ne z} T_{xy}T_{xz}\left[|f(y)|^2 + |f(z)|^2 - \overline{f}(y)f(z) - f(y)\overline{f}(z)\right] \\ &= \frac{1}{2}\sum_{y,z\colon y\ne z} T_{xy}T_{xz}|f(y) - f(z)|^2,\end{aligned}$$

from which the remaining assertions follow. □

Example B.3. In the setting of Proposition B.2, let Φ be given by the stochastic matrix

$$T := \begin{bmatrix} 1 & & & \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ & & & 1 \end{bmatrix} \in \mathbb{R}_+^{4\times 4}.$$

By Proposition B.2, we see that $\mathcal{M}_\Phi = \mathbb{C}1$. On the other hand, it is easy to see that both I and $A := |e_1\rangle\langle e_1| + 2|e_2\rangle\langle e_2| + 2|e_3\rangle\langle e_3| + 3|e_4\rangle\langle e_4|$ are fixed points of Φ, and hence

$$\mathcal{M}_\Phi \subsetneqq \mathcal{F}_\Phi.$$

Moreover, A^2 is not a fixed point of Φ, and hence $\mathcal{F}_\Phi$ is not an algebra.

By Lemma 2.6, Φ cannot have a faithful invariant state. Indeed, it is easy to see that $\Phi^*(\varrho) = \varrho$ if and only if ϱ is diagonal in the given basis, and $\langle e_2, \varrho e_2\rangle = \langle e_3, \varrho e_3\rangle = 0$.

C Example for $\widetilde{S}_f(\varrho\|\sigma)$

For any positive definite $\varrho, \sigma \in \mathcal{B}(\mathcal{H})$, and any function $f : (0, +\infty) \to \mathbb{R}$, let

$$\widetilde{S}_f(\varrho\|\sigma) := \operatorname{Tr} \sigma f(\varrho^{1/2}\sigma^{-1}\varrho^{1/2})$$

as in (3.4). In this section we show that there exists a non-linear operator convex function f such that $\widetilde{S}_f$ is neither monotone increasing, nor monotone decreasing under CPTP maps.

To this end, let

$$f_\delta(x) := 1 - x + \delta(1-x)^2, \qquad x \in [0, +\infty),\ \delta > 0.$$

For every $\delta > 0$, f_δ is a non-linear operator convex function on $(0, +\infty)$; in particular, it is strictly convex. According to the theory of classical f-divergences, if $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_{++}$ commute, and Φ is a trace-preserving positive map such that $\Phi(\varrho)$ and $\Phi(\sigma)$ commute, then

$$\widetilde{S}_{f_\delta}(\Phi(\varrho)\|\Phi(\sigma)) \le \widetilde{S}_{f_\delta}(\varrho\|\sigma), \tag{C.1}$$

and the inequality is in general strict; see, e.g., [34, Proposition A.3] for details.

For every $\varepsilon > 0$ and every $t \in (0,1)$, let

$$\varrho_0 := \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}, \qquad \varrho_\varepsilon := \frac{1}{1+2\varepsilon}(\varrho_0 + \varepsilon I), \qquad \text{and} \qquad \sigma_t := \begin{bmatrix} t & 0 \\ 0 & 1-t \end{bmatrix}.$$

Then

$$\begin{aligned} \widetilde{S}_{f_\delta}(\varrho_\varepsilon\|\sigma_t) &= \operatorname{Tr} \sigma_t \left[I - \varrho_\varepsilon^{1/2}\sigma_t^{-1}\varrho_\varepsilon^{1/2} + \delta(I - \varrho_\varepsilon^{1/2}\sigma_t^{-1}\varrho_\varepsilon^{1/2})^2 \right] \\ &\xrightarrow[\varepsilon,\delta\searrow 0]{} \operatorname{Tr} \sigma_t \left[I - \varrho_0^{1/2}\sigma_t^{-1}\varrho_0^{1/2} \right] = 1 - \frac{1}{4t(1-t)} < 0, \qquad t \in (0,1) \setminus \{1/2\}, \end{aligned}$$

with equality in the last inequality for $t = 1/2$. Taking Φ to be the diagonal pinching, we have $\Phi(\varrho_\varepsilon) = \frac{1}{2}I$, $\Phi(\sigma_t) = \sigma_t$, and

$$\begin{aligned} \widetilde{S}_{f_\delta}(\Phi(\varrho_\varepsilon)\|\Phi(\sigma_t)) &= t f_\delta\left(\frac{1/2}{t}\right) + (1-t) f_\delta\left(\frac{1/2}{1-t}\right) \\ &\xrightarrow[\delta\searrow 0]{} t\left(1 - \frac{1}{2t}\right) + (1-t)\left(1 - \frac{1}{2(1-t)}\right) = 0. \end{aligned}$$

Thus, for every $t \in (0,1) \setminus \{1/2\}$, there exist $\varepsilon_t, \delta_t > 0$ such that for all $0 < \varepsilon < \varepsilon_t$ and $0 < \delta < \delta_t$,

$$\widetilde{S}_{f_\delta}(\Phi(\varrho_\varepsilon)\|\Phi(\sigma_t)) > \widetilde{S}_{f_\delta}(\varrho_\varepsilon\|\sigma_t). \tag{C.2}$$

Together with (C.1), this shows that $\widetilde{S}_{f_\delta}$ is neither increasing nor decreasing under CPTP maps.

