
Limit Distribution Theory for Quantum Divergences

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Abstract

Estimation of quantum relative entropy and its Rényi generalizations is a fundamental statistical task in quantum information theory, physics, and beyond. While several estimators of these divergences have been proposed in the literature along with their computational complexities explored, a limit distribution theory which characterizes the asymptotic fluctuations of the estimation error is still premature. As our main contribution, we characterize these asymptotic distributions in terms of Fréchet derivatives of elementary operator-valued functions. We achieve this by leveraging an operator version of Taylor's theorem and identifying the regularity conditions needed. As an application of our results, we consider an estimator of quantum relative entropy based on Pauli tomography of quantum states and show that the resulting asymptotic distribution is a centered normal, with its variance characterized in terms of the Pauli operators and states. We utilize the knowledge of the aforementioned limit distribution to obtain asymptotic performance guarantees for a multi-hypothesis testing problem.

Index Terms

Quantum divergences, limit distribution, divergence estimation, Fréchet derivative, hypothesis testing

I. INTRODUCTION

Estimation of a quantum state, also known as quantum state tomography, is an important problem in quantum information theory, physics, and quantum machine learning, see e.g., [1]–[8]. In several applications, however, the quantity of interest may not be the entire state, but only a functional of it. Quantum divergences such as quantum relative entropy [9] and its Rényi generalizations [10]–[14] form an important class of such functionals. They play a central role in quantum information theory both in terms of characterizing fundamental limits as well as applications, e.g., see the books [15]–[17]. For instance, the quantum relative entropy characterizes the error-exponent in asymmetric binary quantum hypothesis testing [18] and the Petz-Rényi divergence quantifies the exponent in quantum Chernoff bounds [19], [20]. Owing to their significance, several estimators of these measures have been proposed recently in the literature and their performance investigated in terms of benchmarks such as copy and query complexity (see *Related work* section below). However, a limit distribution theory which characterizes the asymptotic distribution of estimation error is largely unexplored.

Here, we seek a limit distribution theory for the aforementioned quantum divergences. Given two quantum states ρ and σ with corresponding estimators ρ_n and σ_n , respectively, and a divergence $D(\rho, \sigma)$, we want to identify

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the scaling rate r_n (or convergence rate r_n^{-1}) and the limiting variable Z such that the following convergence in distribution (weak convergence) holds:

$$r_n(\mathcal{D}(\rho_n, \sigma_n) - \mathcal{D}(\rho, \sigma)) \xrightarrow{w} Z.$$

Of interest is also the scenario where only one state, say ρ or σ , is estimated and the other is known. Characterization of such limit distributions have several potential applications in quantum statistics and machine learning such as constructing confidence intervals for quantum hypothesis testing, asymptotic analysis of quantum algorithms, and quantum statistics (see [21]–[23] for some classical applications).

While limit distributions fully quantify the asymptotic performance, deriving such results for estimators of quantum divergences are challenging on account of two reasons. Firstly, limit distributions need not always exist, as is well-known for relative entropy in the classical setting. Secondly, the non-commutative framework of quantum theory makes the analysis more involved. For tackling the first challenge, we use an operator version of Taylor's expansion with remainder and ascertain primitive conditions for the existence of limits. The technical core of our contribution entails determining conditions that allow interchange of limiting operations on trace functionals of Fréchet derivatives that appear in such an expansion. For handling issues arising due to non-commutativity, we use appropriate integral expressions for operator functions and dual formulations for divergences.

Applying the aforementioned method to quantum relative entropy, we establish the following convergence in distribution (Theorem 1) when $r_n(\rho_n - \rho) \xrightarrow{w} L_1$ and $r_n(\sigma_n - \sigma) \xrightarrow{w} L_2$ for $\rho \neq \sigma$:

$$r_n(\mathcal{D}(\rho_n \| \sigma_n) - \mathcal{D}(\rho \| \sigma)) \xrightarrow{w} \text{Tr}[L_1(\log \rho - \log \sigma) - \rho D[\log \sigma](L_2)].$$

Here¹, $D[f(A)](B)$ denotes the first-order Fréchet derivative (see Section II for precise definitions) of an operator-valued function f at operator A in the direction of operator B , and L_1 (resp. L_2) denotes the weak limit of the estimator ρ_n (resp. σ_n), appropriately centered and scaled. Analogous to the classical case, a faster convergence rate is achieved when $\rho = \sigma$ with the limit characterized in terms of second-order derivatives. We then consider two prominent quantum Rényi divergences, namely, the Petz-Rényi [11] and the minimal or sandwiched Rényi divergences of order α [13], [14]. While the former admits an analysis similar to Theorem 1, for the latter, we consider a variational form based on dual expressions and derive the limits by applying Taylor's theorem to an intermediate quantity which is easier to analyze. We also use a similar approach to derive the limit distribution for measured relative entropy estimation under a certain assumption on the uniqueness of the optimal measurement.

As an application of our limit distribution results, we characterize the asymptotic distribution of an estimator of quantum relative entropy based on Pauli tomography of quantum states ρ, σ . Specifically, we show that

$$\sqrt{n}(\mathcal{D}(\hat{\rho}_n \| \hat{\sigma}_n) - \mathcal{D}(\rho \| \sigma)) \xrightarrow{w} W,$$

where W is a centered Gaussian variable with a variance that depends on the states and Pauli operators. We then use this result to obtain performance guarantees for a multi-hypothesis testing problem for determining the quantum relative entropy between an unknown state ρ and a known state σ . Assuming that identical copies of the

¹Throughout, we consider logarithms to the base e .

unknown state are available for measurement, we first perform tomography to obtain an estimate of ρ and then use the knowledge of the Gaussian limit to design a test statistic (decision rule) that achieves any desired error level for appropriately chosen thresholds. The test statistic achieves the same performance even when the number of hypotheses scales at a sufficiently slow rate with the number of measurements. Such tests have potential applications to auditing of quantum differential privacy [24], as considered in [22], [25] for the classical case.

A. Related Work

Statistical analysis of estimators of classical information measures and divergences has been an active area of research over the past few decades. The relevant literature pertains broadly to showing consistency, quantifying convergence rates of estimators (or equivalently sample complexity), and characterizing their limiting distributions. Consistency and/or convergence rates for various estimators of f -divergences, which subsumes entropy and mutual information as special cases, have been studied in [26]–[39]. Limit distributions for several f -divergence estimators such as those based on kernel density estimates, k -nearest neighbour methods, and plug-in methods have been established recently [22], [25], [30], [40]–[44], while corresponding results for Rényi divergences have been studied in [23]. Limit distribution theory has also been explored extensively in the optimal transport literature for the class of Wasserstein distances [45]–[52], as well as their regularized versions [50], [53]–[63].

In the quantum setting, computational complexities of various estimators of quantum information measures have been investigated under different input models [64]–[78]. Specifically, [66] established copy complexity bounds characterizing the optimal dimension dependence for quantum Rényi entropy estimation when independent copies of the state are available for measurement. [67], [69] considered entropy estimation under a quantum query model, which assumes access to an oracle that prepares the input quantum state. For limit distributional results in the quantum setting, the asymptotic distribution for spectrum estimation of a quantum state based on the empirical Young’s diagram (EYD) algorithm [79], [80] was determined in [81], [82]. However, to the best of our knowledge, a limit distribution theory for quantum divergences has not been explored before. Here, we study this aspect focusing mostly on finite dimensional quantum systems (except in Section III-C where we treat quantum relative entropy between density operators on an infinite-dimensional separable Hilbert space).

B. Paper Organization

The rest of the paper is organized as follows. Section II introduces the notation and preliminary concepts required for stating our results. The main results on limit distributions of quantum divergences are presented in Section III. The applications, namely limit distributions of quantum relative entropy for tomographic estimators and performance guarantees for a multi-hypothesis testing problem, are discussed in Section IV. This is followed by concluding remarks with avenues for future research in Section V. The proofs of the main results and applications are furnished in Section VI while those of the auxiliary lemmas are provided in the Appendix.

II. PRELIMINARIES

A. Notation

For most part, we consider a finite dimensional complex Hilbert space \mathbb{H}_d of dimension d . Denote the set of linear operators from \mathbb{H}_d to \mathbb{H}_d by $\mathcal{L}(\mathbb{H}_d)$. Without loss of generality, we identify \mathbb{H}_d and $\mathcal{L}(\mathbb{H}_d)$ with \mathbb{C}^d and $\mathbb{C}^{d \times d}$, respectively. Denote the set of all $d \times d$ Hermitian, positive semi-definite, positive definite, and unitary operators by \mathcal{H}_d , \mathcal{P}_d , \mathcal{P}_d^+ and \mathcal{U}_d , respectively. Let \mathcal{S}_d denote the set of density operators, i.e., the set of elements of \mathcal{P}_d with unit trace, and \mathcal{S}_d^+ be its subset with strictly positive eigenvalues. We use $[A, B] := AB - BA$ to represent the commutator of two operators A and B . $\text{Tr}[\cdot]$ and $\|\cdot\|_p$ for $p \geq 1$ signifies the trace operation and Schatten p -norm, respectively. The notation \leq denotes the Löwner partial order in the context of operators, i.e., for $A, B \in \mathcal{H}_d$, $A \leq B$ means that $B - A \in \mathcal{P}_d$. $\mathbb{1}_{\mathcal{X}}$ denotes indicator of a set \mathcal{X} and I denotes the identity operator on \mathbb{H}_d . For linear operators A, B , $A \ll B$ designates that the support of A is contained in that of B , and $A \ll\!\!\ll B$ means that $B \ll A \ll B$. A^{-1} stands for the generalized (Moore–Penrose) inverse of an operator A . For $a, b \in \mathbb{R}$, $a \vee b := \max\{a, b\}$ and $a \wedge b := \min\{a, b\}$. Lastly, we use $a \lesssim_x b$ to denote that $a \leq c_x b$ for some constant $c_x > 0$ which depends only on x .

B. Weak convergence of Random Density Operators

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a sufficiently rich probability space on which all random elements are defined. A sequence of random elements $(X_n)_{n \in \mathbb{N}}$ taking values in a topological space \mathfrak{S} converges weakly to a random element X (taking values in \mathfrak{S}) if $\mathbb{E}[f(X_n)] \rightarrow \mathbb{E}[f(X)]$ for all bounded continuous functions $f : \mathfrak{S} \rightarrow \mathbb{R}$. This is denoted by $X_n \xrightarrow{w} X$. Here, the random element of interest is a random density operator (or operators), which is a Borel-measurable mapping from Ω to the space of density operators, \mathcal{S}_d . The weak limit of a random density operator is unique if it exists (see e.g. [83]). Since density operators have unit trace, the appropriate space \mathfrak{S} to consider weak convergence for our purposes is the space of trace-class operators, i.e., the space of operators with finite trace. In finite dimensions, we may take $\mathfrak{S} = \mathcal{L}(\mathbb{H}_d)$ equipped with any norm since all norms are equivalent.

C. Fréchet Differentiability

Definition 1 (Fréchet differentiability, see e.g. [84]) *For an open set $\mathcal{X} \subseteq \mathbb{R}$, let $f : \mathcal{X} \rightarrow \bar{\mathbb{R}}$ and $A \in \mathcal{H}_d$ with $\text{spec}(A) \subseteq \mathcal{X}$. Then, f is called (Fréchet) differentiable at A if there exists a linear map $D[f(A)] : \mathcal{H}_d \rightarrow \mathcal{H}_d$ such that for all $H \in \mathcal{H}_d$ such that $\text{spec}(A + H) \subseteq \mathcal{X}$,*

$$\|f(A + H) - f(A) - D[f(A)](H)\| = o(\|H\|). \quad (1)$$

Then, $D[f(A)]$ is called the (Fréchet) derivative of f at A and $D[f(A)](H)$ is the directional derivative of f at A in the direction H . The derivative of f induces a map from \mathcal{H}_d into $\mathcal{L}(\mathcal{H}_d)$ given by $D[f] : A \rightarrow D[f(A)]$. If this map is also differentiable at A , then f is said to be twice differentiable at A with the corresponding second-order derivative given by a bilinear map $D^2[f(A)] : \mathcal{H}_d \times \mathcal{H}_d \rightarrow \mathcal{H}_d$.

If f is differentiable at A , then

$$D[f(A)](H) = \frac{d}{dt} f(A + tH) \Big|_{t=0}, \quad \forall H \in \mathcal{H}_d.$$

The chain rule holds: the composition of two differentiable maps f and g is differentiable and $D[g \circ f(A)] = D[g(f(A))]D[f(A)]$. Also, we have the product rule: for two differentiable maps f and g and $h = fg$,

$$D[h(A)](H) = f(A)D[g(A)](H) + D[f(A)](H)g(A).$$

Finally, we will frequently use that

$$D[A^{-1}](H) = -A^{-1}HA^{-1}. \quad (2)$$

D. Bochner Integrability

We need the concept of Bochner-integrability [85] in the proofs of our main results, which we briefly mention. Let $(\mathfrak{X}, \Sigma, \mu)$ be a measure space and \mathfrak{B} be a Banach space. A function $f : \mathfrak{X} \rightarrow \mathfrak{B}$ is said to be integrable (in the sense of Bochner) if there exists a sequence of simple functions g_n such that $g_n \rightarrow f$, μ -a.e., and

$$\lim_{n \rightarrow \infty} \int_{\mathfrak{X}} \|f - g_n\|_{\mathfrak{B}} d\mu = 0,$$

where $\|\cdot\|_{\mathfrak{B}}$ denotes the Banach space norm. A Bochner-measurable function f is integrable if and only if

$$\int_{\mathfrak{X}} \|f\|_{\mathfrak{B}} d\mu < \infty. \quad (3)$$

Moreover, if f is integrable, then

$$\left\| \int_{\mathfrak{X}} f d\mu \right\|_{\mathfrak{B}} \leq \int_{\mathfrak{X}} \|f\|_{\mathfrak{B}} d\mu. \quad (4)$$

E. Quantum Information Measures

The von Neumann entropy of a density operator $\rho \in \mathcal{S}_d$ is

$$H(\rho) := -\text{Tr} [\rho \log \rho],$$

For density operators $\rho, \sigma \in \mathcal{S}_d$, the quantum relative entropy [9] is

$$D(\rho \| \sigma) := \begin{cases} \text{Tr} [\rho (\log \rho - \log \sigma)], & \text{if } \rho \ll \sigma, \\ \infty, & \text{otherwise.} \end{cases}$$

From the above two definitions, it follows that

$$H(\rho) = \log d - D(\rho \| \pi_d), \quad (5)$$

where $\pi_d = I/d$ is the maximally mixed state. By some abuse of notation, the classical relative entropy or Kullback-Leibler (KL) divergence [86] between two distributions P, Q on a discrete alphabet \mathcal{X} is

$$D(P \| Q) := \sum_{x \in \mathcal{X}} P(x) \log \frac{P(x)}{Q(x)},$$

if $P \ll Q$, and ∞ otherwise.

For $\alpha \in (0, 1) \cup (1, \infty)$, the Petz-Rényi divergence [11] between $\rho, \sigma \in \mathcal{S}_d$ is

$$\bar{D}_\alpha(\rho\|\sigma) := \begin{cases} \frac{1}{\alpha-1} \log \text{Tr} [\rho^\alpha \sigma^{1-\alpha}], & \text{if } \rho \ll \sigma \text{ or } \rho \not\ll \sigma \text{ for } \alpha \in (0, 1), \\ \infty, & \text{otherwise.} \end{cases} \quad (6)$$

$\bar{D}_\alpha(\rho\|\sigma)$ satisfies the data-processing inequality for $\alpha \in (0, 2]$. For $\alpha \in (0, 1) \cup (1, \infty)$, the sandwiched Rényi divergence [13], [14] between $\rho, \sigma \in \mathcal{S}_d$ is

$$\tilde{D}_\alpha(\rho\|\sigma) := \begin{cases} \frac{\alpha}{\alpha-1} \log \left\| \rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}} \right\|_\alpha, & \text{if } \rho \ll \sigma \text{ or } \rho \not\ll \sigma \text{ for } \alpha \in (0, 1), \\ \infty, & \text{otherwise.} \end{cases} \quad (7)$$

$\tilde{D}_\alpha(\rho\|\sigma)$ satisfies data-processing inequality for $\alpha \geq 1/2$. Also, note that $\tilde{D}_{1/2}(\rho\|\sigma) = -\log F(\rho, \sigma)$, where $F(\rho, \sigma) := \|\sqrt{\rho}\sqrt{\sigma}\|_1^2 = (\text{Tr} [\sqrt{\rho}\sqrt{\sigma}])^2$ denotes the fidelity [87], [88] between ρ and σ . The max-divergence between states ρ and σ is

$$D_{\max}(\rho\|\sigma) := \lim_{\alpha \rightarrow \infty} \tilde{D}_\alpha(\rho\|\sigma) = \inf \{ \lambda : \rho \leq e^\lambda \sigma \}. \quad (8)$$

This divergence is the unique quantum generalization of the classical Rényi divergence of infinite order that satisfies the data-processing inequality. For further details about the aforementioned information measures, see the books [15], [16].

In the next section, we derive limit distribution for estimators of the aforementioned information measures.

III. MAIN RESULTS

Let ρ_n and σ_n be random density operators such that $\rho_n \xrightarrow{w} \rho$ and $\sigma_n \xrightarrow{w} \sigma$ in *trace norm* (see Section II-B for definitions). Since all norms are equivalent in finite dimensions, the choice of trace norm does not incur any loss of generality. Further, let $(r_n)_{n \in \mathbb{N}}$ denote a diverging positive sequence. In the following, *null* and *alternative* refers to the scenarios $\rho = \sigma$ and $\rho \neq \sigma$, respectively, while *two-sample* signifies that both ρ and σ are estimated.

A. Quantum Relative Entropy

Theorem 1 (Limit distribution for quantum relative entropy) *Let $\rho_n \ll \sigma_n \ll \sigma$ and $\rho_n \ll \rho \ll \sigma$. The following hold:*

(i) *(Two-sample alternative) If $(r_n(\rho_n - \rho), r_n(\sigma_n - \sigma)) \xrightarrow{w} (L_1, L_2)$, then*

$$r_n(D(\rho_n\|\sigma_n) - D(\rho\|\sigma)) \xrightarrow{w} \text{Tr} [L_1(\log \rho - \log \sigma) - \rho D[\log \sigma](L_2)]. \quad (9)$$

(ii) *(Two-sample null) If $\rho = \sigma$ and $(r_n(\rho_n - \rho), r_n(\sigma_n - \rho)) \xrightarrow{w} (L_1, L_2)$, then*

$$r_n^2 D(\rho_n\|\sigma_n) \xrightarrow{w} \text{Tr} [L_1 D[\log \rho](L_1 - L_2)] + \text{Tr} \left[\frac{\rho}{2} D^2[\log \rho](L_1 - L_2, L_1 - L_2) \right]. \quad (10)$$

The proof of Theorem 1 is presented in Section VI-A. The key idea relies on applying an operator version of Taylor's theorem to the function, $(x, y) \mapsto x(\log x - \log y)$, and showing that the remainder terms (e.g., second and higher order terms in the alternative case) vanish under the conditions stated in the theorem. At a technical level,

the arguments use uniform integrability (see Section VI) of the remainder terms (guaranteed under the assumptions) to justify interchange of limits, trace, and integrals. We note that the regularity conditions in Theorem 1 are same as that of [22, Theorem 1] specialized to the discrete setting. Also, observe that analogous to the classical case, the limits depend on whether $\rho = \sigma$ (null) or $\rho \neq \sigma$ (alternative), and that the convergence rate is faster in the former.

Remark 2 (One-sample null and alternative) *The one-sample case refers to the setting when $\sigma_n = \rho$ (null) or $\sigma_n = \sigma$ (alternative) for all $n \in \mathbb{N}$, i.e., when only ρ is approximated by ρ_n . In this case, the respective limits can be obtained by letting $L_2 = 0$ in (9) and (10).*

Simplified expressions for the limit variables in Theorem 1 exist when all relevant density operators commute, as stated in the following corollary.

Corollary 3 (Commutative case) *If all operators in Theorem 1 commute, then*

$$r_n(D(\rho_n \| \sigma_n) - D(\rho \| \sigma)) \xrightarrow{w} \text{Tr} [L_1(\log \rho - \log \sigma) - L_2 \rho \sigma^{-1}]. \quad (11)$$

Additionally, when $\rho = \sigma$, then

$$r_n^2 D(\rho_n \| \sigma_n) \xrightarrow{w} \frac{1}{2} \text{Tr} [(L_1 - L_2)^2 \rho^{-1}]. \quad (12)$$

Equations (11) and (12) recovers [22, Theorem 2] specialized to the discrete setting with finite support, which is the classical analogue of Theorem 1 pertaining to KL divergence. The RHS of (12) is reminiscent of the expression for χ^2 divergence and can be interpreted as a weighted L^2 norm between the limits L_1 and L_2 (see e.g., [89]).

A class of divergences intermediate between the classical and quantum relative entropy are the measured relative entropies [18], [90]–[92], which equals the largest KL divergence between the output probability distributions induced by a set of measurements (quantum to classical channel) on two quantum states. In Appendix B, we characterize the distributional limits for an estimator of this quantity under a uniqueness assumption on the optimal measurement.

Specializing Theorem 1 to von Neumann entropy leads to the following result.

Corollary 4 (Limit distribution for von Neumann entropy) *Let $\rho_n \ll \rho$. If $r_n(\rho_n - \rho) \xrightarrow{w} L$, then*

$$r_n(H(\rho_n) - H(\rho)) \xrightarrow{w} -\text{Tr} [L \log \rho]. \quad (13)$$

Proof. The claim follows from (5) and (9) with $L_1 = L$ and $L_2 = 0$ by noting that the regularity conditions in Part (ii) of Theorem 1 are satisfied with $\sigma_n = \sigma = \pi_d$ for all $n \in \mathbb{N}$. \square

It is well-known that $H(\rho) = H(\lambda)$, where $\lambda \in \mathcal{H}_d$ denotes the diagonal operator comprising of the eigenvalues of ρ arranged in non-increasing order. In other words, $H(\rho)$ equals the Shannon entropy of the probability distribution composed of the eigenvalues of ρ . An unbiased estimator of the spectrum of a quantum state is given by the EYD algorithm [79], [80] that outputs a Young's diagram as its estimate. In [82, Theorem 3.1], the limit distribution of this estimator with a scaling rate $n^{1/2}$ is characterized in terms of a d -dimensional Brownian functional $B = (B_1, \dots, B_d)$. From Corollary 4 and the discussion above, it then follows that the asymptotic distribution of the

EYD algorithm based estimator of $H(\rho)$ is governed by (13) with $r_n = n^{1/2}$, $L = \text{diag}(B)$ and $\rho = \lambda$, where $\text{diag}(\cdot)$ denotes the operation of representing a vector as the diagonal elements of a matrix.