Remark C.1. The above also implies that $\varrho \mapsto \widetilde{S}_{f_\delta}(\varrho\|\sigma_t)$ is not convex on invertible density operators for any $\delta \in (0,\delta_t)$. Indeed, suppose that $\widetilde{S}_{f_\delta}(\varrho\|\sigma_t)$ is convex in ϱ. Since $\Phi(\varrho_\varepsilon) = \int_\Gamma U\varrho_\varepsilon U^*\,dU$, where Γ is the group of diagonal 2×2 unitaries and dU is the Haar probability measure on Γ, one has a contradiction to (C.2) as follows:

$$\widetilde{S}_{f_\delta}(\Phi(\varrho_\varepsilon)\|\sigma_t) \le \int_\Gamma \widetilde{S}_{f_\delta}(U\varrho_\varepsilon U^*\|\sigma_t)\,dU = \int_\Gamma \widetilde{S}_{f_\delta}(U\varrho_\varepsilon U^*\|U\sigma_t U^*)\,dU = \widetilde{S}_{f_\delta}(\varrho_\varepsilon\|\sigma_t),$$

where the unitary invariance $\widetilde{S}_{f_\delta}(U\varrho_\varepsilon U^*\|U\sigma_t U^*) = \widetilde{S}_{f_\delta}(\varrho_\varepsilon\|\sigma_t)$ is obvious.

D Continuity properties of the standard f-divergences

Proof of Proposition 3.8:

(i) Arrange the eigenvalues of ϱ and σ in decreasing order, counted with multiplicities, as

$$\begin{aligned} &a_1 = \cdots = a_{i_1} > a_{i_1+1} = \cdots = a_{i_2} > \cdots > a_{i_{s-1}+1} = \cdots = a_{i_s}, \\ &b_1 = \cdots = b_{j_1} > b_{j_1+1} = \cdots = b_{j_2} > \cdots > b_{j_{r-1}+1} = \cdots = b_{j_r}, \end{aligned}$$

where $i_s = j_r = d = \dim\mathcal{H}$. Let P_l be the spectral projection of ϱ corresponding to a_{i_l}, and Q_k be the spectral projection of σ corresponding to the eigenvalue b_{j_k}. Let $(\varrho_n)_{n\in\mathbb{N}}$ and $(\sigma_n)_{n\in\mathbb{N}}$ be two sequences in $\mathcal{B}(\mathcal{H})_+$ such that $\varrho_n \to \varrho$, $\sigma_n \to \sigma$ as $n \to +\infty$. Choose spectral decompositions $\varrho_n = \sum_{i=1}^d a_i^{(n)} P_i^{(n)}$ with eigenvalues $a_1^{(n)} \ge \cdots \ge a_d^{(n)}$ and orthogonal rank one projections $P_i^{(n)}$, and similarly, $\sigma_n = \sum_{j=1}^d b_j^{(n)} Q_j^{(n)}$ with eigenvalues $b_1^{(n)} \ge \cdots \ge b_d^{(n)}$ and orthogonal rank one projections $Q_j^{(n)}$. Then, as $n \to \infty$, $a_i^{(n)} \to a_i$ and $\sum_{i=i_{l-1}+1}^{i_l} P_i^{(n)} \to P_l$ for every $l = 1,\dots,s$, and similarly, $b_j^{(n)} \to b_j$ and $\sum_{j=j_{k-1}+1}^{j_k} Q_j^{(n)} \to Q_k$ for every $k = 1,\dots,r$, where $i_0 := j_0 := 0$. Then one has

$$S_f(\varrho_n\|\sigma_n) = \sum_{i,j=1}^d P_f\left(a_i^{(n)}, b_j^{(n)}\right) \operatorname{Tr} P_i^{(n)} Q_j^{(n)}. \tag{D.1}$$

Under the assumption that both $f(0^+)$ and $f'(+\infty)$ are finite, the perspective function P_f is continuous on $[0,+\infty)\times[0,+\infty)$, and hence (D.1) converges to the expression in (3.10).