B. Quantum Rényi Divergence

In contrast to the classical case, there is no single definition of quantum Rényi divergence known that satisfies all natural properties desired of a quantum information measure for all α (see [16]). Among the infinite possibilities, the most important ones with direct operational significance are the Petz-Rényi and sandwiched Rényi divergences, which we consider below.

Petz-Rényi divergence: We first derive distributional limits for Petz-Rényi divergence estimators.

Theorem 5 (Limit distribution for Petz-Rényi divergence) *Let $\alpha \in (0, 1) \cup (1, 2]$ and $\bar{\alpha} = 1 - \alpha$. Suppose $\rho_n \ll \sigma_n \ll \sigma$ and $\rho_n \ll \rho \ll \sigma$. Then, the following hold:*

(i) (Two-sample alternative) *If $(r_n(\rho_n - \rho), r_n(\sigma_n - \sigma)) \xrightarrow{w} (L_1, L_2)$, then*

$$r_n(\bar{D}_\alpha(\rho_n \| \sigma_n) - \bar{D}_\alpha(\rho \| \sigma)) \xrightarrow{w} \frac{\text{Tr}[\sigma^{\bar{\alpha}} D[\rho^\alpha](L_1)] + \text{Tr}[\rho^\alpha D[\sigma^{\bar{\alpha}}](L_2)]}{(\alpha - 1) \text{Tr}[\rho^\alpha \sigma^{\bar{\alpha}}]}. \quad (14)$$

(ii) (Two-sample null) *If $\rho = \sigma$ and $(r_n(\rho_n - \rho), r_n(\sigma_n - \rho)) \xrightarrow{w} (L_1, L_2)$, then*

$$r_n^2 \bar{D}_\alpha(\rho_n \| \sigma_n) \xrightarrow{w} \frac{\text{Tr}[\rho^{\bar{\alpha}} D^2[\rho^\alpha](L_1, L_1) + \rho^\alpha D^2[\rho^{\bar{\alpha}}](L_2, L_2) + 2D[\rho^\alpha](L_1)D[\rho^{\bar{\alpha}}](L_2)]}{2(\alpha - 1)}. \quad (15)$$

The proof of Theorem 5 is given in Section VI-B, and utilizes a similar approach as Theorem 1. As in the case of quantum relative entropy, the limits and the scaling rate differ in the null and alternative. Observe that we consider Petz-Rényi divergence of order less than two since it does not satisfy the data-processing inequality above this value. In the commutative case, the expressions in (15) and (14) simplify further, and in particular, we deduce the limit distributions for estimators of classical Rényi divergences as stated below (see [23] for a more general result when the dimension scales with n).

Corollary 6 (Commutative case) *If all operators in Theorem 5 commute, then*

$$r_n(\bar{D}_\alpha(\rho_n \| \sigma_n) - \bar{D}_\alpha(\rho \| \sigma)) \xrightarrow{w} \frac{\alpha \text{Tr}[L_1 \sigma^{\bar{\alpha}} \rho^{-\bar{\alpha}}] + \bar{\alpha} \text{Tr}[L_2 \rho^\alpha \sigma^{-\alpha}]}{(\alpha - 1) \text{Tr}[\rho^\alpha \sigma^{\bar{\alpha}}]}. \quad (16)$$

Moreover, if $\rho = \sigma$, then

$$r_n^2 \bar{D}_\alpha(\rho_n \| \sigma_n) \xrightarrow{w} \frac{\text{Tr}[(L_1 - L_2)^2 \rho^{-1}]}{2(\alpha - 1)}. \quad (17)$$

Sandwiched Rényi divergence: We next consider the minimal or sandwiched Rényi divergence of order α .

Theorem 7 (Limit distribution for sandwiched Rényi divergence) *Let $\alpha \in [0.5, 1) \cup (1, \infty)$ and $\bar{\alpha} = 1 - \alpha$. Suppose $\rho_n \ll \sigma_n \ll \sigma$ and $\rho_n \ll \rho \ll \sigma$. If $(r_n(\rho_n - \rho), r_n(\sigma_n - \sigma)) \xrightarrow{w} (L_1, L_2)$, then*

$$r_n(\tilde{D}_\alpha(\rho_n \| \sigma_n) - \tilde{D}_\alpha(\rho \| \sigma)) \xrightarrow{w} \frac{\alpha}{\alpha - 1} \frac{\text{Tr}\left[\left(D[\rho^{\frac{1}{2}}](L_1)\sigma^{\frac{\bar{\alpha}}{2}}\rho^{\frac{1}{2}} + \rho^{\frac{1}{2}}\sigma^{\frac{\bar{\alpha}}{2}}D[\rho^{\frac{1}{2}}](L_1) + \rho^{\frac{1}{2}}D[\sigma^{\frac{\bar{\alpha}}{2}}](L_2)\rho^{\frac{1}{2}}\right)(\rho^{\frac{1}{2}}\sigma^{\frac{\bar{\alpha}}{2}}\rho^{\frac{1}{2}})^{\alpha-1}\right]}{\|\rho^{\frac{1}{2}}\sigma^{\frac{\bar{\alpha}}{2}}\rho^{\frac{1}{2}}\|_\alpha^\alpha}. \quad (18)$$

If all operators above commute, then (18) simplifies to (16).

The proof of Theorem 7 is given in Section VI-C. Different from the approach used in the previous results, we compute this limit by recasting the term $\|\rho^{1/2}\sigma^{\frac{\alpha}{\alpha}}\rho^{1/2}\|_{\alpha}$ in (7) as a maximization using dual expressions for Schatten norms. However, establishing the desired limit with the new expression is more involved on account of the additional maximization involved. To this end, we consider upper and lower bounds (without the maximization) and show that they coincide with the expression in (18) asymptotically, thus establishing the claim. We mention here that the right-hand side (RHS) of (18) vanishes when $\rho = \sigma$, showing that correct scaling rate in the null setting for a non-degenerate limit should be r_n^2 . However, the above technique does not lead to a proof of this claim due to non-matching upper and lower limits.

As a corollary of Theorem 7, we characterize the limit distributions for fidelity and max-divergence.

Corollary 8 (Fidelity and max-divergence) *Let $\rho_n \ll \sigma_n \ll \sigma$ and $\rho_n \ll \rho \ll \sigma$. If $(r_n(\rho_n - \rho), r_n(\sigma_n - \sigma)) \xrightarrow{w} (L_1, L_2)$, then*

$$r_n(F(\rho_n, \sigma_n) - F(\rho, \sigma)) \xrightarrow{w} (F(\rho, \sigma))^{\frac{1}{2}} \text{Tr} \left[\left(D[\rho^{\frac{1}{2}}](L_1) \sigma \rho^{\frac{1}{2}} + \rho^{\frac{1}{2}} \sigma D[\rho^{\frac{1}{2}}](L_1) + \rho^{\frac{1}{2}} L_2 \rho^{\frac{1}{2}} \right) (\rho^{\frac{1}{2}} \sigma \rho^{\frac{1}{2}})^{-\frac{1}{2}} \right],$$

and

$$r_n(D_{\max}(\rho_n \| \sigma_n) - D_{\max}(\rho \| \sigma)) \xrightarrow{w} e^{-D_{\max}(\rho \| \sigma)} \text{Tr} \left[\left(D[\rho^{\frac{1}{2}}](L_1) \sigma^{-1} \rho^{\frac{1}{2}} + \rho^{\frac{1}{2}} \sigma^{-1} D[\rho^{\frac{1}{2}}](L_1) - \rho^{\frac{1}{2}} \sigma^{-1} L_2 \sigma^{-1} \rho^{\frac{1}{2}} \right) \Pi_{\max} \right],$$

where Π_{\max} denotes the eigenprojection corresponding to the maximal eigenvalue of $\rho^{\frac{1}{2}} \sigma^{-1} \rho^{\frac{1}{2}}$.

C. Generalization to Infinite-dimensional Quantum Systems

Here, we consider a generalization of Theorem 1 to infinite-dimensional quantum systems when the underlying Hilbert space is separable. The appropriate notion of Fréchet differentiability relevant for our purposes is that of an operator-valued function on the space of Hermitian operators with bounded trace-norm, i.e., A and H in Definition 1 are required to have finite trace-norm, and $o(\|H\|)$ is replaced by $o(\|H\|_1)$ in (1). Defining the Fréchet derivative in this manner, the following result (see Section VI-E for proof) provides sufficient conditions under which limit distribution for quantum relative entropy exists.

Theorem 9 (Quantum relative entropy: Infinite dimensional case) *Let $\rho_n \ll \sigma_n \ll \sigma$ and $\rho_n \ll \rho \ll \sigma$ be such that $D(\rho_n \| \sigma_n) < \infty$, $D(\rho \| \sigma) < \infty$, and there exists a constant c satisfying $\mathbb{P}(\|\rho_n \sigma_n^{-1}\|_{\infty} > c) \rightarrow 0$. Then, the following hold:*

- (i) (Two-sample alternative) *If $(r_n(\rho_n - \rho), r_n(\sigma_n - \sigma)) \xrightarrow{w} (L_1, L_2)$ in trace norm, then (9) holds.*
- (ii) (Two-sample null) *If $\rho = \sigma$ and $(r_n(\rho_n - \rho), r_n(\sigma_n - \rho)) \xrightarrow{w} (L_1, L_2)$ in trace norm, then (10) holds.*

We briefly discuss the regularity assumptions in the above theorem. In the infinite dimensional case, $D(\rho \| \sigma)$ can be unbounded even if the support conditions $\rho \ll \sigma$ are satisfied. This necessitates the finiteness assumption on

the quantum relative entropies above. The condition $\mathbb{P}(\|\rho_n \sigma_n^{-1}\|_\infty > c) \rightarrow 0$ imposes a stochastic boundedness assumption on the operator $\rho_n \sigma_n^{-1}$ and is a natural condition for the existence of distributional limits even in the classical case (see [22, Theorem 2 and Remark 1]). To see this, employing the bra-ket notation from quantum theory, take $\rho = \sigma = |0\rangle\langle 0|$, and

$$\begin{aligned}\rho_n &= (1 - n^{-1})|0\rangle\langle 0| + n^{-1}|n\rangle\langle n|, \\ \sigma_n &= (1 - e^{-n^2})|0\rangle\langle 0| + e^{-n^2}|n\rangle\langle n|,\end{aligned}$$

so that $\|\rho_n \sigma_n^{-1}\|_\infty$ diverges. Observe that $\sqrt{n}(\rho_n - \rho) \xrightarrow{w} 0$ and $\sqrt{n}(\sigma_n - \sigma) \xrightarrow{w} 0$, where 0 denotes the zero operator. However, it is easily seen by a straightforward computation that $D(\rho_n \| \sigma_n)$ diverges. Hence, the limit $\sqrt{n}D(\rho_n \| \sigma_n)$ does not exist and Theorem 9 does not hold.

IV. APPLICATION

Limit theorems for classical divergences have several applications in statistics, computational science and biology such as constructing confidence intervals for hypothesis testing [21], auditing of differential privacy [22], and biological data analysis [23]. Here, we consider an application of Theorem 1 in establishing performance guarantees for the problem of testing for the quantum relative entropy between unknown states². The relevant multi-hypothesis testing problem can be formulated as³

$$H_i : \epsilon_i < D(\rho_i \| \sigma_i) \leq \epsilon_{i+1}, \quad (19)$$

where $\epsilon_i \geq 0$ satisfy $\epsilon_{i+1} > \epsilon_i$ for $i \in \mathcal{I} = \{0, \dots, m-1\}$. We are interested in the setting where approximately nd^2 identical copies of the unknown states are available for the tester. The goal then is to design a test $\mathcal{T}_n = \{M_i^{(n)}, i \in \mathcal{I}\}$ with $M_i^{(n)} \geq 0$ for all i , and $\sum_{i \in \mathcal{I}} M_i^{(n)} = I$ that achieves a specified performance, i.e., an m -outcome positive operator-valued measure (POVM) with index set \mathcal{I} (see Appendix B for further details). Denoting the original hypothesis by H and the test outcome by \hat{H} , the performance of \mathcal{T}_n is quantified by the error probabilities

$$\alpha_{i,n}(\mathcal{T}_n, \rho_i^{\otimes n}, \sigma_i^{\otimes n}) := \mathbb{P}(\hat{H} \neq i | H = i) = \text{Tr} \left[(\rho_i^{\otimes n} \otimes \sigma_i^{\otimes n}) \sum_{j \neq i} M_j^{(n)} \right].$$

A test \mathcal{T}_n is said to achieve level τ if $\alpha_{i,n}(\mathcal{T}_n, \rho_i^{\otimes n}, \sigma_i^{\otimes n}) \leq \tau$ for every $i \in \mathcal{I}$. A sequence of tests $(\mathcal{T}_n)_{n \in \mathbb{N}}$ is asymptotically said to achieve level τ if $\limsup_{n \rightarrow \infty} \alpha_{i,n}(\mathcal{T}_n, \rho_i^{\otimes n}, \sigma_i^{\otimes n}) \leq \tau$ for every $i \in \mathcal{I}$.

A pertinent approach to realize a hypothesis test is to first perform tomography of the states to obtain estimates, $\hat{\rho}_n, \hat{\sigma}_n$, and then compute the relative entropy between them. A standard class of tests (motivated from the Neyman-Pearson theorem) then decides in favor of H_i if $t_{i,n} < D(\hat{\rho}_n \| \hat{\sigma}_n) \leq t_{i+1,n}$, where $t_{i,n}$ for $0 \leq i \leq m$ are critical values chosen according to the desired level $\tau_i \in (0, 1]$ for i^{th} error probability. Each such test (statistic) T_n induces a POVM indexed by \mathcal{I} , denoted by $\mathcal{T}_n^{\text{tom}}(\{t_i\}_{i \in \mathcal{I}})$, for which we will use the shorthand $\mathcal{T}_n^{\text{tom}}$. Let

²Since the states under the hypotheses are unknown, the problem is different from testing with known states and computing the quantum relative entropy to decide on the hypotheses.

³Note that here (ρ_i, σ_i) , $1 \leq i \leq m$, denote pairs of quantum states and not random density operators as was used until now.

$\alpha_{i,n}(\mathcal{T}_n^{\text{tom}}, \rho_i^{\otimes n}, \sigma_i^{\otimes n}) = \mathbb{P}(T_n \neq i | H = i)$ denote the error probability for the test statistic T_n given the i^{th} hypothesis is true.

To obtain concrete performance guarantees for the aforementioned hypothesis test, we consider a specific tomographic estimator for density operators based on Pauli measurements. This can be considered as a quantum analogue of the classical plug-in estimator based on empirical probability distributions. The choice of Pauli measurements is mainly due to simplicity of presentation, and our approach will extend to other tomographic schemes that rely on estimating the coefficients in an operator basis expansion using measurements on independent copies of quantum states. In the following, we first describe the estimator and characterize its limiting distribution, which will then be used to construct the test statistic for (19).

A. Tomographic Estimator of Quantum States

Let $d = 2^N$ for some integer N , and $\{\gamma_j\}_{j=0}^{d^2-1}$ denote the set of multi-qubit (N -qubit) Pauli operators constructed as the N -fold tensor product of standard Pauli operators acting on a qubit. Specifically, $\gamma_j = \bigotimes_{i=1}^N \gamma_{j,i}$ with $\gamma_{j,i} \in \{R_k\}_{k=0}^3$, where $\{R_k\}_{k=0}^3$ denotes the single-qubit Pauli basis with the following representations in the standard basis:

$$R_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad R_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad R_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad R_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

We may take $\gamma_0 = I$. The multi-qubit Pauli operators are Hermitian and form an orthogonal operator basis for the real vector space \mathcal{H}_d with respect to the Hilbert-Schmidt inner product. Consequently, any multi-qubit density operator ρ can be written as

$$\rho = \frac{1}{d} \left(I + \sum_{j=1}^{d^2-1} s_j(\rho) \gamma_j \right), \quad (20)$$

with $s_j(\rho) = \text{Tr}[\rho \gamma_j]$. Note that γ_j , for $1 \leq j \leq d^2 - 1$, are traceless and have eigenvalues ± 1 . Moreover, for any $\mathbf{s} = (s_1, \dots, s_{d^2-1}) \in \mathbb{R}^{d^2-1}$, the operator $\frac{1}{d} \left(I + \sum_{j=1}^{d^2-1} s_j \gamma_j \right)$ is Hermitian with unit trace; hence, is a valid density operator provided \mathbf{s} is such that positive semi-definiteness holds. Let P_j^+ and P_j^- denote the projections onto the eigenspace of γ_j corresponding to the eigenvalue $+1$ and -1 , respectively. Then

$$s_j(\rho) = s_j^+(\rho) - s_j^-(\rho),$$

where $s_j^+(\rho) := \text{Tr}[\rho P_j^+]$ and $s_j^-(\rho) := \text{Tr}[\rho P_j^-] = 1 - s_j^+(\rho)$.

Assume that identical copies of ρ and σ are available as desired, on which measurements using Pauli operators can be performed and the outcomes recorded. Let $O_k(j, \rho)$ denote the k^{th} measurement outcome using γ_j on ρ . Denoting by $\mathbb{1}_{\mathcal{A}}$ the indicator of the event \mathcal{A} and by $\Pi_{\mathcal{S}_d}$ the projection (in the sense of Hilbert projection theorem) onto the closed convex set \mathcal{S}_d , a tomographic estimator of ρ and σ is then given by

$$\hat{\rho}_n = \mathbb{1}_{\bar{\rho}_n \geq 0} \bar{\rho}_n + \mathbb{1}_{\bar{\rho}_n \not\geq 0} \Pi_{\mathcal{S}_d}(\bar{\rho}_n), \quad (21a)$$

and

$$\hat{\sigma}_n = \frac{I}{nd} + \left(1 - \frac{1}{n}\right) \left(\mathbb{1}_{\bar{\sigma}_n \geq 0} \bar{\sigma}_n + \mathbb{1}_{\bar{\sigma}_n < 0} \Pi_{S_d}(\bar{\sigma}_n)\right), \quad (21b)$$

respectively, where

$$\begin{aligned} \bar{\rho}_n &:= \frac{1}{d} \left(I + \sum_{j=1}^{d^2-1} \hat{s}_j^{(n)}(\rho) \gamma_j \right), \\ \hat{s}_j^{(n)}(\rho) &:= \frac{1}{n} \sum_{k=1}^n \mathbb{1}_{O_k(j,\rho)=+1} - \mathbb{1}_{O_k(j,\rho)=-1}, \quad j \neq 0, \\ \hat{\mathbf{s}}^{(n)}(\rho) &:= (\hat{s}_1^{(n)}(\rho), \dots, \hat{s}_{d^2-1}^{(n)}(\rho)), \end{aligned}$$

and $\bar{\sigma}_n$, $\hat{s}_j^{(n)}(\sigma)$, and $\hat{\mathbf{s}}^{(n)}(\sigma)$ are defined analogously with ρ replaced by σ in the above expressions. It follows from the above discussion that $\hat{\rho}_n, \hat{\sigma}_n \in \mathcal{S}_d$ for all $n \in \mathbb{N}$. Note that the extra term (negligible asymptotically) I/nd ensures that $\hat{\sigma}_n > 0$ so that $\hat{\rho}_n \ll \hat{\sigma}_n$ and $D(\hat{\rho}_n \| \hat{\sigma}_n)$ is finite. Also, observe that to construct $\hat{\rho}_n$ and $\hat{\sigma}_n$, we need $n(d^2 - 1)$ independent copies, each of ρ and σ , available for measurement.

Let $N(c, v^2)$ denote the one-dimensional normal distribution with mean c and variance v^2 . The following result shows that the limit distribution for estimators of quantum relative entropy based on Pauli tomography is Gaussian.

Proposition 10 (Limit distribution for tomographic estimator) *Let $\rho, \sigma > 0$. Then*

$$\sqrt{n}(D(\hat{\rho}_n \| \sigma) - D(\rho \| \sigma)) \xrightarrow{w} W_1 \sim N(0, v_1^2(\rho, \sigma)), \quad (22a)$$

$$\sqrt{n}(D(\hat{\rho}_n \| \hat{\sigma}_n) - D(\rho \| \sigma)) \xrightarrow{w} W_2 \sim N(0, v_2^2(\rho, \sigma)), \quad (22b)$$

where

$$\begin{aligned} v_1^2(\rho, \sigma) &:= \sum_{j=1}^{d^2-1} \frac{4s_j^+(\rho)s_j^-(\rho)}{d^2} \text{Tr}[\gamma_j(\log \rho - \log \sigma)]^2, \\ v_2^2(\rho, \sigma) &:= v_1^2(\rho, \sigma) + \sum_{j=1}^{d^2-1} \frac{4s_j^+(\sigma)s_j^-(\sigma)}{d^2} \text{Tr}[\rho D[\log \sigma](\gamma_j)]^2. \end{aligned}$$

The proof of Proposition 10 is given in Section VI-F and follows by an application of Theorem 1. The main ingredient of the proof is to show that $(\sqrt{n}(\hat{\rho}_n - \rho), \sqrt{n}(\hat{\sigma}_n - \sigma)) \xrightarrow{w} (L_\rho, L_\sigma)$, where $L_\rho := \sum_{j=1}^{d^2-1} \gamma_j Z_j(\rho)$ and $Z_j(\rho) \sim N(0, 4s_j^+(\rho)s_j^-(\rho)/d^2)$. The claim then follows from (9) by noting that all relevant regularity conditions are satisfied.

B. Performance Guarantees for Multi-hypothesis Testing

For simplicity of presentation, we will assume that $\sigma_i = \sigma$ for all $i \in \mathcal{I}$ with σ known for the test in (19). Such a scenario arises, for instance, when testing for the mixedness of an unknown state ρ with respect to the maximally mixed state, $\sigma = \pi_d$. Also, for $\tau \in [0, 1]$, let

$$Q^{-1}(\tau) = \inf \left\{ z \in \mathbb{R} : (2\pi)^{-1/2} \int_z^\infty e^{-u^2/2} du \leq \tau \right\},$$

be the inverse complimentary cumulative distribution function of the standard normal distribution $N(0, 1)$. The following proposition provides a test statistic for the multi-hypothesis testing problem in (19) by utilizing the limit distribution for quantum relative entropy and characterizes its error probabilities.