(ii) Assume that f is operator convex on $(0,+\infty)$, and let L_n be given as stated. First, by the joint convexity in Proposition 3.10 and Remark 3.11 we see that

$$S_f(\varrho + L_n\|\sigma + L_n) \le S_f(\varrho\|\sigma) + S_f(L_n\|L_n) = S_f(\varrho\|\sigma) + f(1)\operatorname{Tr} L_n$$

so that $\limsup_{n\to\infty} S_f(\varrho + L_n\|\sigma + L_n) \le S_f(\varrho\|\sigma)$. Thus, to obtain the result, it remains to prove that $\liminf_{n\to\infty} S_f(\varrho + L_n\|\sigma + L_n) \ge S_f(\varrho\|\sigma)$. To do this, we use the integral expression (2.2) that we rewrite as

$$f(x) = a + bx + cx^2 + dx^{-1} + \int_{(0,+\infty)} \psi_s(x)\,d\lambda(s), \qquad x \in (0,+\infty), \tag{D.2}$$

where $a, b \in \mathbb{R}$, $c, d \geq 0$, and

$$\psi_s(x) := \frac{(x-1)^2}{x+s}, \qquad s > 0.$$

Now we consider the functions $f_1(x) := a + bx$, $f_2(x) := x^2$, $f_{-1}(x) := x^{-1}$, and $\psi_s(x)$ for $s > 0$, separately. For f_1 and ψ_s we have by the previous point

$$\lim_{n\to\infty} S_{f_1}(\varrho + L_n \| \sigma + L_n) = S_{f_1}(\varrho\|\sigma), \tag{D.3}$$

$$\lim_{n\to\infty} S_{\psi_s}(\varrho + L_n \| \sigma + L_n) = S_{\psi_s}(\varrho\|\sigma), \tag{D.4}$$

where (D.3) is also obvious since $S_{f_1}(\varrho\|\sigma) = a \operatorname{Tr} \sigma + b \operatorname{Tr} \varrho$. For f_2 and f_{-1} we prove the following:

$$\liminf_{n\to\infty} S_{f_2}(\varrho + L_n \| \sigma + L_n) \geq S_{f_2}(\varrho\|\sigma), \tag{D.5}$$

$$\liminf_{n\to\infty} S_{f_{-1}}(\varrho + L_n \| \sigma + L_n) \geq S_{f_{-1}}(\varrho\|\sigma). \tag{D.6}$$

When these have been proved, combining (D.3)–(D.6) yields that

$$\begin{aligned}
\liminf_{n\to\infty} S_f(\varrho + L_n\|\sigma + L_n) &\geq S_{f_1}(\varrho\|\sigma) + cS_{f_2}(\varrho\|\sigma) + dS_{f_{-1}}(\varrho\|\sigma) \\
&\quad + \liminf_{n\to\infty} \int_{(0,+\infty)} S_{\psi_s}(\varrho + L_n\|\sigma + L_n)\, d\lambda(s) \\
&\geq S_{f_1}(\varrho\|\sigma) + cS_{f_2}(\varrho\|\sigma) + dS_{f_{-1}}(\varrho\|\sigma) + \int_{(0,+\infty)} S_{\psi_s}(\varrho\|\sigma)\, d\lambda(s) \\
&= S_f(\varrho\|\sigma),
\end{aligned}$$

where the second inequality in the above is due to Fatou's lemma since $S_{\psi_s}(\varrho + L_n\|\sigma + L_n) \geq 0$ for all $s \in (0, +\infty)$ and $n \in \mathbb{N}$. Thus (D.2) follows. Hence, we are left to prove (D.5) and (D.6).

Proof of (D.5): By (3.10) and Corollary 3.4, note that

$$S_{f_2}(\varrho\|\sigma) = \begin{cases} \operatorname{Tr} \varrho^2\sigma^{-1} & \text{if } \varrho^0 \leq \sigma^0, \\ +\infty & \text{if } \varrho^0 \not\leq \sigma^0, \end{cases}$$

and

$$S_{f_2}(\varrho + L_n\|\sigma + L_n) = \operatorname{Tr}(\varrho + L_n)^2(\sigma + L_n)^{-1}.$$

Assume that $\varrho^0 \leq \sigma^0$. Apply the monotonicity property (Proposition 3.12) to the pinching $\Phi(X) := \sigma^0 X \sigma^0 + (I - \sigma^0)X(I - \sigma^0)$ to obtain

$$\begin{aligned}
&S_{f_2}(\varrho + L_n\|\sigma + L_n) \\
&\quad \geq S_{f_2}(\Phi(\varrho + L_n)\|\Phi(\sigma + L_n)) \\
&\quad = S_{f_2}\big((\varrho + \sigma^0 L_n\sigma^0) + (I - \sigma^0)L_n(I - \sigma^0)\|(\sigma + \sigma^0 L_n\sigma^0) + (I - \sigma^0)L_n(I - \sigma^0)\big) \\
&\quad = \operatorname{Tr}(\varrho + \sigma^0 L_n\sigma^0)^2(\sigma + \sigma^0 L_n\sigma^0)^{-1} + \operatorname{Tr}(I - \sigma^0)L_n(I - \sigma^0).
\end{aligned}$$

Since $\operatorname{Tr}(\varrho + \sigma^0 L_n\sigma^0)^2(\sigma + \sigma^0 L_n\sigma^0)^{-1} \to \operatorname{Tr}\varrho^2\sigma^{-1}$ and $\operatorname{Tr}(I - \sigma^0)L_n(I - \sigma^0) \to 0$ as $n \to \infty$, (D.5) holds in the case $\varrho^0 \leq \sigma^0$.