Proposition 11 (Performance of multi-hypothesis testing) *Let $\tau \in (0, 1]$, and $\rho_i, \sigma > 0$ for $i \in \mathcal{I}$ satisfy the hypotheses in (19) for $\sigma_i = \sigma$ therein. Let $\hat{D}_n = D(\hat{\rho}_n \| \sigma)$ with $\hat{\rho}_n$ given in (21a). Then, the test statistic*

$$T_n = \sum_{i \in \mathcal{I}} i \mathbb{1}_{\hat{D}_n \in \mathcal{L}_{i,n}(c)} \text{ with } \mathcal{L}_{i,n}(c) := (\epsilon_i + cn^{-1/2}, \epsilon_{i+1} + cn^{-1/2}),$$

asymptotically achieves a level τ provided

$$c \geq 2d Q^{-1}(\tau) |\log b|,$$

where b denotes the minimum of the eigenvalues of ρ_i and σ over all $i \in \mathcal{I}$.

The proof of Proposition 11 (see Section VI-G) follows by an application of Proposition 10 and Portmanteau theorem [93, Theorem 2.1]. The threshold c achieving a desired asymptotic level τ is determined by utilizing the knowledge that $\sqrt{n}(\hat{D}_n - D(\rho_i \| \sigma))$ converges in distribution to a centered normal under hypothesis i , whose variance $v_1^2(\rho_i, \sigma)$ can be uniformly bounded for ρ_i, σ with $i \in \mathcal{I}$.

Remark 12 (Growing number of hypotheses) *An inspection of the proof of Proposition 11 reveals that it continues to hold even when the number of hypotheses scales with n , given the new hypotheses boundaries are chosen consistent with the previous ones and are well-separated, i.e., $\min_{i \in \mathcal{I}_n} D(\rho_i \| \sigma) - \epsilon_i = \omega(n^{-1/2})$, where $\omega(\cdot)$ denotes the asymptotic little omega notation and \mathcal{I}_n is the index set of hypotheses that grows with n ($\mathcal{I}_n \subseteq \mathcal{I}_{n+1}$ for every $n \in \mathbb{N}$).*

V. CONCLUDING REMARKS

This paper studied limit distributions for a certain class of estimators of important quantum divergences such as quantum relative entropy, its Rényi generalizations, and measured relative entropy. Taking recourse to an operator version of Taylor's theorem, the limit distributions are characterized in terms of trace functionals of first or second-order Fréchet derivatives of elementary functions. These functions simplify in the commuting case and coincide with previously known expressions in the classical case. We employed the derived results to show that the asymptotic distribution of an estimator of quantum relative entropy based on Pauli tomography of states is normal. We then utilized this knowledge to propose a test statistic for a multi-hypothesis testing problem and characterized its asymptotic performance.

Looking forward, several open questions remain. One pertinent question concerns the rate of convergence of the empirical distribution of the divergence to its limit in the flavor of classical Berry-Esseen theorem. Any progress in this direction would be extremely useful to understand the non-asymptotic behavior of such estimators. Also, accounting for the case of infinite dimensional quantum systems would be a natural extension. In Section III-C, we treated the case of quantum relative entropy for density operators on a separable Hilbert space. We believe that our approach can be extended to more general scenarios with appropriate technical modifications to ensure uniform

integrability of terms that appear in a Taylor's expansion. However, this is beyond the scope of the current article. Of interest further is to understand the asymptotic and non-asymptotic behavior of other classes of estimators such as those based on variational methods, for which the techniques used here may not be directly applicable. Lastly, it would also be beneficial to study the statistical behaviour of estimators of other quantum divergences not considered here such as quantum χ^2 divergence [94] and geometric Rényi divergence [95], [96].

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VI. PROOFS

The following technical lemma will be handy for our purposes. Its proof is given in Appendix A.

Lemma 13 (Properties of trace-class operators) *Let \mathbb{H} be a separable Hilbert space. Then, the following hold:*

- (i) *Let $A, B \in \mathcal{L}(\mathbb{H})$ be such that AB is trace-class. Let P be an orthogonal projection (i.e., Hermitian operator P satisfying $0 \leq P = P^2$) such that $A \ll P$. Then, $\text{Tr}[AB] = \text{Tr}[PAPBP]$.*
- (ii) *Let A, B, C be trace-class Hermitian operators such that $B \leq A \leq C$. Then, $\|A\|_1 \leq \|B\|_1 + \|C\|_1$.*

We next proceed with the proofs of the main results.

A. Proof of Theorem 1

For $A_1, A_2 > 0$, let

$$f(A_1, A_2) = A_1(\log A_1 - \log A_2).$$

Consider the integral representation

$$\begin{aligned} \log A &= \int_0^\infty \left(\frac{1}{(\tau+1)I} - \frac{1}{\tau I + A} \right) d\tau \\ &= \int_0^1 \left(\frac{1}{(\tau+1)I} - \frac{1}{\tau I + A} \right) d\tau + \int_1^\infty \left(\frac{1}{(\tau+1)I} - \frac{1}{\tau I + A} \right) d\tau, \end{aligned} \quad (23)$$

for $A > 0$. We have $D[(\tau I + A)^{-1}](H) = -(\tau I + A)^{-1}H(\tau I + A)^{-1}$ by (2) and

$$D[\log A](H) = \int_0^\infty (\tau I + A)^{-1}H(\tau I + A)^{-1}d\tau.$$

Applying the above, we obtain via the chain rule and product rule for Fréchet derivatives that

$$\begin{aligned} D^{(1,0)}[f(A_1, A_2)](H) &= A_1 \int_0^\infty (\tau I + A_1)^{-1}H(\tau I + A_1)^{-1}d\tau + H(\log A_1 - \log A_2), \\ D^{(0,1)}[f(A_1, A_2)](H) &= -A_1 \int_0^\infty (\tau I + A_2)^{-1}H(\tau I + A_2)^{-1}d\tau, \\ D^{(2,0)}[f(A_1, A_2)](H_1, H_2) &= H_1 \int_0^\infty (\tau I + A_1)^{-1}H_2(\tau I + A_1)^{-1}d\tau \\ &\quad + H_2 \int_0^\infty (\tau I + A_1)^{-1}H_1(\tau I + A_1)^{-1}d\tau \end{aligned}$$

$$\begin{aligned}
& -A_1 \int_0^\infty (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} d\tau \\
& -A_1 \int_0^\infty (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} d\tau, \\
D^{(0,2)}[f(A_1, A_2)](H_1, H_2) &= A_1 \int_0^\infty (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} d\tau \\
& + A_1 \int_0^\infty (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} d\tau, \\
D^{(1,1+)}[f(A_1, A_2)](H_1, H_2) &= -H_1 \int_0^\infty (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} d\tau, \\
D^{(1+,1)}[f(A_1, A_2)](H_1, H_2) &= -H_2 \int_0^\infty (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} d\tau,
\end{aligned}$$

where the notation $D^{(1,1+)}$ means that the order of differentiation is with respect to first coordinate followed by the second, and vice versa for $D^{(1+,1)}$.

Note that $f(A_1, A_2)$ is continuously twice differentiable function from $\mathcal{P}_d^+ \times \mathcal{P}_d^+$ to $\mathcal{L}(\mathbb{H}_d)$. Hence, applying the operator version of multivariate Taylor's theorem (see e.g. [84]), we obtain for $A_1, A_2, B_1, B_2 > 0$ that

$$\begin{aligned}
f(B_1, B_2) &= f(A_1, A_2) + D^{(1,0)}[f(A_1, A_2)](B_1 - A_1) + D^{(0,1)}[f(A_1, A_2)](B_2 - A_2) \\
&+ \int_0^1 (1-t) D^{(2,0)}[f((1-t)A_1 + tB_1, (1-t)A_2 + tB_2)](B_1 - A_1, B_1 - A_1) dt \\
&+ \int_0^1 (1-t) D^{(0,2)}[f((1-t)A_1 + tB_1, (1-t)A_2 + tB_2)](B_2 - A_2, B_2 - A_2) dt \\
&+ \int_0^1 (1-t) D^{(1,1+)}[f((1-t)A_1 + tB_1, (1-t)A_2 + tB_2)](B_1 - A_1, B_2 - A_2) dt \\
&+ \int_0^1 (1-t) D^{(1+,1)}[f((1-t)A_1 + tB_1, (1-t)A_2 + tB_2)](B_2 - A_2, B_1 - A_1) dt. \quad (24)
\end{aligned}$$

Two-sample null: Assume first that $\rho_n, \sigma_n, \rho > 0$. Setting $B_1 = \rho_n$, $B_2 = \sigma_n$ and $A_1 = A_2 = \rho$ in (24), and defining

$$v(\rho_n, \rho, \tau, t) := (\tau I + (1-t)\rho + t\rho_n)^{-1},$$

we have

$$\begin{aligned}
& f(\rho_n, \sigma_n) \\
&= \rho \int_0^\infty (\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} d\tau - \rho \int_0^\infty (\tau I + \rho)^{-1} (\sigma_n - \rho) (\tau I + \rho)^{-1} d\tau \\
&+ 2 \int_0^1 (1-t)(\rho_n - \rho) \int_0^\infty v(\rho_n, \rho, \tau, t)(\rho_n - \rho)v(\rho_n, \rho, \tau, t)d\tau dt \\
&- 2 \int_0^1 (1-t)((1-t)\rho + t\rho_n) \int_0^\infty v(\rho_n, \rho, \tau, t)(\rho_n - \rho)v(\rho_n, \rho, \tau, t)(\rho_n - \rho)v(\rho_n, \rho, \tau, t)d\tau dt \\
&+ 2 \int_0^1 (1-t)((1-t)\rho + t\rho_n) \int_0^\infty v(\sigma_n, \rho, \tau, t)(\sigma_n - \rho)v(\sigma_n, \rho, \tau, t)(\sigma_n - \rho)v(\sigma_n, \rho, \tau, t)d\tau dt \\
&- 2 \int_0^1 (1-t)(\rho_n - \rho) \int_0^\infty v(\sigma_n, \rho, \tau, t)(\sigma_n - \rho)v(\sigma_n, \rho, \tau, t)d\tau dt. \quad (25)
\end{aligned}$$

To extend the validity of the above equation to $0 \leq \rho_n \ll \sigma_n \geq 0$, we consider $f(\tilde{\rho}_n(\epsilon), \tilde{\sigma}_n(\epsilon))$ with

$$\tilde{\rho}_n(\epsilon) := \rho_n + \epsilon \pi_d,$$

$$\tilde{\sigma}_n(\epsilon) := \sigma_n + \epsilon \pi_d,$$

for $\epsilon > 0$, and take limit $\epsilon \rightarrow 0$. Then, the desired expression follows since $f(\tilde{\rho}_n(\epsilon), \tilde{\sigma}_n(\epsilon))$ is continuous in ϵ for $\rho_n \ll \sigma_n$, and uniform integrability conditions which allows for interchange of limits and integral hold for $0 < \epsilon \leq 1$. We illustrate the latter condition for some of the terms above. By using Hölder's inequality for Schatten-norms and $\|A\|_p \geq \|A\|_q$ for a linear operator A and $1 \leq p \leq q \leq \infty$, we have

$$\begin{aligned} \left\| (\tau I + \rho)^{-1} (\tilde{\rho}_n(\epsilon) - \rho) (\tau I + \rho)^{-1} \right\|_1 &\leq \left\| (\tau I + \rho)^{-1} \right\|_\infty \left\| (\tilde{\rho}_n(\epsilon) - \rho) (\tau I + \rho)^{-1} \right\|_1 \\ &\leq \left\| (\tau I + \rho)^{-1} \right\|_\infty^2 \left\| \tilde{\rho}_n(\epsilon) - \rho \right\|_1. \end{aligned} \quad (26)$$

Hence, for all $0 < \epsilon \leq 1$,

$$\begin{aligned} \int_0^\infty \left\| (\tau I + \rho)^{-1} (\tilde{\rho}_n(\epsilon) - \rho) (\tau I + \rho)^{-1} \right\|_1 d\tau &\leq \left\| \tilde{\rho}_n(\epsilon) - \rho \right\|_1 \int_0^\infty \left\| (\tau I + \rho)^{-1} \right\|_\infty^2 d\tau \\ &\lesssim_\rho \left\| \rho_n - \rho \right\|_1 + 1, \end{aligned}$$

where the final inequality follows because of the finiteness of the integral on account of $\rho > 0$. Then, using (3) and (4), we obtain

$$\begin{aligned} \left\| \int_0^\infty (\tau I + \rho)^{-1} (\tilde{\rho}_n(\epsilon) - \rho) (\tau I + \rho)^{-1} d\tau \right\|_1 &\leq \left\| \tilde{\rho}_n(\epsilon) - \rho \right\|_1 \int_0^\infty \left\| (\tau I + \rho)^{-1} \right\|_\infty^2 d\tau \\ &\lesssim_\rho \left\| \rho_n - \rho \right\|_1 + 1. \end{aligned}$$

Thus, the LHS is uniformly integrable independent of ϵ .

Similarly,

$$\begin{aligned} &\left\| (1-t)(\tilde{\rho}_n(\epsilon) - \rho) \int_0^\infty v(\tilde{\rho}_n(\epsilon), \rho, \tau, t) (\tilde{\rho}_n(\epsilon) - \rho) v(\tilde{\rho}_n(\epsilon), \rho, \tau, t) d\tau \right\|_1 \\ &\leq (1-t) \left\| \tilde{\rho}_n(\epsilon) - \rho \right\|_1^2 \int_0^\infty \left\| (\tau I + (1-t)\rho)^{-1} \right\|_\infty^2 d\tau \end{aligned} \quad (27a)$$

$$\begin{aligned} &\lesssim_\rho (1-t) \left\| \tilde{\rho}_n(\epsilon) - \rho \right\|_1^2 (1-t)^{-1} \\ &\lesssim \left\| \rho_n - \rho \right\|_1^2 + 1, \end{aligned} \quad (27b)$$

$$\begin{aligned} &\left\| (1-t)((1-t)\rho + t\tilde{\rho}_n(\epsilon)) \int_0^\infty v(\tilde{\rho}_n(\epsilon), \rho, \tau, t) (\tilde{\rho}_n(\epsilon) - \rho) v(\tilde{\rho}_n(\epsilon), \rho, \tau, t) \right. \\ &\quad \left. (\tilde{\rho}_n(\epsilon) - \rho) v(\tilde{\rho}_n(\epsilon), \rho, \tau, t) d\tau \right\|_1 \\ &\leq (1-t) \left\| \tilde{\rho}_n(\epsilon) - \rho \right\|_1^2 \int_0^\infty \left\| (\tau I + (1-t)\rho)^{-1} \right\|_\infty^2 d\tau \\ &\lesssim_\rho \left\| \rho_n - \rho \right\|_1^2 + 1. \end{aligned} \quad (27c)$$

The uniform integrability for the remaining terms also follows via analogous steps.

Let $g_n := r_n^2 \mathbf{D}(\rho_n \| \sigma_n)$. Multiplying by r_n^2 and taking trace in (25), we obtain

$$g_n = 2 \int_0^1 (1-t) \text{Tr} \left[r_n(\rho_n - \rho) \int_0^\infty v(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] dt$$

$$\begin{aligned}
& -2 \int_0^1 (1-t) \operatorname{Tr} \left[((1-t)\rho + t\rho_n) \int_0^\infty v(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) \right. \\
& \quad \left. v(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] dt \\
& + 2 \int_0^1 (1-t) \operatorname{Tr} \left[((1-t)\rho + t\rho_n) \int_0^\infty v(\sigma_n, \rho, \tau, t) r_n(\sigma_n - \rho) \right. \\
& \quad \left. v(\sigma_n, \rho, \tau, t) r_n(\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) d\tau \right] dt \\
& - 2 \int_0^1 (1-t) \operatorname{Tr} \left[r_n(\rho_n - \rho) \int_0^\infty v(\sigma_n, \rho, \tau, t) r_n(\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) d\tau \right] dt,
\end{aligned} \tag{28}$$

where we used that the first two terms above vanish. To see this for the first term, note that

$$\begin{aligned}
& \int_0^\infty \left\| \rho(\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} \right\|_1 d\tau \\
& = \int_0^1 \left\| \rho(\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} \right\|_1 d\tau + \int_1^\infty \left\| \rho(\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} \right\|_1 d\tau \\
& \leq \|(\rho_n - \rho)\|_1 \|\rho^{-1}\|_1 + \|\rho(\rho_n - \rho)\|_1 \int_1^\infty \tau^{-2} d\tau \\
& \lesssim \|\rho^{-1}\|_\infty + \int_1^\infty \tau^{-2} d\tau \\
& < \infty.
\end{aligned} \tag{29}$$

Similarly,

$$\int_0^\infty \left\| \rho(\rho_n - \rho) (\tau I + \rho)^{-2} \right\|_1 d\tau < \infty. \tag{30}$$

Hence, $\rho(\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1}$ and $\rho(\rho_n - \rho) (\tau I + \rho)^{-2}$ are integrable functions (with respect to Lebesgue measure on $(0, \infty)$). Then, we have

$$\begin{aligned}
\operatorname{Tr} \left[\int_0^\infty \rho(\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} d\tau \right] & \stackrel{(a)}{=} \int_0^\infty \operatorname{Tr} \left[\rho(\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} \right] d\tau \\
& \stackrel{(b)}{=} \int_0^\infty \operatorname{Tr} \left[\rho(\rho_n - \rho) (\tau I + \rho)^{-2} \right] d\tau \\
& \stackrel{(c)}{=} \operatorname{Tr} \left[\rho(\rho_n - \rho) \int_0^\infty (\tau I + \rho)^{-2} d\tau \right] \\
& = \operatorname{Tr} [\rho(\rho_n - \rho)\rho^{-1}] \\
& = \operatorname{Tr} [\rho_n - \rho] \stackrel{(d)}{=} 0,
\end{aligned} \tag{31}$$

where

- (a) follows from (29) by the fact that $\operatorname{Tr}[\cdot]$ is continuous linear (hence bounded) functional on the normed space $\mathcal{L}(\mathbb{H}_d)$ (with $\|\cdot\|_1$ norm);
- (b) uses that $[\rho, (\tau I + \rho)^{-1}] = 0$ and the cyclic property of $\operatorname{Tr}[\cdot]$;
- (c) follows via the same argument as in (a) using (30);
- (d) is because $\operatorname{Tr}[\rho_n] = \operatorname{Tr}[\rho] = 1$ on account of ρ_n and ρ being density operators.

Likewise, it can be shown that

$$\text{Tr} \left[\int_0^\infty \rho (\tau I + \rho)^{-1} (\sigma_n - \rho) (\tau I + \rho)^{-1} d\tau \right] = 0. \quad (32)$$

We next analyze the limit of the expression in (28). To prove the weak convergence of g_n to its desired limit, it suffices to show that for every subsequence of $(g_n)_{n \in \mathbb{N}}$, there exists a further subsequence along which the sequence converges to a unique weak limit (see e.g., [93, Theorem 2.6]). We refer to this as the *subsequence argument*. Let

$$p_n(r_n, t) := (1-t)r_n(\rho_n - \rho) \int_0^\infty v(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau, \quad (33a)$$

$$q_n(r_n, t) := (1-t)((1-t)\rho + t\rho_n) \int_0^\infty v(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) v(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau, \quad (33b)$$

$$\tilde{p}_n(r_n, t) := (1-t)((1-t)\rho + t\rho_n) \int_0^\infty v(\sigma_n, \rho, \tau, t) r_n(\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) r_n(\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) d\tau, \quad (33c)$$

$$\tilde{q}_n(r_n, t) := (1-t)r_n(\rho_n - \rho) \int_0^\infty v(\sigma_n, \rho, \tau, t) r_n(\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) d\tau. \quad (33d)$$

Then, the following bounds hold by using Hölder's inequality for Schatten norms:

$$\|p_n(r_n, t)\|_1 \leq \|r_n(\rho_n - \rho)\|_1^2 \int_0^\infty \|v(\rho_n, \rho, \tau, t)\|_\infty^2 d\tau, \quad (34a)$$

$$\|q_n(r_n, t)\|_1 \leq \|r_n(\rho_n - \rho)\|_1^2 \int_0^\infty \|v(\rho_n, \rho, \tau, t)\|_\infty^3 d\tau, \quad (34b)$$

$$\|\tilde{p}_n(r_n, t)\|_1 \leq \|r_n(\sigma_n - \rho)\|_1^2 \int_0^\infty \|v(\sigma_n, \rho, \tau, t)\|_\infty^3 d\tau, \quad (34c)$$

$$\|\tilde{q}_n(r_n, t)\|_1 \leq \|r_n(\rho_n - \rho)\|_1 \|r_n(\sigma_n - \rho)\|_1 \int_0^\infty \|v(\sigma_n, \rho, \tau, t)\|_\infty^2 d\tau. \quad (34d)$$

To show the aforementioned claim of unique weak limit, consider any subsequence $(n_k)_{k \in \mathbb{N}}$. Then, $((r_{n_k}(\rho_{n_k} - \rho), r_{n_k}(\sigma_{n_k} - \rho))) \xrightarrow{w} (L_1, L_2)$ in $\|\cdot\|_1$ since every subsequence of weakly convergent sequence has the same weak limit. Hence, due to separability of $\mathcal{L}(\mathbb{H}_d)$ (for finite d), by Skorokhods representation theorem (see e.g. [83]), there exists a further subsequence $(n_{k_j})_{j \in \mathbb{N}}$ such that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \rho))) \rightarrow (L_1, L_2)$ in $\|\cdot\|_1$ almost surely (a.s.). Then, since $\sigma_{n_{k_j}} \rightarrow \rho$, we have that $(1-t)\rho + t\sigma_{n_{k_j}} \geq c\rho$ for a constant $0 < c < 1$ (which depends on the realization $\sigma_{n_{k_j}}$) and sufficiently large j . This implies that the integrals in (34) are finite. For instance, the integral in (34a) is $O(1)$ as τ approaches zero and $O(\tau^{-2})$ as τ tends to ∞ . Hence, we obtain

$$\|p_{n_{k_j}}(r_{n_{k_j}}, t)\|_1 \lesssim_\rho \|r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)\|_1^2, \quad (35a)$$

$$\|q_{n_{k_j}}(r_{n_{k_j}}, t)\|_1 \lesssim_\rho \|r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)\|_1^2, \quad (35b)$$

$$\|\tilde{p}_{n_{k_j}}(r_{n_{k_j}}, t)\|_1 \lesssim_\rho \|r_{n_{k_j}}(\sigma_{n_{k_j}} - \rho)\|_1^2, \quad (35c)$$

$$\|\tilde{q}_{n_{k_j}}(r_{n_{k_j}}, t)\|_1 \lesssim_\rho \|r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)\|_1 \|r_{n_{k_j}}(\sigma_{n_{k_j}} - \rho)\|_1. \quad (35d)$$

Next, recall that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \rho))) \rightarrow (L_1, L_2)$ (a.s.) in the space of linear operators with bounded trace norm implies that $(r_{n_{k_j}}(\rho_{n_{k_j}} - \rho))_{j \in \mathbb{N}}$ and $(r_{n_{k_j}}(\sigma_{n_{k_j}} - \rho))_{j \in \mathbb{N}}$ are uniformly integrable sequences (a.s.). This combined with (34) and (35) then shows that $(p_{n_{k_j}}(r_{n_{k_j}}, t))_{j \in \mathbb{N}}$, $(q_{n_{k_j}}(r_{n_{k_j}}, t))_{j \in \mathbb{N}}$, $(\tilde{p}_{n_{k_j}}(r_{n_{k_j}}, t))_{j \in \mathbb{N}}$ and

$(\tilde{q}_{n_{k_j}}(r_{n_{k_j}}, t))_{j \in \mathbb{N}}$ are uniformly integrable sequences. Taking limits $j \rightarrow \infty$, interchanging limits and integral in (28), and noting that $\rho_{n_{k_j}} \rightarrow \rho$, $\sigma_{n_{k_j}} \rightarrow \rho$ a.s. and $\|\cdot\|_1$, yields

$$\begin{aligned} g_{n_{k_j}} &\rightarrow \text{Tr} \left[L_1 \int_0^\infty (\tau I + \rho)^{-1} L_1 (\tau I + \rho)^{-1} d\tau - \rho \int_0^\infty (\tau I + \rho)^{-1} L_1 (\tau I + \rho)^{-1} L_1 (\tau I + \rho)^{-1} d\tau \right] \\ &\quad + \text{Tr} \left[\rho \int_0^\infty (\tau I + \rho)^{-1} L_2 (\tau I + \rho)^{-1} L_2 (\tau I + \rho)^{-1} d\tau - L_1 \int_0^\infty (\tau I + \rho)^{-1} L_2 (\tau I + \rho)^{-1} d\tau \right] \\ &= \text{Tr} [L_1 D[\log \rho](L_1 - L_2)] + \text{Tr} \left[\frac{\rho}{2} D^2[\log \rho](L_1 - L_2, L_1 - L_2) \right]. \end{aligned}$$

Hence, every subsequence $(g_{n_k})_{k \in \mathbb{N}}$ has a further subsequence $(g_{n_{k_j}})_{j \in \mathbb{N}}$ with the same unique limit which implies (10).