Next, assume that $\varrho^0 \not\leq \sigma^0$ (hence $L_n \neq 0$ for all n). Since

$$(\sigma + L_n)^{-1} \geq (\sigma + \|L_n\|_\infty I)^{-1} \geq \|L_n\|_\infty^{-1}(I - \sigma^0)$$

with the operator norm $\|L_n\|_\infty$, one has

$$\operatorname{Tr}(\varrho+L_n)^2(\sigma+L_n)^{-1} \ge \|L_n\|_\infty^{-1} \operatorname{Tr}(\varrho^2+\varrho L_n+L_n\varrho+L_n^2)(I-\sigma^0),$$

which implies (D.5) in this case too, by noting that $\|L_n\|_\infty^{-1} \to +\infty$, $\operatorname{Tr}\varrho^2(I-\sigma^0)>0$ due to $\varrho^0 \not\le \sigma^0$, and $\varrho L_n + L_n\varrho + L_n^2 \to 0$.

Proof of (D.6): The proof is immediate from the above and Proposition 3.7, since $f_{-1}=\widetilde{f}_2$. $\square$

Unlike in the classical case, the continuity property stated in (ii) of Proposition 3.8 may not hold when f is only assumed to be convex, as the following example shows.

Example D.1. Here we give an example where $\varrho=\sigma$ and $\varrho_\varepsilon=\varrho+\varepsilon K$, $\sigma_\varepsilon=\sigma+\varepsilon L$ such that $K,L\ge 0$ and $\varrho+K,\sigma+L>0$, but $\lim_{\varepsilon\searrow 0} S_f(\varrho+\varepsilon K\|\sigma+\varepsilon L) \ne S_f(\varrho\|\sigma)$ for a convex but not operator convex f.

Let $\varrho=\sigma=\begin{bmatrix}1&0\\0&0\end{bmatrix}$ and $K=\begin{bmatrix}0&0\\0&1\end{bmatrix}$, $L=\begin{bmatrix}1/2&1/2\\1/2&1/2\end{bmatrix}$ so that $\varrho+K,\sigma+L>0$. The eigenvalues of $\sigma+\varepsilon L$ are

$$b_1^{(\varepsilon)}=\frac{1+\varepsilon+\sqrt{1+\varepsilon^2}}{2},\qquad b_2^{(\varepsilon)}=\frac{1+\varepsilon-\sqrt{1+\varepsilon^2}}{2},$$

whose unit eigen-vectors are

$$y_1^{(\varepsilon)}=\begin{bmatrix}\frac{\varepsilon}{\left[2(1+\varepsilon^2-\sqrt{1+\varepsilon^2})\right]^{1/2}}\\ \frac{\sqrt{1+\varepsilon^2}-1}{\left[2(1+\varepsilon^2-\sqrt{1+\varepsilon^2})\right]^{1/2}}\end{bmatrix},\qquad y_2^{(\varepsilon)}=\begin{bmatrix}\frac{\varepsilon}{\left[2(1+\varepsilon^2+\sqrt{1+\varepsilon^2})\right]^{1/2}}\\ -\frac{\sqrt{1+\varepsilon^2}+1}{\left[2(1+\varepsilon^2+\sqrt{1+\varepsilon^2}\right]^{1/2}}\end{bmatrix},$$

respectively. Therefore, with $P_1=\begin{bmatrix}1&0\\0&0\end{bmatrix}$, $P_2=\begin{bmatrix}0&0\\0&1\end{bmatrix}$, $Q_1^{(\varepsilon)}=|y_1^{(\varepsilon)}\rangle\langle y_1^{(\varepsilon)}|$ and $Q_2^{(\varepsilon)}=|y_2^{(\varepsilon)}\rangle\langle y_2^{(\varepsilon)}|$, we have

$$\begin{aligned}S_f(\varrho+\varepsilon K\|\sigma+\varepsilon L)&=b_1^{(\varepsilon)}f(1/b_1^{(\varepsilon)})\operatorname{Tr}P_1Q_1^{(\varepsilon)}+b_2^{(\varepsilon)}f(1/b_2^{\varepsilon})\operatorname{Tr}P_1Q_2^{(\varepsilon)}\\&\quad+b_1^{(\varepsilon)}f(\varepsilon/b_1^{(\varepsilon)})\operatorname{Tr}P_2Q_1^{(\varepsilon)}+b_2^{(\varepsilon)}f(\varepsilon/b_2^{(\varepsilon)})\operatorname{Tr}P_2Q_2^{(\varepsilon)}.\end{aligned}\tag{D.7}$$

Since $b_1^{(\varepsilon)}\to 1$ and $y_1^{(\varepsilon)}\to\begin{bmatrix}1\\0\end{bmatrix}$ so that $Q_1^{(\varepsilon)}\to P_1$, we have as $\varepsilon\searrow 0$,

$$b_1^{(\varepsilon)}f(1/b_1^{(\varepsilon)})\operatorname{Tr}P_1Q_1^{(\varepsilon)}\ \longrightarrow\ f(1)=S_f(\varrho\|\sigma).$$

On the other hand,

$$\begin{aligned}b_2^{(\varepsilon)}f(1/b_2^{(\varepsilon)})\operatorname{Tr}P_1Q_2^{(\varepsilon)}&=\frac{1+\varepsilon-\sqrt{1+\varepsilon^2}}{2}\,f\left(\frac{2}{1+\varepsilon-\sqrt{1+\varepsilon^2}}\right)\frac{\varepsilon^2}{2(1+\varepsilon^2+\sqrt{1+\varepsilon^2})}\\&=\frac{\varepsilon^3}{2(1+\varepsilon+\sqrt{1+\varepsilon^2})(1+\varepsilon^2+\sqrt{1+\varepsilon^2})}\,f\left(\frac{1+\varepsilon+\sqrt{1+\varepsilon^2}}{\varepsilon}\right).\end{aligned}$$

For example, when $f(x)=x^\alpha$ where $\alpha>0$, we find that

$$b_2f(1/b_2^{\varepsilon})\operatorname{Tr}P_1Q_2^{(\varepsilon)}=\frac{\varepsilon^{3-\alpha}(1+\varepsilon+\sqrt{1+\varepsilon^2})^{\alpha-1}}{2(1+\varepsilon^2+\sqrt{1+\varepsilon^2})}\ \longrightarrow\ \begin{cases}0&\text{if } 0<\alpha<3\\1&\text{if }\alpha=3\\+\infty&\text{if }\alpha>3\end{cases}$$

Since the other two terms in (D.7) are non-negative, we have

$$\lim_{\varepsilon \searrow 0} S_f(\varrho + \varepsilon K \| \sigma + \varepsilon L) = +\infty \neq S_f(\varrho \| \sigma)$$

for $f(x) = x^\alpha$ with $\alpha > 3$.

We also have the following one-sided continuity result:

Proposition D.2. Let $\varrho, \sigma \in \mathcal{B}(\mathcal{H})_+$ and let f be an operator convex function on $(0, +\infty)$.

(i) If $f(0^+) < +\infty$ and $\varrho^0 \leq \sigma^0$, then

$$S_f(\varrho \| \sigma) = \lim_{n \to \infty} S_f(\varrho \| \sigma + L_n)$$

for any sequence $L_n \in \mathcal{B}(\mathcal{H})_+$ with $L_n \to 0$.

(ii) If $f'(+\infty) < +\infty$ and $\sigma^0 \leq \varrho^0$, then

$$S_f(\varrho \| \sigma) = \lim_{n \to \infty} S_f(\varrho + K_n \| \sigma)$$

for any sequence $K_n \in \mathcal{B}(\mathcal{H})_+$ with $K_n \to 0$.

Proof. By Remark 3.11,

$$S_f(\varrho \| \sigma + L_n) \leq S_f(\varrho \| \sigma) + S_f(0 \| L_n) = S_f(\varrho \| \sigma) + f(0^+) \operatorname{Tr} L_n,$$

so it is enough to prove that $\liminf_{n \to \infty} S_f(\varrho \| \sigma + L_n) \geq S_f(\varrho \| \sigma)$. The assumption $f(0^+) < +\infty$ guarantees that the f_{-1} term does not appear in the integral representation (D.2). Moreover, by (i) of Proposition 3.8, we have

$$\lim_{n \to \infty} S_{f_1}(\varrho \| \sigma + L_n) = S_{f_1}(\varrho \| \sigma), \qquad \lim_{n \to \infty} S_{\psi_s}(\varrho \| \sigma + L_n) = S_{\psi_s}(\varrho \| \sigma). \tag{D.8}$$

Thus, it is enough to show show that $\liminf_{n \to \infty} S_{f_2}(\varrho \| \sigma + L_n) \geq S_{f_2}(\varrho \| \sigma)$. This is easy as in the above proof of (D.5):

$$\begin{aligned} S_{f_2}(\varrho \| \sigma + L_n) &\geq S_{f_2}\big(\varrho \| (\sigma + \sigma^0 L_n \sigma^0) + (I - \sigma^0) L_n (I - \sigma^0)\big) \\ &= \operatorname{Tr} \varrho^2 (\sigma + \sigma^0 L_n \sigma^0)^{-1} \ \longrightarrow \ \operatorname{Tr} \varrho^2 \sigma^{-1} = S_{f_2}(\varrho \| \sigma), \end{aligned}$$

where the convergence holds due to the assumption $\varrho^0 \leq \sigma^0$. This proves (i), and (ii) follows by using $S_f(\varrho \| \sigma) = S_{\widetilde{f}}(\sigma \| \varrho)$. □

Again, assuming only convexity of f is not sufficient for the above proposition.