If $[\rho_n, \rho] = 0$, then $[r_n(\rho_n - \rho), \rho] = 0$. Consider a subsequence $r_{n_j}(\rho_{n_j} - \rho) \rightarrow L_1$ a.s. Since the commutator is a continuous linear functional of its individual arguments, we have

$$[L_1, \rho] = \lim_{j \rightarrow \infty} [r_{n_j}(\rho_{n_j} - \rho), \rho] = 0, \text{ a.s.} \quad (36)$$

Hence, L_1 and ρ commutes. The proof of $[L_1, L_2] = [L_2, \rho] = 0$ under the conditions $[\rho_n, \rho] = [\sigma_n, \rho] = [\sigma_n, \rho_n] = 0$ follow similarly. Under this scenario, the expression in the RHS of (10) simplifies to

$$\begin{aligned} &\text{Tr} \left[L_1^2 \int_0^\infty (\tau I + \rho)^{-2} d\tau \right] - \text{Tr} \left[L_1^2 \rho \int_0^\infty (\tau I + \rho)^{-3} d\tau \right] + \text{Tr} \left[L_2^2 \rho \int_0^\infty (\tau I + \rho)^{-3} d\tau \right] \\ &\quad - \text{Tr} \left[L_1 L_2 \int_0^\infty (\tau I + \rho)^{-2} d\tau \right] \\ &= \frac{1}{2} \text{Tr} [L_1^2 \rho^{-1}] + \frac{1}{2} \text{Tr} [L_2^2 \rho^{-1}] - \text{Tr} [L_1 L_2 \rho^{-1}] \\ &= \frac{1}{2} \text{Tr} [(L_1 - L_2)^2 \rho^{-1}]. \end{aligned}$$

Finally, consider the case $\rho \geq 0$. Note that the left-hand side (LHS) and RHS of (10) is invariant to restricting the space to the support of ρ . To see this, let $P_\rho = \sum_{i=1}^r |e_i\rangle\langle e_i|$ be the projector onto the eigenspace pertaining to the non-zero eigenvalues of ρ , where r is the rank of ρ and $(|e_i\rangle)_{i=1}^r$ are the corresponding orthonormal eigenvectors. Setting $\tilde{\rho} = P_\rho \rho P_\rho$, $\tilde{\rho}_n = P_\rho \rho_n P_\rho$, $\tilde{\sigma}_n = P_\rho \sigma_n P_\rho$, and noting that $\rho_n \ll \sigma_n \ll \rho \ll P_\rho$, it follows from Lemma 13(i) that

$$\begin{aligned} D(\rho_n || \sigma_n) &= \text{Tr} [\rho_n \log \rho_n] - \text{Tr} [\rho_n \log \sigma_n] \\ &= \text{Tr} [P_\rho \rho_n P_\rho \log \rho_n P_\rho] - \text{Tr} [P_\rho \rho_n P_\rho \log \sigma_n P_\rho] \\ &= \text{Tr} [\tilde{\rho}_n \log \tilde{\rho}_n] - \text{Tr} [\tilde{\rho}_n \log \tilde{\sigma}_n]. \end{aligned}$$

Note that $\tilde{\rho} > 0$ and $\tilde{\rho}_n, \tilde{\sigma}_n \geq 0$ are density operators.

Next, to see that the RHS of (10) is invariant to restricting to support of ρ , we first note that the support of L_1 and L_2 is contained in that of ρ . To show this, notice that for every $n \in \mathbb{N}$, $\rho_n - \rho \ll \rho$ and $\sigma_n - \rho \ll \rho$ because $\rho_n, \sigma_n \ll \rho$ by assumption. By Portmanteau's theorem [83, Theorem 1.3.4 (vii)], since $r_n(\rho_n - \rho) \xrightarrow{w} L_1$, we have

$$\liminf \mathbb{E}[f(r_n(\rho_n - \rho))] \geq f(L_1), \quad (37)$$

for every bounded Lipschitz continuous (w.r.t. to trace norm) non-negative f . Let P_ρ^\perp denote the projector onto the orthogonal complement of the support of ρ . Applying (37) to the bounded Lipschitz continuous function $f_M(L) = \|P_\rho^\perp L P_\rho^\perp\|_1 \wedge M$ on the space of trace-class operators, where $M > 0$, we obtain

$$0 = \liminf r_n \mathbb{E} \left[\|P_\rho^\perp (\rho_n - \rho) P_\rho^\perp\|_1 \right] \geq r_n \|P_\rho^\perp L_1 P_\rho^\perp\|_1 \wedge M \geq 0.$$

Since r_n is positive and the above equation has to hold for every M , taking limit $M \rightarrow \infty$ implies that $\|P_\rho^\perp L_1 P_\rho^\perp\|_1 = 0$. Hence, the support of L_1 is contained in that of ρ . Similar claim also holds for L_2 . Thus, the RHS is also invariant to replacing all operators by their sandwiched versions obtained by left and right multiplying with P_ρ . Finally, observe that $(r_n(\rho_n - \rho), r_n(\sigma_n - \rho)) \xrightarrow{w} (L_1, L_2)$ implies $(r_n(\tilde{\rho}_n - \tilde{\rho}), r_n(\tilde{\sigma}_n - \tilde{\rho})) \xrightarrow{w} (P_\rho L_1 P_\rho, P_\rho L_2 P_\rho)$ by an application of Slutsky's theorem [83]. Hence, the previous proof applies and the claim follows.

Two-sample alternative: Assume first that $\rho_n, \sigma_n, \rho, \sigma > 0$. Setting $B_1 = \rho_n$, $B_2 = \sigma_n$, $A_1 = \rho$ and $A_2 = \sigma \neq \rho$ in (24), we have

$$\begin{aligned} f(\rho_n, \sigma_n) &= f(\rho, \sigma) + \rho \int_0^\infty (\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} d\tau - \rho \int_0^\infty (\tau I + \sigma)^{-1} (\sigma_n - \sigma) (\tau I + \sigma)^{-1} d\tau \\ &\quad + (\rho_n - \rho) (\log \rho - \log \sigma) + 2 \int_0^1 (1-t)(\rho_n - \rho) \int_0^\infty v(\rho_n, \rho, \tau, t)(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau dt \\ &\quad - 2 \int_0^1 (1-t)((1-t)\rho + t\rho_n) \int_0^\infty v(\rho_n, \rho, \tau, t)(\rho_n - \rho) v(\rho_n, \rho, \tau, t)(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau dt \\ &\quad + 2 \int_0^1 (1-t)((1-t)\rho + t\rho_n) \int_0^\infty v(\sigma_n, \sigma, \tau, t)(\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t)(\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) d\tau dt \\ &\quad - 2 \int_0^1 (1-t)(\rho_n - \rho) \int_0^\infty v(\sigma_n, \sigma, \tau, t)(\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) d\tau dt. \end{aligned} \quad (38)$$

This equation extends to $0 \leq \rho_n \ll \sigma_n \geq 0$ via similar arguments in Part (i). Multiplying by r_n and taking trace, we obtain

$$\begin{aligned} g_n &:= r_n (\mathcal{D}(\rho_n \| \sigma_n) - \mathcal{D}(\rho \| \sigma)) \\ &= \text{Tr} \left[r_n (\rho_n - \rho) (\log \rho - \log \sigma) - \rho \int_0^\infty (\tau I + \sigma)^{-1} r_n (\sigma_n - \sigma) (\tau I + \sigma)^{-1} d\tau \right] \\ &\quad + \text{Tr} \left[2 \int_0^1 (1-t) r_n^{\frac{1}{2}} (\rho_n - \rho) \int_0^\infty v(\rho_n, \rho, \tau, t) r_n^{\frac{1}{2}} (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] dt \\ &\quad - 2 \int_0^1 (1-t) \text{Tr} \left[((1-t)\rho + t\rho_n) \int_0^\infty v(\rho_n, \rho, \tau, t) r_n^{\frac{1}{2}} (\rho_n - \rho) v(\rho_n, \rho, \tau, t) r_n^{\frac{1}{2}} (\rho_n - \rho) \right. \\ &\quad \left. v(\rho_n, \rho, \tau, t) d\tau \right] dt \\ &\quad + 2 \int_0^1 (1-t) \text{Tr} \left[((1-t)\rho + t\rho_n) \int_0^\infty v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}} (\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}} (\sigma_n - \sigma) \right. \\ &\quad \left. v(\sigma_n, \sigma, \tau, t) d\tau \right] dt \\ &\quad - 2 \int_0^1 (1-t) \text{Tr} \left[r_n^{\frac{1}{2}} (\rho_n - \rho) \int_0^\infty v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}} (\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) d\tau \right] dt, \end{aligned} \quad (39)$$

where we used (31).

Let

$$\bar{p}_n(r_n, t) := (1-t)((1-t)\rho + t\rho_n) \int_0^\infty v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}}(\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}}(\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) d\tau, \quad (40a)$$

$$\bar{q}_n(r_n, t) := (1-t)r_n^{\frac{1}{2}}(\rho_n - \rho) \int_0^\infty v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}}(\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) d\tau. \quad (40b)$$

Then, via steps akin to (34), we have

$$\begin{aligned} \|\bar{p}_n(r_n, t)\|_1 &\leq \left\| r_n^{\frac{1}{2}}(\sigma_n - \sigma) \right\|_1^2 \int_0^\infty \|v(\sigma_n, \sigma, \tau, t)\|_\infty^3 d\tau, \\ \|\bar{q}_n(r_n, t)\|_1 &\leq \left\| r_n^{\frac{1}{2}}(\rho_n - \rho) \right\|_1 \left\| r_n^{\frac{1}{2}}(\sigma_n - \sigma) \right\|_1 \int_0^\infty \|v(\sigma_n, \sigma, \tau, t)\|_\infty^2 d\tau. \end{aligned}$$

As in Part (i), for any subsequence $(n_k)_{k \in \mathbb{N}}$, consider a further subsequence $(n_{k_j})_{j \in \mathbb{N}}$ such that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)) \rightarrow (L_1, L_2)$ in $\|\cdot\|_1$ a.s. Noting that there exists a constant $0 < c < 1$ such that $(1-t)\sigma + t\sigma_{n_{k_j}} \geq c\sigma$ for sufficiently large j , we have

$$\left\| \bar{p}_{n_{k_j}}(r_{n_{k_j}}, t) \right\|_1 \lesssim_\sigma \left\| r_{n_{k_j}}^{\frac{1}{2}}(\sigma_{n_{k_j}} - \sigma) \right\|_1^2, \quad (41a)$$

$$\left\| \bar{q}_{n_{k_j}}(r_{n_{k_j}}, t) \right\|_1 \lesssim_\sigma \left\| r_{n_{k_j}}^{\frac{1}{2}}(\rho_{n_{k_j}} - \rho) \right\|_1 \left\| r_{n_{k_j}}^{\frac{1}{2}}(\sigma_{n_{k_j}} - \sigma) \right\|_1. \quad (41b)$$

The above equations and (35) subsequently implies that $(p_{n_{k_j}}(r_{n_{k_j}}, t))_{j \in \mathbb{N}}$, $(q_{n_{k_j}}(r_{n_{k_j}}, t))_{j \in \mathbb{N}}$, $(\bar{p}_{n_{k_j}}(r_{n_{k_j}}, t))_{j \in \mathbb{N}}$ and $(\bar{q}_{n_{k_j}}(r_{n_{k_j}}, t))_{j \in \mathbb{N}}$ are uniformly integrable. Moreover, $((r_{n_{k_j}}^{1/2}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}^{1/2}(\sigma_{n_{k_j}} - \sigma)) \rightarrow (0, 0)$. Taking limits $j \rightarrow \infty$ and interchanging limits and integral yields

$$\begin{aligned} g_{n_{k_j}} &\rightarrow \text{Tr} \left[L_1 (\log \rho - \log \sigma) - \rho \int_0^\infty (\tau I + \sigma)^{-1} L_2 (\tau I + \sigma)^{-1} d\tau \right] \\ &= \text{Tr} [L_1 (\log \rho - \log \sigma)] - \text{Tr} [\rho D[\log \sigma](L_2)]. \end{aligned}$$

This implies (11) via the subsequence argument mentioned in Part (i).

In the commutative case, we observe similar to (36) that $[L_1, L_2] = [L_1, \rho] = [L_1, \sigma] = [L_2, \rho] = [L_2, \sigma] = 0$ when $[\rho_n, \rho] = [\sigma_n, \sigma] = [\rho, \sigma] = [\sigma_n, \rho_n] = [\sigma_n, \rho] = [\sigma, \rho_n] = 0$. In this case, the above limit simplifies as

$$\text{Tr} \left[\rho \int_0^\infty (\tau I + \sigma)^{-1} L_2 (\tau I + \sigma)^{-1} d\tau \right] = \text{Tr} [L_2 \rho \sigma^{-1}].$$

Finally, consider the case $0 \leq \rho \ll \sigma \geq 0$ and P_ρ be the projector onto support of ρ as defined in Part (i). Since $\rho_n \ll \rho \ll P_\rho$, we have $P_\rho \rho_n = \rho_n P_\rho = \rho_n$ and by cyclicity of trace

$$\begin{aligned} D(\rho_n \| \sigma_n) - D(\rho \| \sigma) &= \text{Tr} [\rho_n (\log \rho_n - \log \sigma_n)] - \text{Tr} [\rho (\log \rho - \log \sigma)] \\ &= \text{Tr} [P_\rho \rho_n (\log \rho_n - \log \sigma_n) P_\rho] - \text{Tr} [P_\rho \rho (\log \rho - \log \sigma) P_\rho]. \end{aligned}$$

Since $\rho_n, \sigma_n, \rho \ll \sigma$, we may assume without loss of generality that $\sigma > 0$ by restricting the underlying Hilbert space to the support of σ . Note that $P_\rho L_1 = L_1$ and $P_\rho \rho = \rho$ due to $\rho_n, L_1 \ll \rho$. Consider the function $f(A_1, A_2) = P_\rho A_1 (\log A_1 - \log A_2) P_\rho$. Note that $f(A_1, A_2)$ is continuously twice differentiable at (A_1, A_2) such

that $0 \leq A_1 \ll \rho$ and $A_2 > 0$. Then, applying the operator version of Taylor's theorem at (ρ, σ) and following similar steps as above (for the case $\rho, \sigma > 0$) yields

$$\begin{aligned} r_n(D(\rho_n \|\sigma_n) - D(\rho \|\sigma)) &\xrightarrow{w} \text{Tr}[P_\rho L_1(\log \rho - \log \sigma) P_\rho] - \text{Tr}[P_\rho \rho D[\log \sigma](L_2) P_\rho] \\ &= \text{Tr}[L_1(\log \rho - \log \sigma)] - \text{Tr}[\rho D[\log \sigma](L_2)], \end{aligned}$$

provided $(P_\rho p_n(r_n, t) P_\rho)_{n \in \mathbb{N}}$, $(P_\rho q_n(r_n, t) P_\rho)_{n \in \mathbb{N}}$, $(P_\rho \bar{p}_n(r_n, t) P_\rho)_{n \in \mathbb{N}}$ and $(P_\rho \bar{q}_n(r_n, t) P_\rho)_{n \in \mathbb{N}}$ (see (35) and (40)) are uniformly integrable along the subsequence $(n_{k_j})_{j \in \mathbb{N}}$ such that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)) \rightarrow (L_1, L_2)$ in $\|\cdot\|_1$ a.s. The uniform integrability of the last two subsequences follow via analogous arguments leading to (41) since $\sigma > 0$. Moreover, we have

$$\begin{aligned} P_\rho p_n(r_n, t) P_\rho &:= P_\rho(1-t)r_n(\rho_n - \rho) \int_0^\infty v(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau P_\rho \\ &= (1-t)r_n(\rho_n - \rho) \int_0^\infty \bar{v}(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) \bar{v}(\rho_n, \rho, \tau, t) d\tau, \end{aligned}$$

where $\bar{v}(\rho_n, \rho, \tau, t) := P_\rho(\tau I + (1-t)\rho + t\rho_n)^{-1} P_\rho \ll \rho$. The last equality follows since the operators coincide on the support ρ and, otherwise act as zero operator on the kernel of ρ . Then, via similar arguments leading to (35a) and (35a), we have

$$\begin{aligned} \|P_\rho p_{n_{k_j}}(r_{n_{k_j}}, t) P_\rho\|_1 &\leq \|r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)\|_1^2 \int_0^\infty \|\bar{v}(\rho_{n_{k_j}}, \rho, \tau, t)\|_\infty^2 d\tau \lesssim_\rho \|r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)\|_1^2, \\ \|P_\rho q_{n_{k_j}}(r_{n_{k_j}}, t) P_\rho\|_1 &\leq \|r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)\|_1^2 \int_0^\infty \|\bar{v}(\rho_{n_{k_j}}, \rho, \tau, t)\|_\infty^3 d\tau \lesssim_\rho \|r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)\|_1^2, \end{aligned}$$

from which the uniform integrability of the first two sequences follow. This completes the proof.

B. Proof of Theorem 5

In the following, we will assume without loss of generality that $\rho, \sigma > 0$. The proofs for extending to the general case $\rho \ll \sigma$ follows via similar arguments as given in the proof of Theorem 1. We first prove Part (ii).

Two-sample alternative: Consider the case $\alpha \in (0, 1)$, $\bar{\alpha} := 1 - \alpha$, and $Q_\alpha(\rho, \sigma) := \text{Tr}[\rho^\alpha \sigma^{\bar{\alpha}}]$. We will initially show that

$$\begin{aligned} r_n(Q_\alpha(\rho_n, \sigma_n) - Q_\alpha(\rho, \sigma)) &\xrightarrow{w} \text{Tr}[\sigma^{\bar{\alpha}} D[\rho^\alpha](L_1)] + \text{Tr}[\rho^\alpha D[\sigma^{\bar{\alpha}}](L_2)] \\ &= c_\alpha \text{Tr} \left[\int_0^\infty \tau^\alpha (\tau I + \rho)^{-1} L_1 (\tau I + \rho)^{-1} d\tau \sigma^{\bar{\alpha}} \right] \\ &\quad + c_{\bar{\alpha}} \text{Tr} \left[\rho^\alpha \int_0^\infty \tau^{\bar{\alpha}} (\tau I + \sigma)^{-1} L_2 (\tau I + \sigma)^{-1} d\tau \right], \end{aligned}$$

where $c_\alpha = \pi / \sin(\pi\alpha)$. Then, applying the functional delta method [83, Theorem 3.9.4] with $\phi(x) = \log x / (\alpha - 1)$ at $x = Q_\alpha(\rho, \sigma)$ leads to

$$r_n(\bar{D}_\alpha(\rho_n \|\sigma_n) - \bar{D}_\alpha(\rho \|\sigma)) \xrightarrow{w} \frac{\text{Tr}[\sigma^{\bar{\alpha}} D[\rho^\alpha](L_1)] + \text{Tr}[\rho^\alpha D[\sigma^{1-\alpha}](L_2)]}{(\alpha - 1) \text{Tr}[\rho^\alpha \sigma^{\bar{\alpha}}]}, \quad (42)$$

as claimed in (14).