Example D.3. Let ϱ, σ and L as in Example D.1, and $f(x) := x^\alpha$ with some fixed $\alpha > 3$. Then $f(0^+) = 0$, $\varrho^0 \leq \sigma^0$, and the same calculation as in Example D.1 shows that

$$\lim_{\varepsilon \searrow 0} S_f(\varrho \| \sigma + \varepsilon L) = +\infty \neq S_f(\varrho \| \sigma)$$

for $f(x) = x^\alpha$ with $\alpha > 3$.

E Proof of Proposition 3.26

Proof of (i). Since f is operator convex, $g(x) := (f(x) - f(1))/(x-1)$ where $g(1) := f'(1)$ is an operator monotone function on $(0, +\infty)$, and $f(0^+) < +\infty$ implies that $g(0) := g(0^+)$ is finite. Thus, $h(x) := g(x) - g(0^+)$ is a non-negative operator monotone function on $[0, +\infty)$, so that

$$f(x) = \alpha + \beta x + (x-1)h(x), \qquad x \in (0, \infty),$$

where $\alpha, \beta \in \mathbb{R}$. If $h(1) = 0$ then h is identically zero, and the assertion is trivial, so for the rest we can assume that $h(1) = 1$, by possibly replacing h with $h/h(1)$. Then we can write

$$\begin{aligned}
&P_f(\varrho + K_n, \sigma + K_n) \\
&\quad = \alpha(\sigma + K_n) + \beta(\varrho + K_n) \\
&\qquad + (\sigma + K_n)^{1/2}\big[(\sigma + K_n)^{-1/2}(\varrho + K_n)(\sigma + K_n)^{-1/2} - I\big] \\
&\qquad\qquad \times h\big((\sigma + K_n)^{-1/2}(\varrho + K_n)(\sigma + K_n)^{1/2}\big)(\sigma + K_n)^{1/2} \\
&\quad = \alpha(\sigma + K_n) + \beta(\varrho + K_n) + \big[(\varrho + K_n)(\sigma + K_n)^{-1} - I\big]\big[(\sigma + K_n)\,\tau_h\,(\varrho + K_n)\big].
\end{aligned}$$

On the other hand, we write

$$\begin{aligned}
\sigma^{1/2} f(\sigma^{-1/2}\varrho\sigma^{-1/2})\sigma^{1/2} &= \alpha\sigma + \beta\varrho + \sigma^{1/2}(\sigma^{-1/2}\varrho\sigma^{-1/2} - P)h(\sigma^{-1/2}\varrho\sigma^{-1/2})\sigma^{1/2} \\
&= \alpha\sigma + \beta\varrho + (\varrho\sigma^{-1} - P)(\sigma\,\tau_h\,\varrho),
\end{aligned}$$

where $P := \sigma^0$ and the operator mean $\sigma\,\tau_h\,\varrho$ is defined as an operator in $\mathcal{B}(P\mathcal{H})$. Set

$$Y_n := \big[(\varrho + K_n)(\sigma + K_n)^{-1} - I\big]\big[(\sigma + K_n)\,\tau_h\,(\varrho + K_n)\big], \tag{E.1}$$

and write Y_n in the form of 2×2 block matrices under the decomposition $\mathcal{H} = P\mathcal{H} \oplus (I-P)\mathcal{H}$ as

$$Y_n = \begin{bmatrix} Y_{11}^{(n)} & Y_{12}^{(n)} \\ Y_{21}^{(n)} & Y_{22}^{(n)} \end{bmatrix}, \qquad (Y_{12}^{(n)})^* = Y_{21}^{(n)}.$$

What we need to prove is that, as $n \to \infty$,

$$Y_{11}^{(n)} \longrightarrow (\varrho\sigma^{-1} - P)(\sigma\,\tau_h\,\varrho), \quad Y_{12}^{(n)} \longrightarrow 0 \;\; (\text{hence } \; Y_{21}^{(n)} \longrightarrow 0), \quad Y_{22}^{(n)} \longrightarrow 0. \tag{E.2}$$

We also write

$$K_n := \begin{bmatrix} K_{11}^{(n)} & K_{12}^{(n)} \\ K_{21}^{(n)} & K_{22}^{(n)} \end{bmatrix}, \qquad (K_{12}^{(n)})^* = K_{21}^{(n)}.$$