To show the above, we compute the Fréchet derivatives of the operator-valued function $f(A_1, A_2) = A_1^\alpha A_2^{1-\alpha}$. Using the integral representation [97, Lemma 2.8]

$$A^\alpha = c_\alpha \int_0^\infty \tau^\alpha \left(\frac{1}{\tau I} - \frac{1}{\tau I + A} \right), \quad \alpha \in (0, 1),$$

we have via chain and product rule for Fréchet derivatives that

$$\begin{aligned} D^{(1,0)}[f(A_1, A_2)](H) &= c_\alpha \int_0^\infty \tau^\alpha (\tau I + A_1)^{-1} H (\tau I + A_1)^{-1} d\tau A_2^{\bar{\alpha}}, \\ D^{(0,1)}[f(A_1, A_2)](H) &= c_{\bar{\alpha}} A_1^\alpha \int_0^\infty \tau^{\bar{\alpha}} (\tau I + A_2)^{-1} H (\tau I + A_2)^{-1} d\tau, \\ D^{(2,0)}[f(A_1, A_2)](H_1, H_2) &= -c_\alpha \int_0^\infty \tau^\alpha (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} d\tau A_2^{\bar{\alpha}} \\ &\quad - c_\alpha \int_0^\infty \tau^\alpha (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} d\tau A_2^{\bar{\alpha}}, \\ D^{(0,2)}[f(A_1, A_2)](H_1, H_2) &= -c_{\bar{\alpha}} A_1^\alpha \int_0^\infty \tau^{\bar{\alpha}} (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} d\tau \\ &\quad - c_{\bar{\alpha}} A_1^\alpha \int_0^\infty \tau^{\bar{\alpha}} (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} d\tau, \\ D^{(1,1+)}[f(A_1, A_2)](H_1, H_2) &= c_\alpha c_{\bar{\alpha}} \int_0^\infty \tau^\alpha (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} d\tau \\ &\quad \int_0^\infty \tau^{\bar{\alpha}} (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} d\tau, \\ D^{(1+,1)}[f(A_1, A_2)](H_1, H_2) &= c_\alpha c_{\bar{\alpha}} \int_0^\infty \tau^\alpha (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} d\tau \\ &\quad \int_0^\infty \tau^{\bar{\alpha}} (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} d\tau. \end{aligned}$$

Then, from (24) with $B_1 = \rho_n$, $B_2 = \sigma_n$, $A_1 = \rho$, and $A_2 = \sigma$ and $v(\rho_n, \rho, \tau, t) := (\tau I + (1-t)\rho + t\rho_n)^{-1}$, we obtain

$$\begin{aligned} \rho_n^\alpha \sigma_n^{\bar{\alpha}} &= \rho^\alpha \sigma^{\bar{\alpha}} + c_\alpha \int_0^\infty \tau^\alpha (\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} d\tau \sigma^{\bar{\alpha}} \\ &\quad + c_{\bar{\alpha}} \rho^\alpha \int_0^\infty \tau^{\bar{\alpha}} (\tau I + \sigma)^{-1} (\sigma_n - \sigma) (\tau I + \sigma)^{-1} d\tau \\ &\quad - 2c_\alpha \int_0^1 (1-t) \left[\int_0^\infty \tau^\alpha v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] \\ &\quad \quad \quad ((1-t)\sigma + t\sigma_n)^{\bar{\alpha}} dt \\ &\quad - 2c_{\bar{\alpha}} \int_0^1 (1-t) ((1-t)\rho + t\rho_n)^\alpha \left[\int_0^\infty \tau^{\bar{\alpha}} v(\sigma_n, \sigma, \tau, t) (\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) (\sigma_n - \sigma) \right. \\ &\quad \quad \quad \left. v(\sigma_n, \sigma, \tau, t) d\tau \right] dt \\ &\quad + 2c_\alpha c_{\bar{\alpha}} \int_0^1 (1-t) \left[\int_0^\infty \tau^\alpha v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] \\ &\quad \quad \quad \left[\int_0^\infty \tau^{\bar{\alpha}} v(\sigma_n, \sigma, \tau, t) (\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) d\tau \right] dt. \end{aligned}$$

Multiplying by r_n , taking trace, and subsequent limits leads to (42) using similar arguments as in Theorem 1, provided

$$\begin{aligned}\bar{p}_n(r_n, t) &:= (1-t) \left[\int_0^\infty \tau^\alpha v(\rho_n, \rho, \tau, t) r_n^{\frac{1}{2}}(\rho_n - \rho) v(\rho_n, \rho, \tau, t) r_n^{\frac{1}{2}}(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] \\ &\quad \left(((1-t)\sigma + t\sigma_n)^\alpha \right), \\ \bar{q}_n(r_n, t) &:= (1-t) \left((1-t)\rho + t\rho_n \right)^\alpha \left[\int_0^\infty \tau^{\bar{\alpha}} v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}}(\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}}(\sigma_n - \sigma) \right. \\ &\quad \left. v(\sigma_n, \sigma, \tau, t) d\tau \right], \\ \bar{s}_n(r_n, t) &:= (1-t) \left[\int_0^\infty \tau^\alpha v(\rho_n, \rho, \tau, t) r_n^{\frac{1}{2}}(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] \left[\int_0^\infty \tau^{\bar{\alpha}} v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}}(\sigma_n - \sigma) \right. \\ &\quad \left. v(\sigma_n, \sigma, \tau, t) d\tau \right],\end{aligned}$$

are uniformly integrable sequences along a subsequence $(n_{k_j})_{j \in \mathbb{N}}$ such that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)) \rightarrow (L_1, L_2)$ in $\|\cdot\|_1$ a.s. To see the required uniform integrability, observe that

$$\|\bar{p}_n(r_n, t)\|_1 \leq \left\| r_n^{\frac{1}{2}}(\rho_n - \rho) \right\|_1^2 \left[\int_0^\infty \tau^\alpha \|v(\rho_n, \rho, \tau, t)\|_\infty^3 d\tau \right] \left\| ((1-t)\sigma + t\sigma_n)^\alpha \right\|_1, \quad (43a)$$

$$\|\bar{q}_n(r_n, t)\|_1 \leq \left\| r_n^{\frac{1}{2}}(\sigma_n - \sigma) \right\|_1^2 \left[\int_0^\infty \tau^{\bar{\alpha}} \|v(\sigma_n, \sigma, \tau, t)\|_\infty^3 d\tau \right] \left\| ((1-t)\rho + t\rho_n)^\alpha \right\|_1, \quad (43b)$$

$$\|\bar{s}_n(r_n, t)\|_1 \leq \left\| r_n^{\frac{1}{2}}(\rho_n - \rho) \right\|_1 \left\| r_n^{\frac{1}{2}}(\sigma_n - \sigma) \right\|_1 \left[\int_0^\infty \tau^\alpha \|v(\rho_n, \rho, \tau, t)\|_\infty^2 d\tau \right] \left[\int_0^\infty \|v(\sigma_n, \sigma, \tau, t)\|_\infty^2 d\tau \right]. \quad (43c)$$

For $\alpha \in (0, 1)$, we have by concavity of the function $x \mapsto x^\alpha$ for $x \geq 0$ that

$$\left\| ((1-t)\sigma + t\sigma_n)^\alpha \right\|_1 = \sum_{i=1}^d \lambda_i^{\bar{\alpha}} \leq d \left(\frac{1}{d} \sum_{i=1}^d \lambda_i \right)^{\bar{\alpha}} = d^\alpha \left\| ((1-t)\sigma + t\sigma_n) \right\|_1^{\bar{\alpha}} \leq d^\alpha.$$

Here, $\{\lambda_i\}_{i=1}^d$ denotes the set of eigenvalues of $(1-t)\sigma + t\sigma_n$, and we used that for $A \geq 0$, the eigenvalues of A^α are equal to the eigenvalues of A raised to the power α . Similarly,

$$\left\| ((1-t)\rho + t\rho_n)^\alpha \right\|_1 \leq d^{\bar{\alpha}} \left\| (1-t)\rho + t\rho_n \right\|_1^\alpha \leq d^{\bar{\alpha}}. \quad (44)$$

Next, since $\rho_{n_{k_j}} \rightarrow \rho$ and $\sigma_{n_{k_j}} \rightarrow \sigma$ in $\|\cdot\|_1$ a.s., we have that $(1-t)\rho + t\rho_{n_{k_j}} \geq c\rho$ and $(1-t)\sigma + t\sigma_{n_{k_j}} \geq c\sigma$ a.s. for a constant $0 < c < 1$ and sufficiently large j . Consequently, we obtain that the integrals in (43) are finite for $\alpha \in (0, 1)$. For instance, the integrand in (43a) is $O(\tau^\alpha)$ for τ close to zero and $O(\tau^{\alpha-3})$ as $\tau \rightarrow \infty$ which implies its finiteness. Hence,

$$\left\| \bar{p}_{n_{k_j}}(r_{n_{k_j}}, t) \right\|_1 \lesssim_{d, \rho, \alpha} \left\| r_{n_{k_j}}^{\frac{1}{2}}(\rho_{n_{k_j}} - \rho) \right\|_1^2, \quad (45a)$$

$$\left\| \bar{q}_{n_{k_j}}(r_{n_{k_j}}, t) \right\|_1 \lesssim_{d, \sigma, \alpha} \left\| r_{n_{k_j}}^{\frac{1}{2}}(\sigma_{n_{k_j}} - \sigma) \right\|_1^2, \quad (45b)$$

$$\left\| \bar{s}_{n_{k_j}}(r_{n_{k_j}}, t) \right\|_1 \lesssim_{d, \rho, \sigma, \alpha} \left\| r_{n_{k_j}}^{\frac{1}{2}}(\rho_{n_{k_j}} - \rho) \right\|_1 \left\| r_{n_{k_j}}^{\frac{1}{2}}(\sigma_{n_{k_j}} - \sigma) \right\|_1. \quad (45c)$$

Then, the desired uniform integrability follows from those of the sequences $((r_{n_{k_j}}^{1/2}(\rho_{n_{k_j}} - \rho))_{j \in \mathbb{N}}$ and $(r_{n_{k_j}}^{1/2}(\sigma_{n_{k_j}} - \sigma))_{j \in \mathbb{N}}$. This completes the proof of the claim for $\alpha \in (0, 1)$.

Next, consider the case $\alpha \in (1, 2)$. Using the integral representation [97, Lemma 2.8]

$$A^\alpha = c_{\alpha-1} \int_0^\infty (\tau^{\alpha-2} A + \tau^\alpha (\tau I + A)^{-1} - \tau^{\alpha-1} I) d\tau, \quad (46a)$$

$$A^{\bar{\alpha}} = c_{\bar{\alpha}+1} \int_0^\infty \tau^{\bar{\alpha}} (\tau I + A)^{-1} d\tau, \quad (46b)$$

we have

$$\begin{aligned} D^{(1,0)}[f(A_1, A_2)](H) &= c_{\alpha-1} \int_0^\infty (\tau^{\alpha-2} H - \tau^\alpha (\tau I + A_1)^{-1} H (\tau I + A_1)^{-1}) d\tau A_2^{\bar{\alpha}}, \\ D^{(0,1)}[f(A_1, A_2)](H) &= -c_{\bar{\alpha}+1} A_1^\alpha \int_0^\infty \tau^{\bar{\alpha}} (\tau I + A_2)^{-1} H (\tau I + A_2)^{-1} d\tau, \\ D^{(2,0)}[f(A_1, A_2)](H_1, H_2) &= c_{\alpha-1} \int_0^\infty \tau^\alpha (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} d\tau A_2^{\bar{\alpha}} \\ &\quad + c_{\alpha-1} \int_0^\infty \tau^\alpha (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} d\tau A_2^{\bar{\alpha}}, \\ D^{(0,2)}[f(A_1, A_2)](H_1, H_2) &= c_{\bar{\alpha}+1} A_1^\alpha \int_0^\infty \tau^{\bar{\alpha}} (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} d\tau \\ &\quad + c_{\bar{\alpha}+1} A_1^\alpha \int_0^\infty \tau^{\bar{\alpha}} (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} d\tau, \\ D^{(1,1+)}[f(A_1, A_2)](H_1, H_2) &= -c_{\alpha-1} c_{\bar{\alpha}+1} \left[\int_0^\infty (\tau^{\alpha-2} H_1 - \tau^\alpha (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1}) d\tau \right] \\ &\quad \left[\int_0^\infty \tau^{\bar{\alpha}} (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} d\tau \right], \\ D^{(1+,1)}[f(A_1, A_2)](H_1, H_2) &= -c_{\bar{\alpha}+1} c_{\alpha-1} \left[\int_0^\infty (\tau^{\alpha-2} H_2 - \tau^\alpha (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1}) d\tau \right] \\ &\quad \left[\int_0^\infty \tau^{\bar{\alpha}} (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} d\tau \right]. \end{aligned}$$

Substituting $B_1 = \rho_n$, $B_2 = \sigma_n$, $A_1 = \rho$, and $A_2 = \sigma$, multiplying by r_n , taking trace and following similar arguments as above leads to the claim provided

$$\begin{aligned} \tilde{p}_n(r_n, t) &:= (1-t) \left[\int_0^\infty \tau^\alpha v(\rho_n, \rho, \tau, t) r_n^{\frac{1}{2}} (\rho_n - \rho) v(\rho_n, \rho, \tau, t) r_n^{\frac{1}{2}} (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] \\ &\quad ((1-t)\sigma + t\sigma_n)^{\bar{\alpha}}, \\ \tilde{q}_n(r_n, t) &:= (1-t)((1-t)\rho + t\rho_n)^\alpha \left[\int_0^\infty \tau^{\bar{\alpha}} v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}} (\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}} (\sigma_n - \sigma) \right. \\ &\quad \left. v(\sigma_n, \sigma, \tau, t) d\tau \right], \\ \tilde{s}_n(r_n, t) &:= (1-t) \left[\int_0^\infty \left(\tau^{\alpha-2} r_n^{\frac{1}{2}} (\rho_n - \rho) - \tau^\alpha v(\rho_n, \rho, \tau, t) r_n^{\frac{1}{2}} (\rho_n - \rho) v(\rho_n, \rho, \tau, t) \right) d\tau \right] \\ &\quad \left[\int_0^\infty \tau^{\bar{\alpha}} v(\sigma_n, \sigma, \tau, t) r_n^{\frac{1}{2}} (\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) d\tau \right], \end{aligned}$$

are uniformly integrable along a subsequence $(n_{k_j})_{j \in \mathbb{N}}$ satisfying $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)) \rightarrow (L_1, L_2)$ in $\|\cdot\|_1$ a.s. Observe that

$$\|\tilde{p}_n(r_n, t)\|_1 \lesssim_{d,\alpha} \left\| r_n^{\frac{1}{2}} (\rho_n - \rho) \right\|_1^2 \left[\int_0^\infty \tau^\alpha \|v(\rho_n, \rho, \tau, t)\|_\infty^3 d\tau \right], \quad (47a)$$

$$\|\tilde{q}_n(r_n, t)\|_1 \lesssim_{d, \alpha} \left\| r_n^{\frac{1}{2}}(\sigma_n - \sigma) \right\|_1^2 \left[\int_0^\infty \tau^{\bar{\alpha}} \|v(\sigma_n, \sigma, \tau, t)\|_\infty^3 d\tau \right], \quad (47b)$$

$$\|\tilde{s}_n(r_n, t)\|_1 \lesssim_{d, \alpha} \left\| r_n^{\frac{1}{2}}(\sigma_n - \sigma) \right\|_1 \int_0^\infty \tau^{\bar{\alpha}} \|v(\sigma_n, \sigma, \tau, t)\|_\infty^2 d\tau \left[\int_0^\infty \left\| \tau^{\alpha-2} r_n^{\frac{1}{2}}(\rho_n - \rho) - \tau^\alpha v(\rho_n, \rho, \tau, t) r_n^{\frac{1}{2}}(\rho_n - \rho) v(\rho_n, \rho, \tau, t) \right\|_1 d\tau \right]. \quad (47c)$$

It is straightforward to see the finiteness of the integrals in (47), except perhaps the last integral in (47c). For the latter, observe that along a subsequence $(n_{k_j})_{j \in \mathbb{N}}$ such that $\rho_{n_{k_j}} \rightarrow \rho$, $\sigma_{n_{k_j}} \rightarrow \rho$ in $\|\cdot\|_1$ (a.s.), there exists constants $c, c' > 0$ (depending on ρ and the realizations $\rho_{n_{k_j}}, \sigma_{n_{k_j}}$) such that

$$cI \leq (1-t)\rho + t\rho_{n_{k_j}}, (1-t)\rho + t\sigma_{n_{k_j}} \leq c'I.$$

Then, we have

$$\begin{aligned} (\tau^{\alpha-2} - \tau^\alpha(\tau + c')^{-2}) (\rho_{n_{k_j}} - \rho) &\geq \tau^{\alpha-2}(\rho_{n_{k_j}} - \rho) - \tau^\alpha v(\rho_{n_{k_j}}, \rho, \tau, t) (\rho_{n_{k_j}} - \rho) v(\rho_{n_{k_j}}, \rho, \tau, t) \\ &\geq (\tau^{\alpha-2} - \tau^\alpha(\tau + c)^{-2}) (\rho_{n_{k_j}} - \rho). \end{aligned}$$

From Lemma 13(ii), it then follows that

$$\begin{aligned} &\int_0^\infty \left\| \tau^{\alpha-2} r_{n_{k_j}}^{\frac{1}{2}} (\rho_{n_{k_j}} - \rho) - \tau^\alpha v(\rho_{n_{k_j}}, \rho, \tau, t) r_{n_{k_j}}^{\frac{1}{2}} (\rho_{n_{k_j}} - \rho) v(\rho_{n_{k_j}}, \rho, \tau, t) \right\|_1 d\tau \\ &\leq \left\| r_{n_{k_j}}^{\frac{1}{2}} (\rho_{n_{k_j}} - \rho) \right\|_1 \left(\int_0^\infty (\tau^{\alpha-2} - \tau^\alpha(\tau + c)^{-2}) d\tau + \int_0^\infty (\tau^{\alpha-2} - \tau^\alpha(\tau + c')^{-2}) d\tau \right). \end{aligned}$$

The last two integrals are finite for $\alpha \in (1, 2)$. Thus, the RHS of the equations in (47) are bounded similar to the RHS of (45), and the desired integrability follows. This completes the proof of (14) for $\alpha \in (0, 2)$. The case $\alpha = 2$ is simpler as $f(A_1, A_2) = A_1^2 A_2^{-1}$ and the relevant derivatives can be computed using the rules $D[A^2](H) = AH + HA$ and (2). Since rest of the proof is similar to above, we omit the details.

Two-sample null: Consider $\alpha \in (0, 1)$. We will show that

$$\begin{aligned} r_n^2(Q_\alpha(\rho_n, \sigma_n) - Q_\alpha(\rho, \rho)) &= r_n^2(Q_\alpha(\rho_n, \sigma_n) - 1) \xrightarrow{w} \frac{1}{2} \text{Tr} [\rho^{\bar{\alpha}} D^2[\rho^\alpha](L_1, L_1) + \rho^\alpha D^2[\rho^{\bar{\alpha}}](L_2, L_2) \\ &\quad + 2D[\rho^\alpha](L_1)D[\rho^{\bar{\alpha}}](L_2)]. \end{aligned} \quad (48)$$

Then, an application of the functional delta method yields the claim in (15) by noting that $\log 1 = 0$. From (24)

with $B_1 = \rho_n$, $B_2 = \sigma_n$, $A_1 = A_2 = \rho$, and $v(\rho_n, \rho, \tau, t) := (\tau I + (1-t)\rho + t\rho_n)^{-1}$, we obtain

$$\begin{aligned} &\rho_n^\alpha \sigma_n^{\bar{\alpha}} \\ &= \rho + c_\alpha \int_0^\infty \tau^\alpha (\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} d\tau \rho^{\bar{\alpha}} + c_{\bar{\alpha}} \rho^\alpha \int_0^\infty \tau^{\bar{\alpha}} (\tau I + \rho)^{-1} (\sigma_n - \rho) (\tau I + \rho)^{-1} d\tau \\ &\quad - 2c_\alpha \int_0^1 (1-t) \left[\int_0^\infty \tau^\alpha v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] \\ &\quad \quad \quad ((1-t)\rho + t\sigma_n)^{\bar{\alpha}} dt \\ &\quad - 2c_{\bar{\alpha}} \int_0^1 (1-t) ((1-t)\rho + t\rho_n)^\alpha \left[\int_0^\infty \tau^{\bar{\alpha}} v(\sigma_n, \rho, \tau, t) (\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) (\sigma_n - \rho) \right. \\ &\quad \quad \quad \left. v(\sigma_n, \rho, \tau, t) d\tau \right] dt \end{aligned}$$

$$+ 2c_\alpha c_{\bar{\alpha}} \int_0^1 (1-t) \left[\int_0^\infty \tau^\alpha v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] \\ \left[\int_0^\infty \tau^{\bar{\alpha}} v(\sigma_n, \rho, \tau, t) (\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) d\tau \right] dt.$$

Multiplying by r_n^2 , taking trace and following similar arguments as above leads to (48), provided

$$\text{Tr} \left[\int_0^\infty \tau^\alpha (\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} d\tau \rho^{\bar{\alpha}} \right] = 0, \quad (49a)$$

$$\text{Tr} \left[\rho^\alpha \int_0^\infty \tau^{\bar{\alpha}} (\tau I + \rho)^{-1} (\sigma_n - \rho) (\tau I + \rho)^{-1} d\tau \right] = 0, \quad (49b)$$

and the sequences

$$\begin{aligned} \bar{p}_n(r_n, t) &:= (1-t) \left[\int_0^\infty \tau^\alpha v(\rho_n, \rho, \tau, t) r_n (\rho_n - \rho) v(\rho_n, \rho, \tau, t) r_n (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] ((1-t)\rho + t\sigma_n)^{\bar{\alpha}}, \\ \tilde{q}_n(r_n, t) &:= (1-t) ((1-t)\rho + t\rho_n)^\alpha \left[\int_0^\infty \tau^{\bar{\alpha}} v(\sigma_n, \rho, \tau, t) r_n (\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) r_n (\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) d\tau \right], \\ \tilde{s}_n(r_n, t) &:= (1-t) \left[\int_0^\infty (\tau^{\alpha-2} r_n (\rho_n - \rho) - \tau^\alpha v(\rho_n, \rho, \tau, t) r_n (\rho_n - \rho) v(\rho_n, \rho, \tau, t)) d\tau \right] \\ &\quad \left[\int_0^\infty \tau^{\bar{\alpha}} v(\sigma_n, \rho, \tau, t) r_n (\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) d\tau \right], \end{aligned}$$

are uniformly integrable along a subsequence $(n_{k_j})_{j \in \mathbb{N}}$ satisfying $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \rho)) \rightarrow (L_1, L_2)$ in $\|\cdot\|_1$ a.s. To show (49a), note that we have

$$\begin{aligned} \text{Tr} \left[\int_0^\infty \tau^\alpha (\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} d\tau \rho^{\bar{\alpha}} \right] &\stackrel{(a)}{=} \text{Tr} \left[(\rho_n - \rho) \rho^{\bar{\alpha}} \int_0^\infty \tau^\alpha (\tau I + \rho)^{-2} d\tau \right] \\ &\stackrel{(b)}{=} c_\alpha^{-1} \text{Tr} [\rho_n - \rho] = 0, \end{aligned}$$

where (a) follows by similar arguments leading to (31) and (b) is due to

$$\int_0^\infty \tau^\alpha (\tau I + \rho)^{-2} d\tau = -\tau^\alpha (\tau I + \rho)^{-1} \Big|_0^\infty - \alpha \int_0^\infty \tau^{\alpha-1} (\tau I + \rho)^{-1} d\tau = c_\alpha^{-1} \rho^{-\bar{\alpha}}.$$

In the above, the first equality uses integration by parts and the second equality uses (46b). Similarly, (49b) also holds. The desired integrability can be shown similar to (45). This completes the proof of (15) for the case $\alpha \in (0, 1)$.