Since $K_n \ge 0$, we note (see, e.g., [12, Proposition 1.3.2]) that

$$K_{12}^{(n)} = (K_{11}^{(n)})^{1/2} W_n (K_{22}^{(n)})^{1/2}, \quad K_{21}^{(n)} = (K_{22}^{(n)})^{1/2} W_n^* (K_{11}^{(n)})^{1/2} \quad \text{with} \quad \|W_n\| \le 1, \tag{E.3}$$

and $K_n \to 0$ means that $K_{ij}^{(n)} \to 0$ $(i, j = 1, 2)$ as $n \to \infty$. Furthermore, we write

$$(\varrho + K_n)(\sigma + K_n)^{-1} = \begin{bmatrix} X_{11}^{(n)} & X_{12}^{(n)} \\ X_{21}^{(n)} & X_{22}^{(n)} \end{bmatrix}. \tag{E.4}$$

We will perform the following computations, for the sake of brevity, with disregarding the superscript $^{(n)}$. Since

$$\begin{bmatrix} \varrho + K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} \sigma + K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix},$$

we have

$$\varrho + K_{11} = X_{11}(\sigma + K_{11}) + X_{12}K_{21}, \tag{E.5}$$
$$K_{12} = X_{11}K_{12} + X_{12}K_{22}, \tag{E.6}$$
$$K_{21} = X_{21}(\sigma + K_{11}) + X_{22}K_{21}, \tag{E.7}$$
$$K_{22} = X_{21}K_{12} + X_{22}K_{22}. \tag{E.8}$$

Note that $K_{22} > 0$ since $\sigma + K_n > 0$. By (E.3) and (E.6) one finds

$$\begin{aligned} X_{12}K_{21} &= X_{12}K_{22}^{1/2}W_n^*K_{11}^{1/2} = (I_1 - X_{11})K_{12}K_{22}^{-1/2}W_n^*K_{11}^{1/2} \\ &= (I_1 - X_{11})K_{11}^{1/2}W_nW_n^*K_{11}^{1/2}. \end{aligned}$$

Therefore, by (E.5),

$$\varrho + K_{11} = X_{11}(\sigma + K_{11}) + (I_1 - X_{11})K_{11}^{1/2}W_nW_n^*K_{11}^{1/2}$$

so that

$$X_{11} = \left(\varrho + K_{11} - K_{11}^{1/2}W_nW_n^*K_{11}^{1/2}\right)\left(\sigma + K_{11} - K_{11}^{1/2}W_nW_n^*K_{11}^{1/2}\right)^{-1} \tag{E.9}$$

for sufficiently large n. Here, note that the operator in the second bracket above is invertible for large n. By (E.7), (E.3) and (E.8) one further finds

$$\begin{aligned} X_{21}(\sigma + K_{11}) &= K_{21} - X_{22}K_{21} = K_{21} - X_{22}K_{22}^{1/2}W_n^*K_{11}^{1/2} \\ &= K_{21} - (K_{22} - X_{21}K_{12})K_{22}^{-1/2}W_n^*K_{11}^{1/2} \\ &= K_{21} - K_{22}^{1/2}W_n^*K_{11}^{1/2} + X_{21}K_{11}^{1/2}W_nW_n^*K_{11}^{1/2}, \end{aligned}$$

which implies that

$$X_{21} = \left(K_{21} - K_{22}^{1/2}W_n^*K_{11}^{1/2}\right)\left(\sigma + K_{11} - K_{11}^{1/2}W_nW_n^*K_{11}^{1/2}\right)^{-1} \tag{E.10}$$

for sufficiently large n. Furthermore, by (E.6) and (E.3) one has

$$X_{12}K_{22}^{1/2} = (I_1 - X_{11})K_{12}K_{22}^{-1/2} = (I_1 - X_{11})K_{11}^{1/2}W_n. \tag{E.11}$$

Now, via (E.9), (E.10), (E.11) and (E.8) we obtain the convergences

$$X_{11}^{(n)} \longrightarrow \varrho\sigma^{-1}, \quad X_{21}^{(n)} \longrightarrow 0, \quad X_{12}^{(n)}(K_{22}^{(n)})^{1/2} \longrightarrow 0, \quad X_{22}^{(n)}K_{22}^{(n)} \longrightarrow 0. \tag{E.12}$$

We next write

$$(\sigma + K_n)\,\tau_h\,(\varrho + K_n) = \begin{bmatrix} A_{11}^{(n)} & A_{12}^{(n)} \\ A_{21}^{(n)} & A_{22}^{(n)} \end{bmatrix}, \qquad (A_{12}^{(n)})^* = A_{21}^{(n)}, \tag{E.13}$$

and note as in (E.3) that

$$A_{21}^{(n)} = (A_{22}^{(n)})^{1/2}V_n(A_{11}^{(n)})^{1/2} \quad \text{with} \quad \|V_n\| \le 1. \tag{E.14}$$