The proof when $\alpha \in (1, 2]$ is similar and hence omitted.

If $[\rho_n, \rho] = [\sigma_n, \rho] = [\sigma_n, \rho_n] = 0$ for all n sufficiently large, then $[L_1, L_2] = [L_1, \rho] = [L_2, \rho] = 0$. Hence,

$$\rho^{\bar{\alpha}} D^2[\rho^\alpha](L_1, L_1) = -2\rho^{\bar{\alpha}} L_1^2 c_\alpha \int_0^\infty \tau^\alpha (\tau I + \rho)^{-3} d\tau = \rho^{\bar{\alpha}} L_1^2 \rho^{\alpha-2} = L_1^2 \rho^{-1}.$$

Similarly,

$$\begin{aligned} \rho^\alpha D^2[\rho^{\bar{\alpha}}](L_2, L_2) &= L_2^2 \rho^{-1}, \\ 2D[\rho^\alpha](L_1) D[\rho^{\bar{\alpha}}](L_2) &= 2L_1 L_2 \rho^{-1}. \end{aligned}$$

Substituting this in (15) leads to (17).

C. Proof of Theorem 7

We will prove the claim for $\rho, \sigma > 0$. The general case $\rho \ll \sigma$ can be handled via similar arguments as in the proof of Theorem 1. We begin by noting that the following variational form holds for the sandwiched Rényi divergence as given in [13] (see [98] for a further application of this form in generalizing sandwiched Rényi divergence to infinite dimensional quantum settings):

$$\tilde{D}_\alpha(\rho\|\sigma) := \frac{\alpha}{\alpha-1} \log \left\| \rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}} \right\|_\alpha = \max_{\substack{\eta \geq 0, \\ \|\eta\|_{\frac{\alpha}{\alpha-1}} \leq 1}} \tilde{D}_\alpha(\rho\|\sigma; \eta), \quad (50)$$

where

$$\tilde{D}_\alpha(\rho\|\sigma; \eta) := (\alpha/(\alpha-1)) \log \text{Tr} \left[\rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}} \eta \right].$$

The maximum above is achieved by

$$\eta = \eta^*(\rho, \sigma, \alpha) := (\rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}})^{\alpha-1} / \left\| \rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}} \right\|_\alpha^{\alpha-1}. \quad (51)$$

Defining $\eta_n^* := \eta^*(\rho_n, \sigma_n, \alpha)$, we have

$$r_n(\tilde{D}_\alpha(\rho_n\|\sigma_n) - \tilde{D}_\alpha(\rho\|\sigma)) \leq r_n(\tilde{D}_\alpha(\rho_n\|\sigma_n; \eta_n^*) - \tilde{D}_\alpha(\rho\|\sigma; \eta_n^*)), \quad (52a)$$

$$r_n(\tilde{D}_\alpha(\rho_n\|\sigma_n) - \tilde{D}_\alpha(\rho\|\sigma)) \geq r_n(\tilde{D}_\alpha(\rho_n\|\sigma_n; \eta^*) - \tilde{D}_\alpha(\rho\|\sigma; \eta^*)). \quad (52b)$$

We will show that the limit on the RHS of (52a) and (52b) coincides with the RHS of (18), thus proving the desired claim.

To establish that the former limit equals the RHS of (18), it is sufficient to show that

$$\begin{aligned} & r_n \left(\text{Tr} \left[\rho_n^{\frac{1}{2}} \sigma_n^{\frac{\alpha}{\alpha-1}} \rho_n^{\frac{1}{2}} \eta_n^* \right] - \text{Tr} \left[\rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}} \eta_n^* \right] \right) \\ & \xrightarrow{w} \frac{\text{Tr} \left[\left(D[\rho^{\frac{1}{2}}](L_1) \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}} + \rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} D[\rho^{\frac{1}{2}}](L_1) + \rho^{\frac{1}{2}} D[\sigma^{\frac{\alpha}{\alpha-1}}](L_2) \rho^{\frac{1}{2}} \right) (\rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}})^{\alpha-1} \right]}{\left\| \rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}} \right\|_\alpha^{\alpha-1}}. \end{aligned} \quad (53)$$

Then, the functional delta-method (specifically [83, Theorem 3.9.5 and Lemma 3.9.7]) applied to the continuously differentiable function $x \mapsto \alpha \log x / (\alpha - 1)$ at $x = \left\| \rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}} \right\|_\alpha > 0$ yields

$$\begin{aligned} & r_n(\tilde{D}_\alpha(\rho_n\|\sigma_n; \eta_n^*) - \tilde{D}_\alpha(\rho\|\sigma; \eta_n^*)) \\ & \xrightarrow{w} \frac{\alpha}{\alpha-1} \frac{\text{Tr} \left[\left(D[\rho^{\frac{1}{2}}](L_1) \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}} + \rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} D[\rho^{\frac{1}{2}}](L_1) + \rho^{\frac{1}{2}} D[\sigma^{\frac{\alpha}{\alpha-1}}](L_2) \rho^{\frac{1}{2}} \right) (\rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}})^{\alpha-1} \right]}{\left\| \rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{\alpha-1}} \rho^{\frac{1}{2}} \right\|_\alpha^\alpha}, \end{aligned}$$

as desired. Further, invoking the subsequence argument, it suffices to prove (53) along a subsequence $(n_{k_j})_{j \in \mathbb{N}}$ such that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)) \rightarrow (L_1, L_2)$ in trace-norm a.s.

To show (53), we compute the Fréchet derivatives of

$$f(A_1, A_2) = A_1^{\frac{1}{2}} A_2^{\frac{\alpha}{\alpha-1}} A_1^{\frac{1}{2}}.$$

Consider $\alpha \in (0.5, 1) \cup (1, \infty)$. Since $\bar{\alpha}/\alpha \in (0, 1) \cup (-1, 0)$, the following integral representations given in [97, Lemma 2.8] are relevant for our purpose:

$$A^\alpha = c_\alpha \int_0^\infty \tau^\alpha \left(\frac{1}{\tau I} - \frac{1}{\tau I + A} \right) d\tau, \quad \alpha \in (0, 1),$$

$$A^\alpha = c_{\alpha+1} \int_0^\infty \frac{\tau^\alpha}{\tau I + A} d\tau, \quad \alpha \in (-1, 0).$$

We have via the chain and product rule for Fréchet derivatives that

$$\begin{aligned} D^{(1,0)}[f(A_1, A_2)](H) &= c_{\frac{1}{2}} \int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H (\tau I + A_1)^{-1} d\tau A_2^{\frac{\alpha}{2}} A_1^{\frac{1}{2}} \\ &\quad + c_{\frac{1}{2}} A_1^{\frac{1}{2}} A_2^{\frac{\alpha}{2}} \int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H (\tau I + A_1)^{-1} d\tau, \\ D^{(0,1)}[f(A_1, A_2)](H) &= -c_{\frac{\alpha}{\alpha}+1} A_1^{\frac{1}{2}} \left[\int_0^\infty \tau^{\frac{\alpha}{2}} (\tau I + A_2)^{-1} H (\tau I + A_2)^{-1} d\tau \right] A_1^{\frac{1}{2}}, \\ D^{(2,0)}[f(A_1, A_2)](H_1, H_2) &= -c_{\frac{1}{2}} \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} d\tau \right. \\ &\quad + \int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} d\tau \left. \right] A_2^{\frac{\alpha}{2}} A_1^{\frac{1}{2}} \\ &\quad - c_{\frac{1}{2}} A_1^{\frac{1}{2}} A_2^{\frac{\alpha}{2}} \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} d\tau \right. \\ &\quad + \int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} d\tau \left. \right] \\ &\quad + c_{\frac{1}{2}}^2 \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} d\tau \right] A_2^{\frac{\alpha}{2}} \\ &\quad \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} d\tau \right] \\ &\quad + c_{\frac{1}{2}}^2 \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} d\tau \right] A_2^{\frac{\alpha}{2}} \\ &\quad \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} d\tau \right], \\ D^{(0,2)}[f(A_1, A_2)](H_1, H_2) &= c_{\frac{\alpha}{\alpha}+1} A_1^{\frac{1}{2}} \left[\int_0^\infty \tau^{\frac{\alpha}{2}} (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} d\tau \right. \\ &\quad + \int_0^\infty \tau^{\frac{\alpha}{2}} (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} d\tau \left. \right] A_1^{\frac{1}{2}}, \\ D^{(1,1+)}[f(A_1, A_2)](H_1, H_2) &= -c_{\frac{1}{2}} c_{\frac{\alpha}{\alpha}+1} \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} d\tau \right] \\ &\quad \left[\int_0^\infty \tau^{\frac{\alpha}{2}} (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} d\tau \right] A_1^{\frac{1}{2}} \\ &\quad - c_{\frac{1}{2}} c_{\frac{\alpha}{\alpha}+1} A_1^{\frac{1}{2}} \left[\int_0^\infty \tau^{\frac{\alpha}{2}} (\tau I + A_2)^{-1} H_2 (\tau I + A_2)^{-1} d\tau \right] \\ &\quad \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_1 (\tau I + A_1)^{-1} d\tau \right], \\ D^{(1+,1)}[f(A_1, A_2)](H_1, H_2) &= -c_{\frac{1}{2}} c_{\frac{\alpha}{\alpha}+1} \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} d\tau \right] \\ &\quad \left[\int_0^\infty \tau^{\frac{\alpha}{2}} (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} d\tau \right] A_1^{\frac{1}{2}} \\ &\quad - c_{\frac{1}{2}} c_{\frac{\alpha}{\alpha}+1} A_1^{\frac{1}{2}} \left[\int_0^\infty \tau^{\frac{\alpha}{2}} (\tau I + A_2)^{-1} H_1 (\tau I + A_2)^{-1} d\tau \right] \\ &\quad \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + A_1)^{-1} H_2 (\tau I + A_1)^{-1} d\tau \right]. \end{aligned}$$

Then, substituting the expressions for Fréchet derivatives derived above in (24) with $B_1 = \rho_n$, $B_2 = \sigma_n$, $A_1 = \rho$, and $A_2 = \sigma$ leads to

$$\begin{aligned} \rho_n^{\frac{1}{2}} \sigma_n^{\frac{\bar{\alpha}}{\alpha}} \rho_n^{\frac{1}{2}} \eta_n^* &= \rho^{\frac{1}{2}} \sigma^{\frac{\bar{\alpha}}{\alpha}} \rho^{\frac{1}{2}} \eta_n^* + c_{\frac{1}{2}} \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} d\tau \right] \sigma^{\frac{\bar{\alpha}}{\alpha}} \rho^{\frac{1}{2}} \eta_n^* \\ &\quad + c_{\frac{1}{2}} \rho^{\frac{1}{2}} \sigma^{\frac{\bar{\alpha}}{\alpha}} \left[\int_0^\infty \tau^{\frac{1}{2}} (\tau I + \rho)^{-1} (\rho_n - \rho) (\tau I + \rho)^{-1} d\tau \right] \eta_n^* \\ &\quad - c_{\frac{1}{\alpha}} \rho^{\frac{1}{2}} \left[\int_0^\infty \tau^{\frac{\bar{\alpha}}{\alpha}} (\tau I + \sigma)^{-1} (\sigma_n - \sigma) (\tau I + \sigma)^{-1} d\tau \right] \rho^{\frac{1}{2}} \eta_n^* + R_n \eta_n^*, \end{aligned} \quad (54)$$

where $R_n := R_{1,n} + R_{2,n} + R_{3,n}$, and with $v(\rho_n, \rho, \tau, t) := (\tau I + (1-t)\rho + t\rho_n)^{-1}$,

$$\begin{aligned} R_{1,n} &:= -2c_{\frac{1}{2}} \int_0^1 (1-t) \int_0^\infty \tau^{\frac{1}{2}} v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \\ &\quad \left((1-t)\sigma + t\sigma_n \right)^{\frac{\bar{\alpha}}{\alpha}} \left((1-t)\rho + t\rho_n \right)^{\frac{1}{2}} dt \\ &\quad - 2c_{\frac{1}{2}} \int_0^1 (1-t) \left((1-t)\rho + t\rho_n \right)^{\frac{1}{2}} \left((1-t)\sigma + t\sigma_n \right)^{\frac{\bar{\alpha}}{\alpha}} \\ &\quad \int_0^\infty \tau^{\frac{1}{2}} v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau dt \\ &\quad + 4c_{\frac{1}{2}}^2 \int_0^1 (1-t) \left[\int_0^\infty \tau^{\frac{1}{2}} v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] \left((1-t)\sigma + t\sigma_n \right)^{\frac{\bar{\alpha}}{\alpha}} \\ &\quad \left[\int_0^\infty \tau^{\frac{1}{2}} v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] dt, \\ R_{2,n} &:= 2c_{\frac{1}{\alpha}} \int_0^1 (1-t) \left((1-t)\rho + t\rho_n \right)^{\frac{1}{2}} \left[\int_0^\infty \tau^{\frac{\bar{\alpha}}{\alpha}} v(\sigma_n, \sigma, \tau, t) (\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) (\sigma_n - \sigma) \right. \\ &\quad \left. v(\sigma_n, \sigma, \tau, t) d\tau \right] \left((1-t)\rho + t\rho_n \right)^{\frac{1}{2}} dt, \\ R_{3,n} &:= -2c_{\frac{1}{\alpha}} c_{\frac{1}{2}} \int_0^1 (1-t) \left[\int_0^\infty \tau^{\frac{1}{2}} v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] \\ &\quad \left[\int_0^\infty \tau^{\frac{\bar{\alpha}}{\alpha}} v(\sigma_n, \sigma, \tau, t) (\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) d\tau \right] \left((1-t)\rho + t\rho_n \right)^{\frac{1}{2}} dt \\ &\quad - 2c_{\frac{1}{\alpha}} c_{\frac{1}{2}} \int_0^1 (1-t) \left((1-t)\rho + t\rho_n \right)^{\frac{1}{2}} \left[\int_0^\infty \tau^{\frac{1}{2}} v(\rho_n, \rho, \tau, t) (\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau \right] \\ &\quad \left[\int_0^\infty \tau^{\frac{\bar{\alpha}}{\alpha}} v(\sigma_n, \sigma, \tau, t) (\sigma_n - \sigma) v(\sigma_n, \sigma, \tau, t) d\tau \right] dt. \end{aligned}$$

Multiplying by r_n and taking limits, the desired claim will follow provided $\text{Tr}[r_n R_n \eta_n^*] \rightarrow 0$ along the subsequence $(n_{k_j})_{j \in \mathbb{N}}$ mentioned above. To show this, we require an interchange of limits and integral which can be justified via the uniform integrability conditions stated below:

$$\begin{aligned} &\|r_n R_{1,n} \eta_n^*\|_1 \\ &\lesssim_{d,\alpha} \left\| r_n^{\frac{1}{2}} (\rho_n - \rho) \right\|_1^2 \left[\int_0^\infty \tau^{\frac{1}{2}} \|v(\rho_n, \rho, \tau, t)\|_\infty^3 d\tau \right] \|(1-t)\sigma + t\sigma_n\|_1^{\frac{\bar{\alpha}}{\alpha}} \|(1-t)\rho + t\rho_n\|_1^{\frac{1}{2}} \|\eta_n^*\|_1 \\ &\quad + \left\| r_n^{\frac{1}{2}} (\rho_n - \rho) \right\|_1^2 \|(1-t)\sigma + t\sigma_n\|_1^{\frac{\bar{\alpha}}{\alpha}} \left[\int_0^\infty \tau^{\frac{1}{2}} \|v(\rho_n, \rho, \tau, t)\|_\infty^2 d\tau \right]^2 \|\eta_n^*\|_1, \\ &\|r_n R_{2,n} \eta_n^*\|_1 \lesssim_{d,\alpha} \|(1-t)\rho + t\rho_n\|_1 \left\| r_n^{\frac{1}{2}} (\sigma_n - \sigma) \right\|_1^2 \left[\int_0^\infty \tau^{\frac{\bar{\alpha}}{\alpha}} \|v(\sigma_n, \sigma, \tau, t)\|_\infty^3 d\tau \right] \|\eta_n^*\|_1, \end{aligned}$$

$$\|r_n R_{3,n} \eta_n^*\|_1 \lesssim_{d,\alpha} \left\| r_n^{\frac{1}{2}} (\rho_n - \rho) \right\|_1 \left\| r_n^{\frac{1}{2}} (\sigma_n - \sigma) \right\|_1 \left\| (1-t)\rho + t\rho_n \right\|_1^{\frac{1}{2}} \left[\int_0^\infty \tau^{\frac{1}{2}} \|v(\rho_n, \rho, \tau, t)\|_\infty^2 d\tau \right] \\ \left[\int_0^\infty \tau^{\frac{\alpha}{2}} \|v(\sigma_n, \sigma, \tau, t)\|_\infty^2 d\tau \right] \|\eta_n^*\|_1.$$

To obtain these bounds, we used Hölders inequality similar to (26) along with (44), which applies due to concavity of the map $x \mapsto x^{\bar{\alpha}/\alpha}$ for $\bar{\alpha}/\alpha \in (-1, 0) \cup (0, 1)$. Hence, analogous to (45), the integrals above are finite, and

$$\left\| r_{n_{k_j}} R_{1,n_{k_j}} \eta_{n_{k_j}}^* \right\|_1 \lesssim_{d,\rho,\sigma,\alpha} \left\| r_{n_{k_j}}^{\frac{1}{2}} (\rho_{n_{k_j}} - \rho) \right\|_1^2, \\ \left\| r_{n_{k_j}} R_{2,n_{k_j}} \eta_{n_{k_j}}^* \right\|_1 \lesssim_{d,\rho,\sigma,\alpha} \left\| r_{n_{k_j}}^{\frac{1}{2}} (\rho_{n_{k_j}} - \rho) \right\|_1^2, \\ \left\| r_{n_{k_j}} R_{3,n_{k_j}} \eta_{n_{k_j}}^* \right\|_1 \lesssim_{d,\rho,\sigma,\alpha} \left\| r_{n_{k_j}}^{\frac{1}{2}} (\rho_{n_{k_j}} - \rho) \right\|_1 \left\| r_{n_{k_j}}^{\frac{1}{2}} (\sigma_{n_{k_j}} - \sigma) \right\|_1,$$

holds a.s. along the subsequence $(n_{k_j})_{j \in \mathbb{N}}$. From this, the desired integrability follows from those of the terms in the RHS of the equations above, and moreover, $\text{Tr}[r_{n_{k_j}} R_{n_{k_j}} \eta_{n_{k_j}}^*] \rightarrow 0$. Also, note that since $\rho_{n_{k_j}} \rightarrow \rho$ and $\sigma_{n_{k_j}} \rightarrow \sigma$ a.s. in trace norm, $\eta_{n_{k_j}}^*$ converges a.s. in trace norm to η^* due to $\rho, \sigma > 0$. This is because for all sufficiently large j (depending on the realizations), the eigenvalues (and eigenvectors) of both $\rho_{n_{k_j}}$ and $\sigma_{n_{k_j}}$ are arbitrarily close to that of ρ and σ , respectively, which are all bounded away from zero. Consequently, $r_n(\text{Tr}[\rho_n^{\frac{1}{2}} \sigma_n^{\frac{\alpha}{2}} \rho_n^{\frac{1}{2}} \eta_n^*] - \text{Tr}[\rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{2}} \rho^{\frac{1}{2}} \eta^*])$ converges to the RHS of (53) along $(n_{k_j})_{j \in \mathbb{N}}$. In a similar vein, $r_n(\text{Tr}[\rho_n^{\frac{1}{2}} \sigma_n^{\frac{\alpha}{2}} \rho_n^{\frac{1}{2}} \eta_n^*] - \text{Tr}[\rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{2}} \rho^{\frac{1}{2}} \eta^*])$ converges a.s. to RHS of (53) along the same subsequence, thus proving (53) and completing the proof of (18) when $\alpha \in (0.5, 1) \cup (1, \infty)$. The proof for $\alpha = 0.5$ can be shown similar to above by applying Taylor's theorem to $f(A_1, A_2) = A_1^{\frac{1}{2}} A_2 A_1^{\frac{1}{2}}$, for which the Fréchet derivatives are relatively easier to compute.

To see that (18) simplifies to (16) when all relevant operators commute, observe that $D[\rho^{\frac{1}{2}}](L_1) = L_1 \rho^{\frac{1}{2}}/2$ and $D[\sigma^{\frac{\alpha}{2}}](L_2) = (\bar{\alpha}/\alpha) L_2 \sigma^{\frac{\alpha}{2}-1}$, and hence

$$\left(D[\rho^{\frac{1}{2}}](L_1) \sigma^{\frac{\alpha}{2}} \rho^{\frac{1}{2}} + \rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{2}} D[\rho^{\frac{1}{2}}](L_1) + \rho^{\frac{1}{2}} D[\sigma^{\frac{\alpha}{2}}](L_2) \rho^{\frac{1}{2}} \right) (\rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{2}} \rho^{\frac{1}{2}})^{\alpha-1} = L_1 \sigma^{\bar{\alpha}} \rho^{-\bar{\alpha}} + L_2 \frac{\bar{\alpha}}{\alpha} \sigma^{-\alpha} \rho^{\alpha}.$$

Substituting this in (18) and noting that $\|\rho^{\frac{1}{2}} \sigma^{\frac{\alpha}{2}} \rho^{\frac{1}{2}}\|_\alpha^\alpha = \text{Tr}[\rho^\alpha \sigma^{\bar{\alpha}}]$ proves the claim.

D. Proof of Corollary 8

By setting $\alpha = 0.5$ in (18), we obtain

$$r_n \left(\tilde{D}_{\frac{1}{2}}(\rho_n \| \sigma_n) - \tilde{D}_{\frac{1}{2}}(\rho \| \sigma) \right) \xrightarrow{w} \frac{-\text{Tr} \left[\left(D[\rho^{\frac{1}{2}}](L_1) \sigma \rho^{\frac{1}{2}} + \rho^{\frac{1}{2}} \sigma D[\rho^{\frac{1}{2}}](L_1) + \rho^{\frac{1}{2}} L_2 \rho^{\frac{1}{2}} \right) (\rho^{\frac{1}{2}} \sigma \rho^{\frac{1}{2}})^{-\frac{1}{2}} \right]}{\sqrt{F(\rho, \sigma)}}.$$

The claim for fidelity then follows by noting that $F(\rho, \sigma) = e^{-\tilde{D}_{1/2}(\rho \| \sigma)}$, and applying the functional delta method to the above equation for the map $x \mapsto e^{-x}$ at $x = \tilde{D}_{1/2}(\rho \| \sigma)$.

Next, consider max-divergence given in (8) which corresponds to infinite-order sandwiched Rényi divergence. The variational form in (50) with $\alpha = \infty$ becomes

$$D_{\max}(\rho \| \sigma) = \max_{\eta \geq 0: \|\eta\|_1 \leq 1} D_{\max}(\rho \| \sigma; \eta),$$

where

$$D_{\max}(\rho\|\sigma; \eta) := \log \text{Tr} \left[\rho^{\frac{1}{2}} \sigma^{-1} \rho^{\frac{1}{2}} \eta \right].$$

The maximum above is achieved by $\eta^* = \Pi_{\max}$, where Π_{\max} is the eigenprojection corresponding to the maximal eigenvalue of $\rho^{1/2} \sigma^{-1} \rho^{1/2}$. The rest of the proof is similar to that of Theorem 7 and proceeds by arguing that

$$\eta_n^* = \Pi_{n, \max} \rightarrow \Pi_{\max},$$

a.s. in trace norm,

$$\begin{aligned} & r_n \left(\text{Tr} \left[\rho_n^{\frac{1}{2}} \sigma_n^{-1} \rho_n^{\frac{1}{2}} \Pi_{n, \max} \right] - \text{Tr} \left[\rho^{\frac{1}{2}} \sigma^{-1} \rho^{\frac{1}{2}} \Pi_{n, \max} \right] \right) \\ & \xrightarrow{w} \text{Tr} \left[\left(D[\rho^{\frac{1}{2}}](L_1) \sigma^{-1} \rho^{\frac{1}{2}} + \rho^{\frac{1}{2}} \sigma^{-1} D[\rho^{\frac{1}{2}}](L_1) + \rho^{\frac{1}{2}} D[\sigma^{-1}](L_2) \rho^{\frac{1}{2}} \right) \Pi_{\max} \right], \\ & r_n \left(\text{Tr} \left[\rho_n^{\frac{1}{2}} \sigma_n^{-1} \rho_n^{\frac{1}{2}} \Pi_{\max} \right] - \text{Tr} \left[\rho^{\frac{1}{2}} \sigma^{-1} \rho^{\frac{1}{2}} \Pi_{\max} \right] \right) \\ & \xrightarrow{w} \text{Tr} \left[\left(D[\rho^{\frac{1}{2}}](L_1) \sigma^{-1} \rho^{\frac{1}{2}} + \rho^{\frac{1}{2}} \sigma^{-1} D[\rho^{\frac{1}{2}}](L_1) + \rho^{\frac{1}{2}} D[\sigma^{-1}](L_2) \rho^{\frac{1}{2}} \right) \Pi_{\max} \right], \end{aligned}$$

where $\Pi_{n, \max}$ is the eigenprojection corresponding to the maximal eigenvalue of $\rho_n^{1/2} \sigma_n^{-1} \rho_n^{1/2}$. These together imply that

$$\begin{aligned} & r_n \left(e^{D_{\max}(\rho_n\|\sigma_n)} - e^{D_{\max}(\rho\|\sigma)} \right) \\ & \xrightarrow{w} \text{Tr} \left[\left(D[\rho^{\frac{1}{2}}](L_1) \sigma^{-1} \rho^{\frac{1}{2}} + \rho^{\frac{1}{2}} \sigma^{-1} D[\rho^{\frac{1}{2}}](L_1) + \rho^{\frac{1}{2}} D[\sigma^{-1}](L_2) \rho^{\frac{1}{2}} \right) \Pi_{\max} \right]. \end{aligned}$$

Then, applying the functional delta-method to $x \mapsto \log x$ at $x = e^{D_{\max}(\rho\|\sigma)}$ yields the desired claim.

E. Proof of Theorem 9

We will prove the claim assuming $\rho, \sigma > 0$. The general case $\rho \ll \sigma$ follows using similar arguments as in the proof of Theorem 1. Following the proof of Theorem 1, it suffices to show that the terms in a Taylor's expansion of the quantum relative entropy are well-defined and the uniform integrability of the remainder terms are ensured. Note that $D(\rho_n\|\sigma_n) < \infty$ for all $n \in \mathbb{N}$ and $D(\rho\|\sigma) < \infty$ by assumption.

Two-sample null: Consider a subsequence $(n_{k_j})_{j \in \mathbb{N}}$ such that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)) \rightarrow (L_1, L_2)$ in $\|\cdot\|_1$ a.s. This is again possible by Skorokhods representation theorem by separability of the space of trace-class operators (i.e., set of operators with finite trace norm). However, the key difference from the finite dimensional case is that the argument that there exists a constant $0 < c < 1$ such that $(1-t)\rho + t\sigma_{n_{k_j}} \geq c\rho$ for sufficiently large j does not hold. Hence, we need a different argument to ensure uniform integrability of the terms which we provide next under the additional assumption that $\mathbb{P}(\|\rho_n \sigma_n^{-1}\|_{\infty} > c) \rightarrow 0$.

Since the high-level proof is similar to that of Theorem 1, we will only highlight the differences. To begin, we note that the steps from (24) to (32) hold. Next, we show uniform integrability of the terms defined in (33):

$$p_n(r_n, t) := (1-t)r_n(\rho_n - \rho) \int_0^\infty v(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau, \quad (55a)$$

$$q_n(r_n, t) := (1-t)((1-t)\rho + t\rho_n) \int_0^\infty v(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) v(\rho_n, \rho, \tau, t) r_n(\rho_n - \rho) v(\rho_n, \rho, \tau, t) d\tau, \quad (55b)$$

$$\tilde{p}_n(r_n, t) := (1-t)((1-t)\rho + t\rho_n) \int_0^\infty v(\sigma_n, \rho, \tau, t) r_n(\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) r_n(\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) d\tau, \quad (55c)$$

$$\tilde{q}_n(r_n, t) := (1-t)r_n(\rho_n - \rho) \int_0^\infty v(\sigma_n, \rho, \tau, t) r_n(\sigma_n - \rho) v(\sigma_n, \rho, \tau, t) d\tau, \quad (55d)$$

where $v(\rho_n, \rho, \tau, t) := (\tau I + (1-t)\rho + t\rho_n)^{-1}$. The first and last term can be bounded as

$$\begin{aligned} \|p_n(r_n, t)\|_1 &\leq (1-t) \|r_n(\rho_n - \rho)\|_1^2 \int_0^\infty \|v(\rho_n, \rho, \tau, t)\|_\infty^2 d\tau \\ &\lesssim_\rho (1-t) \|r_n(\rho_n - \rho)\|_1^2 (1-t)^{-1} \\ &= \|r_n(\rho_n - \rho)\|_1^2, \end{aligned} \quad (56a)$$

$$\begin{aligned} \|\tilde{q}_n(r_n, t)\|_1 &\leq (1-t) \|r_n(\rho_n - \rho)\|_1 \|r_n(\sigma_n - \rho)\|_1 \int_0^\infty \|v(\sigma_n, \rho, \tau, t)\|_\infty^2 d\tau \\ &\lesssim_\rho \|r_n(\rho_n - \rho)\|_1 \|r_n(\sigma_n - \rho)\|_1. \end{aligned} \quad (56b)$$

For the second and third terms, we have by using Hölder's inequality for Schatten-norms and $\|A\|_p \geq \|A\|_q$ for any linear operator A and $1 \leq p \leq q \leq \infty$, that

$$\begin{aligned} \|q_n(r_n, t)\|_1 &\leq (1-t) \|r_n(\rho_n - \rho)\|_1^2 \int_0^\infty \|((1-t)\rho + t\rho_n)v(\rho_n, \rho, \tau, t)\|_\infty \|v(\rho_n, \rho, \tau, t)\|_\infty^2 d\tau \\ &\stackrel{(a)}{\leq} (1-t) \|r_n(\rho_n - \rho)\|_1^2 \int_0^\infty \|v(\rho_n, \rho, \tau, t)\|_\infty^2 d\tau \\ &\lesssim_\rho (1-t) \|r_n(\rho_n - \rho)\|_1^2 (1-t)^{-1} \\ &= \|r_n(\rho_n - \rho)\|_1^2, \\ \|\tilde{p}_n(r_n, t)\|_1 &\leq (1-t) \|r_n(\sigma_n - \rho)\|_1^2 \int_0^\infty \|((1-t)\rho + t\rho_n)v(\sigma_n, \rho, \tau, t)\|_\infty \|v(\sigma_n, \rho, \tau, t)\|_\infty^2 d\tau \\ &\stackrel{(b)}{\leq} (1-t) \|r_n(\sigma_n - \rho)\|_1^2 \|I + \rho_n \sigma_n^{-1}\|_\infty \int_0^\infty \|v(\sigma_n, \rho, \tau, t)\|_\infty^2 d\tau. \end{aligned}$$

Here, we used

$$\begin{aligned} v^{\frac{1}{2}}(\rho_n, \rho, \tau, t)((1-t)\rho + t\rho_n)v^{\frac{1}{2}}(\rho_n, \rho, \tau, t) &\leq I, \\ v^{\frac{1}{2}}(\sigma_n, \rho, \tau, t)((1-t)\rho + t\rho_n)v^{\frac{1}{2}}(\sigma_n, \rho, \tau, t) &\leq I + \rho_n \sigma_n^{-1}, \end{aligned}$$

in (a) and (b), respectively. Since $\mathbb{P}(\|\rho_n \sigma_n^{-1}\|_\infty > c) \rightarrow 0$, by an application of Borel-Cantelli lemma, there exists a subsequence $(n_{k_j})_{j \in \mathbb{N}}$ such that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \rho)) \rightarrow (L_1, L_2)$ in $\|\cdot\|_1$ and $\|\rho_{n_{k_j}} \sigma_{n_{k_j}}^{-1}\|_\infty \leq c$ a.s. Hence, along this subsequence, we have

$$\|p_{n_{k_j}}(r_{n_{k_j}}, t)\|_1 \lesssim_\rho \|r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)\|_1^2, \quad (57a)$$

$$\|\tilde{q}_{n_{k_j}}(r_{n_{k_j}}, t)\|_1 \lesssim_\rho \|r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)\|_1 \|r_{n_{k_j}}(\sigma_{n_{k_j}} - \rho)\|_1, \quad (57b)$$

$$\|q_{n_{k_j}}(r_{n_{k_j}}, t)\|_1 \lesssim_\rho \|r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)\|_1^2, \quad (57c)$$

$$\|\tilde{p}_{n_{k_j}}(r_{n_{k_j}}, t)\|_1 \lesssim_{\rho, c} \|r_{n_{k_j}}(\sigma_{n_{k_j}} - \rho)\|_1^2. \quad (57d)$$

This verifies the required uniform integrability conditions. The rest of the proof is same as that of Theorem 1, and hence omitted.

Two-sample alternative: Consider the expansions in (38). By taking trace, we obtain (39) using (32) as well as $D(\rho_n \|\sigma_n) < \infty$ and $D(\rho \|\sigma) < \infty$. We need to verify that the remaining terms in the expansion are well-defined and that the second-order terms satisfy a uniform integrability condition along a subsequence $(n_{k_j})_{j \in \mathbb{N}}$ such that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)) \rightarrow (L_1, L_2)$ in $\|\cdot\|_1$ and $\|\rho_{n_{k_j}} \sigma_{n_{k_j}}^{-1}\|_\infty \leq c$ a.s. Note that since $\rho, \sigma > 0$, we have

$$\begin{aligned} \|r_n(\rho_n - \rho)(\log \rho - \log \sigma)\|_1 &\leq \|r_n(\rho_n - \rho)\|_1 \|\log \rho - \log \sigma\|_\infty, \\ \left\| \rho \int_0^\infty (\tau I + \sigma)^{-1} r_n(\sigma_n - \sigma) (\tau I + \sigma)^{-1} d\tau \right\|_1 &\leq \|r_n(\sigma_n - \sigma)\|_1 \int_0^\infty \|(\tau I + \sigma)^{-1}\|_\infty^2 d\tau \lesssim_\sigma \|r_n(\sigma_n - \sigma)\|_1. \end{aligned}$$

Hence, the first two terms in (39) are well defined. Taking limits along the subsequence $(n_{k_j})_{j \in \mathbb{N}}$ yields

$$\begin{aligned} &\text{Tr} \left[r_{n_{k_j}}(\rho_{n_{k_j}} - \rho)(\log \rho - \log \sigma) - \rho \int_0^\infty (\tau I + \sigma)^{-1} r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma) (\tau I + \sigma)^{-1} d\tau \right] \\ &\xrightarrow{w} \text{Tr} \left[L_1(\log \rho - \log \sigma) - \rho \int_0^\infty (\tau I + \sigma)^{-1} L_2(\tau I + \sigma)^{-1} d\tau \right]. \end{aligned}$$

It remains to show that $p_n(r_n, t)$, $q_n(r_n, t)$, $\bar{p}_n(r_n, t)$, $\bar{q}_n(r_n, t)$ as defined in (33) and (40b) are uniformly integrable along the subsequence $(n_{k_j})_{j \in \mathbb{N}}$. But, this follows similar to (57), completing the proof.

F. Proof of Proposition 10

Recall that $\hat{\mathbf{s}}^{(n)}(\rho) := (\hat{s}_1^{(n)}(\rho), \dots, \hat{s}_{d^2-1}^{(n)}(\rho))$, where

$$\hat{s}_j^{(n)}(\rho) := \frac{1}{n} \sum_{k=1}^n \mathbb{1}_{O_k(j, \rho)=+1} - \mathbb{1}_{O_k(j, \rho)=-1}, \quad 1 \leq j \leq d^2 - 1.$$

With $\gamma_0 = I$ and $\hat{s}_0^{(n)}(\rho) = 1$, we have

$$\sqrt{n}(\hat{\rho}_n - \rho) = \sqrt{n}(\hat{\rho}_n - \bar{\rho}_n) + \sqrt{n}(\bar{\rho}_n - \rho), \quad (58)$$

where recall that

$$\bar{\rho}_n = \frac{1}{d} \sum_{j=0}^{d^2-1} \hat{s}_j^{(n)}(\rho) \gamma_j.$$

Note that the first term above can be written as

$$\sqrt{n}(\hat{\rho}_n - \bar{\rho}_n) = \mathbb{1}_{\bar{\rho}_n \neq 0} \sqrt{n} \left(\Pi_{\mathcal{S}_d}(\bar{\rho}_n) - \frac{1}{d} \sum_{j=0}^{d^2-1} \hat{s}_j^{(n)}(\rho) \gamma_j \right).$$

We have $|\hat{s}_j^{(n)}(\rho)| \leq 1$ for all j, n . Moreover, the entries of γ_j are bounded, and so is $\Pi_{\mathcal{S}_d}(\bar{\rho}_n)$ being a projection onto the space of density operators. From this, it follows that

$$\sqrt{n} \|\hat{\rho}_n - \bar{\rho}_n\|_1 \lesssim_d \sqrt{n}.$$

Consequently,

$$\mathbb{E} \left[\sqrt{n} \left\| \hat{\rho}_n - \frac{1}{d} \sum_{j=0}^{d^2-1} \hat{s}_j^{(n)}(\rho) \gamma_j \right\|_1 \right] \lesssim_d \mathbb{P}(\bar{\rho}_n \neq 0) \sqrt{n}. \quad (59)$$

For $\mathbf{s} = (s_1, \dots, s_{d^2-1}) \in \mathbb{R}^{d^2-1}$, let $\omega(\mathbf{s}) := \frac{1}{d} \left(I + \sum_{j=1}^{d^2-1} s_j \gamma_j \right)$. Note that the set $\mathcal{C} := \{\mathbf{s} \in \mathbb{R}^{d^2-1} : \omega(\mathbf{s}) \geq 0\}$ is a convex set⁴. Recalling that $\mathbf{s}(\rho) = (s_1(\rho), \dots, s_{d^2-1}(\rho))$ with $s_j(\rho) = \text{Tr}[\rho \gamma_j]$ and $\rho, \sigma > 0$, we have $\mathbf{s}(\rho), \mathbf{s}(\sigma) \in \text{int}(\mathcal{C})$, where $\text{int}(\mathcal{C})$ denotes the interior of \mathcal{C} . The set $\text{int}(\mathcal{C})$ corresponds to \mathbf{s} such that the eigenvalues $\omega(\mathbf{s})$ are strictly positive. Let $\{\lambda_i(\mathbf{s})\}_{i=1}^{d^2}$ denote the eigenvalues of $\omega(\mathbf{s})$ such that $\lambda_i(\mathbf{s}) \leq \lambda_j(\mathbf{s})$ when $j \leq i$. Note that these eigenvalues satisfy $\sum_{i=1}^{d^2} \lambda_i(\mathbf{s}) = 1$ and are the roots of a characteristic polynomial of $\omega(\mathbf{s})$. Let

$$\delta(\rho) := \min_{1 \leq i \leq d^2} \{\lambda_i(\mathbf{s}(\rho))/2\}$$

and consider the event

$$\mathcal{E}_i := \{|\lambda_i(\hat{\mathbf{s}}^n(\rho)) - \lambda_i(\mathbf{s}(\rho))| \geq \delta(\rho)\}.$$

For $\rho, \sigma > 0$, we have $\delta(\rho) \wedge \delta(\sigma) > 0$. By the continuity of the roots of a polynomial as specified in [99, Theorem 1.4], there exists an $\epsilon_{\delta(\rho)} > 0$ such that $\|\mathbf{s} - \tilde{\mathbf{s}}\|_1 \leq \epsilon_{\delta(\rho)}$ implies that $|\lambda_i(\mathbf{s}) - \lambda_i(\tilde{\mathbf{s}})| \leq \delta(\rho)$ for all $1 \leq i \leq d^2$. Hence,

$$\{\bar{\rho}_n \not\geq 0\} \subseteq \cup_{i=1}^{d^2} \mathcal{E}_i \subseteq \{\|\hat{\mathbf{s}}^n(\rho) - \mathbf{s}(\rho)\|_2 > \epsilon_{\delta(\rho)}\}.$$

Now, since $\mathbb{E}[\hat{\mathbf{s}}^n(\rho)] = \mathbf{s}(\rho)$, we have by an application of Hoeffding's inequality that

$$\mathbb{P}(\bar{\rho}_n \not\geq 0) \leq \mathbb{P}(\|\hat{\mathbf{s}}^n(\rho) - \mathbf{s}(\rho)\|_2 \geq \epsilon_{\delta(\rho)}) \leq e^{-nc_i(\rho, d)},$$

where $c_i(\rho, d) > 0$ is some constant that depends on ρ, d . Consequently, the LHS of (59) converges to zero which implies that the first term in the RHS of (58) converges weakly to zero.

Next, consider the second term in the RHS of (58). Since the measurements for different Pauli operators are done on independent copies of ρ , $\hat{s}_j^{(n)}(\rho)$ are independent across different j . Setting $X_k(j, \rho) := \mathbb{1}_{O_k(j, \rho)=+1} - \mathbb{1}_{O_k(j, \rho)=-1}$ and noting that $\mathbb{E}[X_k(j, \rho)] = s_j(\rho)$, we have by the classical central limit theorem (CLT) that

$$\sqrt{n} \left(\frac{1}{d} \sum_{j=1}^{d^2-1} \hat{s}_j^{(n)}(\rho) \gamma_j - \rho \right) = \sum_{j=1}^{d^2-1} \frac{\gamma_j n^{-\frac{1}{2}}}{d} \sum_{k=1}^n (X_k(j, \rho) - s_j(\rho)) \xrightarrow{w} \underbrace{\sum_{j=1}^{d^2-1} \gamma_j Z_j(\rho)}_{L_\rho},$$

where $Z_j(\rho) \sim N(0, 4s_j^+(\rho)s_j^-(\rho)/d^2)$ are independent for different j . From this and the fact that the first term in the RHS of (58) converges weakly to zero, an application of Slutsky's theorem yields $\sqrt{n}(\hat{\rho}_n - \rho) \xrightarrow{w} L_\rho$. Repeating the same arguments with $\rho, \bar{\rho}_n$ replaced by $\sigma, \bar{\sigma}_n$, and noting that $\|I\|_1/n \rightarrow 0$ leads to $\sqrt{n}(\hat{\sigma}_n - \sigma) \xrightarrow{w} L_\sigma$. Consequently, $(\sqrt{n}(\hat{\rho}_n - \rho), \sqrt{n}(\hat{\sigma}_n - \sigma)) \xrightarrow{w} (L_\rho, L_\sigma)$, where L_ρ and L_σ are independent due to the independence of the measurements on ρ and σ . Moreover, $\hat{\rho}_n \ll \hat{\sigma}_n \ll \sigma$ and $\hat{\rho}_n \ll \rho \ll \sigma$ since $\hat{\rho}_n \ll \hat{\sigma}_n$ and $\rho, \sigma > 0$. Hence, Theorem 1 applies and (9) yields

$$\begin{aligned} \sqrt{n}(\mathcal{D}(\hat{\rho}_n \| \hat{\sigma}_n) - \mathcal{D}(\rho \| \sigma)) &\xrightarrow{w} \text{Tr}[L_\rho(\log \rho - \log \sigma) - \rho D[\log \sigma](L_\sigma)] \\ &= \sum_{j=1}^{d^2-1} Z_j(\rho) \text{Tr}[\gamma_j(\log \rho - \log \sigma)] - Z_j(\sigma) \text{Tr}[\rho D[\log \sigma](\gamma_j)] \end{aligned}$$

⁴This set has a simple characterization when $d = 2$, given by $\mathcal{C} = \{\mathbf{s} \in \mathbb{R}^{d^2-1} : \|\mathbf{s}\|_2 \leq 1\}$. This is due to the fact that the eigenvalues of $\omega(\mathbf{s})$ are equal to $(1 \pm \|\mathbf{s}\|_2)/2$.

$$\sim N(0, v_2^2(\rho, \sigma)),$$

where $v_2^2(\rho, \sigma)$ is defined in Proposition 10. This completes the proof.