Since $(\sigma + K_n)\,\tau_h\,(\varrho + K_n) \to \sigma\,\tau_h\,\varrho$, we have

$$A_{11}^{(n)} \longrightarrow \sigma\,\tau_h\,\varrho, \qquad A_{12}^{(n)} \longrightarrow 0, \qquad A_{22}^{(n)} \longrightarrow 0. \tag{E.15}$$

Moreover, since

$$(\sigma + K_n)\,\tau_h\,(\varrho + K_n) \geq K_n\,\tau_h\,K_n = K_n,$$

we have $A_{22}^{(n)} \geq K_{22}^{(n)}$. On the other hand, by the transformer inequality,

$$\begin{aligned} A_{22}^{(n)} &= P^\perp\big[(\sigma + K_n)\,\tau_h\,(\varrho + K_n)\big]P^\perp \\ &\leq \big(P^\perp(\sigma + K_n)P^\perp\big)\,\tau_h\,\big(P^\perp(\varrho + K_n)P^\perp\big) \\ &= (P^\perp K_n P^\perp)\,\tau_h\,(P^\perp K_n P^\perp) = K_{22}^{(n)}. \end{aligned}$$

Therefore,

$$A_{22}^{(n)} = K_{22}^{(n)}. \tag{E.16}$$

Finally, since (E.1), (E.4) and (E.13) give

$$Y_n = \begin{bmatrix} X_{11}^{(n)} - I_1 & X_{12}^{(n)} \\ X_{21}^{(n)} & X_{22}^{(n)} - I_2 \end{bmatrix} \begin{bmatrix} A_{11}^{(n)} & A_{12}^{(n)} \\ A_{21}^{(n)} & A_{22}^{(n)} \end{bmatrix},$$

we have, by (E.14) and (E.16),

$$\begin{aligned} Y_{11}^{(n)} &= (X_{11}^{(n)} - I_1)A_{11}^{(n)} + X_{12}^{(n)}(K_{22}^{(n)})^{1/2}V_n(A_{11}^{(n)})^{1/2}, \\ Y_{12}^{(n)} &= (X_{11}^{(n)} - I_1)A_{12}^{(n)} + X_{12}^{(n)}K_{22}^{(n)}, \\ Y_{22}^{(n)} &= X_{21}^{(n)}A_{12}^{(n)} + (X_{22}^{(n)} - I_2)K_{22}^{(n)}. \end{aligned}$$

Together with (E.12) and (E.15) these yield the required convergences in (E.2).

Proof of (ii). This follows from (i) by Lemma 2.1.

Proof of (iii). From the integral expression (2.2) we define

$$\begin{aligned} f_0(x) &:= f(1) + f'(1)(x-1) + c(x-1)^2 + \int_{[1,+\infty)} \frac{(x-1)^2}{x+s}\,d\lambda(s), \\ f_1(x) &:= \int_{[0,1)} \frac{(x-1)^2}{x+s}\,d\lambda(s), \qquad x \in (0,+\infty). \end{aligned}$$

Then f_0 and f_1 are operator convex functions on $(0,+\infty)$ such that $f = f_0 + f_1$. Since $\int_{[0,+\infty)}(1+s)^{-1}\,d\lambda(s) < +\infty$, note that

$$\int_{[1,+\infty)} \frac{1}{s}\,d\lambda(s) < +\infty, \qquad \int_{[0,1)} d\lambda(s) < +\infty.$$

Hence it is easy to see that $f_0(0^+) < +\infty$ and $f_1'(+\infty) < +\infty$. So one can apply (i) to f_0 and (ii) to f_1 to obtain

$$\lim_{n\to\infty} P_{f_0}(\varrho + K_n, \sigma + K_n) = \sigma^{1/2} f_0\left(\sigma^{-1/2}\varrho\sigma^{-1/2}\right)\sigma^{1/2} \tag{E.17}$$

$$\lim_{n\to\infty} P_{f_1}(\varrho + K_n, \sigma + K_n) = \varrho^{1/2} \widetilde{f}_1\left(\varrho^{-1/2}\sigma\varrho^{-1/2}\right)\varrho^{1/2}. \tag{E.18}$$

Since the assumption $\varrho^0 = \sigma^0$ gives

$$\sigma^{1/2} f_k\left(\sigma^{-1/2}\varrho\sigma^{-1/2}\right)\sigma^{1/2} = \varrho^{1/2}\widetilde{f}_k\left(\varrho^{-1/2}\sigma\varrho^{-1/2}\right)\varrho^{1/2}, \qquad k = 0, 1,$$

the conclusion of (iii) follows by adding (E.17) and (E.18) together. □

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