G. Proof of Proposition 11

We will use Proposition 10 to prove the claim. To that end, we first bound the relevant variances $v_1^2(\rho_k, \sigma)$ for $k \in \mathcal{I}$ given by

$$v_1^2(\rho_k, \sigma) := \sum_{j=1}^{d^2-1} \frac{4s_j^+(\rho_k)s_j^-(\rho_k)}{d^2} \text{Tr} [\gamma_j(\log \rho_k - \log \sigma)]^2.$$

Observe that $s_j^+(\rho_k)s_j^-(\rho_k) \leq 1/4$ since $0 \leq s_j^+(\rho_k) = 1 - s_j^-(\rho_k) \leq 1$. Hence, we have

$$\begin{aligned} v_1^2(\rho_k, \sigma) &\leq \frac{1}{d^2} \sum_{j=1}^{d^2-1} \text{Tr} [\gamma_j(\log \rho_k - \log \sigma)]^2 \\ &\leq \frac{2}{d^2} \left(\sum_{j=1}^{d^2-1} \text{Tr} [\gamma_j \log \rho_k]^2 + \text{Tr} [\gamma_j \log \sigma]^2 \right) \\ &\leq \frac{2}{d^2} \left(\sum_{j=1}^{d^2-1} \|\gamma_j\|_2^2 \|\log \rho_k\|_2^2 + \|\gamma_j\|_2^2 \|\log \sigma\|_2^2 \right) \\ &\leq 4d^2(\log b)^2, \end{aligned}$$

where the second inequality uses $(a - b)^2 \leq 2(a^2 + b^2)$ for $a, b \in \mathbb{R}$, the penultimate inequality follows by Cauchy-Schwarz, and the final inequality uses $\|\gamma_j\|_2^2 \leq d$ and $\|\log \sigma\|_2^2 \vee \|\log \rho_k\|_2^2 \leq d(\log b)^2$ for all $k \in \mathcal{I}$. Then,

$$\begin{aligned} \alpha_{i,n}(\mathcal{T}_n^{\text{tom}}, \rho_i^{\otimes n}, \sigma_i^{\otimes n}) &= \mathbb{P}(\hat{D}_n \notin (\epsilon_i + cn^{-\frac{1}{2}}, \epsilon_{i+1} + cn^{-\frac{1}{2}}) | H = i) \\ &= \mathbb{P}(\hat{D}_n - D(\rho_i \| \sigma) \notin (\epsilon_i - D(\rho_i \| \sigma) + cn^{-\frac{1}{2}}, \epsilon_{i+1} - D(\rho_i \| \sigma) + cn^{-\frac{1}{2}}) | H = i) \\ &\leq \mathbb{P}(n^{\frac{1}{2}}(\hat{D}_n - D(\rho_i \| \sigma)) \notin (n^{\frac{1}{2}}(\epsilon_i - D(\rho_i \| \sigma)) + c, c) | H = i), \end{aligned}$$

where the final inequality follows because $D(\rho_i \| \sigma) \leq \epsilon_{i+1}$. Note that $n^{\frac{1}{2}}(\hat{D}_n - D(\rho_i \| \sigma)) \xrightarrow{w} W_1 \sim N(0, v_1^2(\rho_i, \sigma))$ given H_i is the true hypothesis by (22a) in Proposition 10. Then, taking limits in the equation above and applying Portmanteaus theorem [93, Theorem 2.1] yields

$$\begin{aligned} \limsup_{n \rightarrow \infty} \alpha_{i,n}(\mathcal{T}_n^{\text{tom}}, \rho_i^{\otimes n}, \sigma_i^{\otimes n}) &\leq \limsup_{n \rightarrow \infty} \mathbb{P}(n^{\frac{1}{2}}(\hat{D}_n - D(\rho_i \| \sigma)) \notin (n^{\frac{1}{2}}(\epsilon_i - D(\rho_i \| \sigma)) + c, c) | H = i) \\ &= \mathbb{P}(W_1 \notin (-\infty, c)) \\ &= Q(c/v_1(\rho_i, \sigma)), \end{aligned}$$

where $Q(x) := (2\pi)^{-1/2} \int_x^\infty e^{-x^2} dx$ is the complementary error function. Setting $c = 2dQ^{-1}(\tau)|\log b|$, the RHS above is bounded by τ for all $i \in \mathcal{I}$.

APPENDIX A

PROOF OF LEMMA 13

To prove (i), note that since $A \ll P$ with P being a projection, we have $PAP = A$. Hence,

$$\mathrm{Tr}[AB] = \mathrm{Tr}[PAPB] = \mathrm{Tr}[PAPBP],$$

where the final inequality follows since $PAPB$ is trace-class and P is bounded (being a projection), and using the fact that $\mathrm{Tr}[MN] = \mathrm{Tr}[NM]$ when M and N are trace-class and bounded linear operators, respectively.

To prove (ii), first consider the case that \mathbb{H} is finite dimensional, i.e., $\mathbb{H} = \mathbb{H}_d$. By the spectral theorem, we have $A = \sum_{i=1}^d \lambda_{i,A} |e_{i,A}\rangle\langle e_{i,A}|$, where $\{\lambda_{i,A}\}_{i=1}^d$ and $\{e_{i,A}\}_{i=1}^d$ are the set of eigenvalues and corresponding set of orthonormal eigenvectors of A , respectively. Similarly, let $B = \sum_{i=1}^d \lambda_{i,B} |e_{i,B}\rangle\langle e_{i,B}|$ and $C = \sum_{i=1}^d \lambda_{i,C} |e_{i,C}\rangle\langle e_{i,C}|$ be the spectral decomposition of B and C , respectively. Then, $B \leq A \leq C$ implies that for all $1 \leq j \leq d$,

$$\sum_{i=1}^d \lambda_{i,B} |\langle e_{j,A}, e_{i,B} \rangle|^2 \leq \langle e_{j,A} | A | e_{j,A} \rangle = \lambda_{j,A} \leq \sum_{i=1}^d \lambda_{i,C} |\langle e_{j,A}, e_{i,C} \rangle|^2.$$

Hence, we have

$$\begin{aligned} \|A\|_1 &= \sum_{j=1}^d |\lambda_{j,A}| \leq \sum_{j=1}^d \max \left\{ \sum_{i=1}^d |\lambda_{i,B}| |\langle e_{j,A}, e_{i,B} \rangle|^2, \sum_{i=1}^d |\lambda_{i,C}| |\langle e_{j,A}, e_{i,C} \rangle|^2 \right\} \\ &\leq \sum_{j=1}^d \sum_{i=1}^d |\lambda_{i,B}| |\langle e_{j,A}, e_{i,B} \rangle|^2 + |\lambda_{i,C}| |\langle e_{j,A}, e_{i,C} \rangle|^2 \\ &= \sum_{i=1}^d |\lambda_{i,B}| + |\lambda_{i,C}| = \|B\|_1 + \|C\|_1, \end{aligned} \quad (60)$$

where in the penultimate inequality, we upper bounded maximum of positive numbers by its sum, and in the penultimate equality, we used that the eigenvectors form an orthonormal basis implying that

$$\sum_{j=1}^d |\langle e_{j,A}, e_{i,B} \rangle|^2 = \sum_{j=1}^d |\langle e_{j,A}, e_{i,C} \rangle|^2 = 1, \quad \forall 1 \leq i \leq d.$$

For the case of separable \mathbb{H} , let $(e_n)_{n \in \mathbb{N}}$ be a sequence of orthonormal basis elements, and $(P_n)_{n \in \mathbb{N}}$, with $P_n := \sum_{i=1}^n |e_i\rangle\langle e_i|$, be an increasing sequence of orthogonal projections. Then, setting $A_n = P_n A P_n$, $B_n = P_n B P_n$, $C_n = P_n C P_n$ and noting that $B_n \leq A_n \leq C_n$, (60) implies that $\|A_n\|_1 \leq \|B_n\|_1 + \|C_n\|_1$. Taking limits $n \rightarrow \infty$ and observing that $A_n \rightarrow A$, $B_n \rightarrow B$ and $C_n \rightarrow C$ in trace norm, completes the proof.

APPENDIX B

LIMIT DISTRIBUTIONS FOR MEASURED RELATIVE ENTROPY

Here, we derive limit distributions for estimators of measured relative entropy with respect to a general class of measurements (see [18], [90]–[92] for certain important classes). Before stating our result, we need to introduce some terminology. Let \mathcal{M} denote a set of POVMs (see the books [15]–[17]), where a POVM here refers to a set $M = \{M_i\}_{i \in \mathcal{I}}$ of operators indexed by a discrete set \mathcal{I} satisfying $0 \leq M_i \leq I$ and $\sum_{i \in \mathcal{I}} M_i = I$. The measured relative entropy between density operators ρ and σ with respect to \mathcal{M} is

$$D_{\mathcal{M}}(\rho \| \sigma) := \sup_{M \in \mathcal{M}} D(P_{\rho, M} \| P_{\sigma, M}), \quad (61)$$

where $P_{\rho,M}$ denotes the probability measure defined via $P_{\rho,M}(i) := \text{Tr}[M_i\rho]$. In what follows, we will also use the notation $P_{A,M}(\cdot)$ for a general operator A and POVM M , in which case it is no longer necessarily a probability distribution.

Each POVM M defines a measurement (quantum to classical) channel given by $M(\rho) := \sum_{i \in \mathcal{I}} \text{Tr}[M_i\rho] |i\rangle\langle i|$, where $|i\rangle$ denotes the i^{th} computational basis element. We will use the same notation M for the POVM and the measurement channel (linear superoperator) induced by it, with the usage being evident from the context. With this notation, $D_{\mathcal{M}}(\rho\|\sigma) = \sup_{M \in \mathcal{M}} D(M(\rho)\|M(\sigma))$. We identify two POVMs M and \tilde{M} in \mathcal{M} if for every $\rho, \sigma \in \mathcal{S}_d$, $P_{\rho,M}(\cdot)$ and $P_{\sigma,M}(\cdot)$ are equivalent (up to the same permutation) to $P_{\rho,\tilde{M}}(\cdot)$ and $P_{\sigma,\tilde{M}}(\cdot)$, respectively, since measured relative entropy remains the same with this identification. Also, we will restrict to \mathcal{M} such that $|\mathcal{I}| \leq m$ for all $M \in \mathcal{M}$ and some $m \in \mathbb{N}$. This is not a restriction when \mathcal{M} contains the set of all projective measurements (see [100]). By adding zero matrices as necessary, we may assume without loss of generality that $\mathcal{I} = \{0, \dots, m-1\}$. We will view \mathcal{M} as a subset of the space of linear superoperators equipped with operator norm topology.

Let $M^*(\rho, \sigma, \mathcal{M})$ denote an optimizer achieving the supremum (if it exists) in (61). The next result characterizes limit distribution for measured relative entropy estimation in terms of quantities induced by optimal measurement.

Theorem 14 (Limit distribution for measured relative entropy) *Let $\rho_n \ll \sigma_n \ll \sigma$, $\rho_n \ll \rho \ll \sigma$, and \mathcal{M} be compact such that $M^* := M^*(\rho, \sigma, \mathcal{M})$ is unique with the identification of POVMs as mentioned above. If $(r_n(\rho_n - \rho), r_n(\sigma_n - \sigma)) \xrightarrow{w} (L_1, L_2)$, then*

$$r_n(D_{\mathcal{M}}(\rho_n\|\sigma_n) - D_{\mathcal{M}}(\rho\|\sigma)) \xrightarrow{w} \sum_{i \in \mathcal{I}} P_{L_1, M^*}(i) \log \frac{P_{\rho, M^*}(i)}{P_{\sigma, M^*}(i)} - \frac{P_{L_2, M^*}(i) P_{\rho, M^*}(i)}{P_{\sigma, M^*}(i)}. \quad (62)$$

Before, we proceed with the proof of Proposition 14, a few remarks are in order. Since the definition of $D_{\mathcal{M}}$ itself involves a supremum, a method of proof similar to that of Theorem 7 applies. However, a key technical difference arises due to the fact that without additional assumptions, the maximizer in (61) is not unique. Moreover, the maximizer does not have a closed form expression in general. Hence, to establish the above claim, our proof involves showing that the optimal measurement POVM of the empirical measured relative entropy, $D_{\mathcal{M}}(\rho_n\|\sigma_n)$, converges to M^* in operator norm. This convergence necessitates the requirement of a unique M^* as stated above.

Proof. It suffices to show that for every subsequence of \mathbb{N} , there exists a further subsequence along which the convergence in (62) holds. Let n_{k_j} be a subsequence such that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)) \rightarrow (L_1, L_2)$ in trace-norm a.s., which exists by the same reasons stated in the proof of Theorem 1. Let M_n^* be such that

$$D_{\mathcal{M}}(\rho_n\|\sigma_n) = D(P_{\rho_n, M_n^*} \| P_{\sigma_n, M_n^*}).$$

Such an M_n^* exists since \mathcal{M} is compact and $D(P_{\rho_n, M} \| P_{\sigma_n, M})$ is a continuous functional of M for $\rho_n \ll \sigma_n$.

We will show that $M_n^* \rightarrow M^*$ a.s. in operator norm. Note that since $\rho \ll \sigma$, there exists constants $c_1, c_2 > 0$ such that $c_1\sigma \leq \rho \leq c_2\sigma$. Since a quantum channel is a completely positive linear map, we also have $c_1M(\sigma) \leq M(\rho) \leq c_2M(\sigma)$. Moreover, since $\rho_{n_{k_j}} \rightarrow \rho$ and $\sigma_{n_{k_j}} \rightarrow \sigma$ in trace norm a.s., there exists constants \tilde{c}_1, \tilde{c}_2 (depending on the realization $\rho_{n_{k_j}}$ and $\sigma_{n_{k_j}}$) such that for all j sufficiently large, $0 < \tilde{c}_1 \leq c_1$, $0 < c_2 \leq \tilde{c}_2$,

$\tilde{c}_1 \sigma_{n_{k_j}} \leq \rho_{n_{k_j}} \leq \tilde{c}_2 \sigma_{n_{k_j}}$ and $\tilde{c}_1 M(\sigma_{n_{k_j}}) \leq M(\rho_{n_{k_j}}) \leq \tilde{c}_2 M(\sigma_{n_{k_j}})$. Then, denoting by A_- , the negative part of $A = A_+ - A_-$, we have

$$\begin{aligned} D(M(\rho) \| M(\sigma)) &\stackrel{(a)}{=} \int_{\tilde{c}_1}^{\tilde{c}_2} \frac{ds}{s} \text{Tr} \left[(M(\rho) - sM(\sigma))_- \right] + \log \tilde{c}_2 + 1 - \tilde{c}_2 \\ &\stackrel{(b)}{=} \int_{\tilde{c}_1}^{\tilde{c}_2} \frac{ds}{2s} (s - 1 + \| (M(\rho) - sM(\sigma)) \|_1) + \log \tilde{c}_2 + 1 - \tilde{c}_2, \end{aligned}$$

where (a) follows from the integral representation of quantum relative entropy (see [101, Theorem 6] and [102, Corollary 1]), while (b) uses $\|A\|_1 = A_+ + A_-$ and $\text{Tr} [M(\rho) - sM(\sigma)] = 1 - s$. Using similar representation for $D(M(\rho_{n_{k_j}}) \| M(\sigma_{n_{k_j}}))$ and subtracting from previous equation, we have

$$\begin{aligned} &\left| D(M(\rho) \| M(\sigma)) - D(M(\rho_{n_{k_j}}) \| M(\sigma_{n_{k_j}})) \right| \\ &= \left| \int_{\tilde{c}_1}^{\tilde{c}_2} \frac{ds}{2s} \|M(\rho) - sM(\sigma)\|_1 - \|M(\rho_{n_{k_j}}) - sM(\sigma_{n_{k_j}})\|_1 \right| \\ &\leq \int_{\tilde{c}_1}^{\tilde{c}_2} \frac{ds}{2s} \left| \|M(\rho) - sM(\sigma)\|_1 - \|M(\rho_{n_{k_j}}) - sM(\sigma_{n_{k_j}})\|_1 \right| \\ &\stackrel{(a)}{\leq} \int_{\tilde{c}_1}^{\tilde{c}_2} \frac{ds}{2s} \|M(\rho) - M(\rho_{n_{k_j}}) - sM(\sigma) + sM(\sigma_{n_{k_j}})\|_1 \\ &\stackrel{(b)}{\leq} \int_{\tilde{c}_1}^{\tilde{c}_2} \frac{ds}{2s} (\|M(\rho) - M(\rho_{n_{k_j}})\|_1 + s\|M(\sigma) - M(\sigma_{n_{k_j}})\|_1) \\ &\stackrel{(c)}{\leq} \int_{\tilde{c}_1}^{\tilde{c}_2} \frac{ds}{2s} (\|\rho - \rho_{n_{k_j}}\|_1 + s\|\sigma - \sigma_{n_{k_j}}\|_1), \end{aligned}$$

where (a) and (b) follows from triangle inequality, while (c) is due to data processing inequality for trace norm. By setting $h_n(M) = D(M(\rho_n) \| M(\sigma_n))$, it follows from the above inequality that $h_{n_{k_j}}(M)$ converges uniformly to $D(M(\rho) \| M(\sigma))$ (as a function of M) given $\rho_{n_{k_j}} \rightarrow \rho$ and $\sigma_{n_{k_j}} \rightarrow \sigma$. Also, note that for any $M, \tilde{M} \in \mathcal{M}$, we have via similar steps as above that

$$\begin{aligned} \left| D(M(\rho) \| M(\sigma)) - D(\tilde{M}(\rho) \| \tilde{M}(\sigma)) \right| &\leq \int_{c_1}^{c_2} \frac{ds}{2s} (\|M(\rho) - \tilde{M}(\rho)\|_1 + s\|M(\sigma) - \tilde{M}(\sigma)\|_1) \\ &\leq \int_{c_1}^{c_2} \frac{ds}{2s} \|M - \tilde{M}\| (s + 1) \\ &\leq \frac{\|M - \tilde{M}\|}{2} \left(\ln \frac{c_2}{c_1} + c_2 - c_1 \right), \end{aligned}$$

where $\|\cdot\|$ in the last two inequalities denotes the operator norm. Hence, $D(M(\rho) \| M(\sigma))$ is a uniformly continuous functional of M in operator norm. Since \mathcal{M} is compact in the operator norm topology and $M^* = \arg \max_{\mathcal{M}} D(\rho \| \sigma)$ is unique, the aforementioned uniform convergence implies that $M_{n_{k_j}}^* \rightarrow M^*$ a.s. in operator norm.

Equipped with the above, we next prove (62). Observe that by definition of M_n^* and M^* , we have

$$r_n (D_{\mathcal{M}}(\rho_n \| \sigma_n) - D_{\mathcal{M}}(\rho \| \sigma)) \leq r_n (D(P_{\rho_n, M_n^*} \| P_{\sigma_n, M_n^*}) - D(P_{\rho, M_n^*} \| P_{\sigma, M_n^*})), \quad (63a)$$

$$r_n (D_{\mathcal{M}}(\rho_n \| \sigma_n) - D_{\mathcal{M}}(\rho \| \sigma)) \geq r_n (D(P_{\rho_n, M^*} \| P_{\sigma_n, M^*}) - D(P_{\rho, M^*} \| P_{\sigma, M^*})). \quad (63b)$$

Denoting the LHS and RHS of (62) by $g_n(\rho_n, \sigma_n)$ and $g(L_1, L_2)$, respectively, we will show that along the subsequence $(n_{k_j})_{j \in \mathbb{N}}$, the RHS of (63a) and (63b) converge a.s. to $g(L_1, L_2)$. This then implies that $g_{n_{k_j}} \rightarrow g(L_1, L_2)$ a.s. and also weakly.

From Taylor expansion applied to the function $f(x, y) = x \log \frac{x}{y}$, we have⁵ for u, v, \bar{u}, \bar{v} such that $u \geq 0, v, \bar{u}, \bar{v} > 0$ or $u = 0, v \geq 0, \bar{u}, \bar{v} > 0$ that

$$\begin{aligned} u \log \frac{u}{v} &= \bar{u} \log \frac{\bar{u}}{\bar{v}} + \left(1 + \log \frac{\bar{u}}{\bar{v}}\right) (u - \bar{u}) - \frac{\bar{u}}{\bar{v}} (v - \bar{v}) + \int_0^1 \frac{(1-\tau)(u - \bar{u})^2}{(1-\tau)\bar{u} + \tau u} d\tau \\ &\quad + \int_0^1 \frac{(1-\tau)((1-\tau)\bar{u} + \tau u)(v - \bar{v})^2}{((1-\tau)\bar{v} + \tau v)^2} d\tau - 2 \int_0^1 \frac{(1-\tau)(u - \bar{u})(v - \bar{v})}{((1-\tau)\bar{v} + \tau v)^2} d\tau. \end{aligned} \quad (64)$$

Let $u = P_{\rho_n, M_n^*}(i)$, $v = P_{\sigma_n, M_n^*}(i)$, $\bar{u} = P_{\rho, M_n^*}(i)$, $\bar{v} = P_{\sigma, M_n^*}(i)$ for $i \in \mathcal{I}$ and note that the aforementioned constraints on u, v, \bar{u}, \bar{v} are satisfied since $P_{\rho_n, M_n^*} \ll P_{\rho, M_n^*} \ll P_{\sigma, M_n^*}$ and $P_{\rho_n, M_n^*} \ll P_{\sigma_n, M_n^*} \ll P_{\sigma, M_n^*}$ due to $\rho_n \ll \sigma_n \ll \sigma$ and $\rho_n \ll \rho \ll \sigma$. Substituting the above and summing the resulting expression over i in the above equation leads to

$$\begin{aligned} f_n &:= r_n (\mathcal{D}(M_n^*(\rho_n) \| M_n^*(\sigma_n)) - \mathcal{D}(M_n^*(\rho) \| M_n^*(\sigma))) \\ &= \sum_{i \in \mathcal{I}} r_n (P_{\rho_n, M_n^*}(i) - P_{\rho, M_n^*}(i)) \log \frac{P_{\rho, M_n^*}(i)}{P_{\sigma, M_n^*}(i)} - \sum_{i \in \mathcal{I}} r_n (P_{\sigma_n, M_n^*}(i) - P_{\sigma, M_n^*}(i)) \frac{P_{\rho, M_n^*}(i)}{P_{\sigma, M_n^*}(i)} + R_n, \end{aligned}$$

where $R_n = R_{n,1} + R_{n,2} - 2R_{n,3}$, and

$$\begin{aligned} R_{n,1} &:= \sum_{i \in \mathcal{I}} \int_0^1 \frac{(1-\tau) \left(r_n^{\frac{1}{2}} (P_{\rho_n, M_n^*}(i) - P_{\rho, M_n^*}(i)) \right)^2}{(1-\tau)P_{\rho, M_n^*}(i) + \tau P_{\rho_n, M_n^*}(i)} d\tau, \\ R_{n,2} &:= \sum_{i \in \mathcal{I}} \int_0^1 \frac{(1-\tau) ((1-\tau)P_{\rho, M_n^*}(i) + \tau P_{\rho_n, M_n^*}(i)) \left(r_n^{\frac{1}{2}} ((P_{\sigma_n, M_n^*}(i) - P_{\sigma, M_n^*}(i))) \right)^2}{((1-\tau)P_{\sigma_n, M_n^*}(i) + \tau P_{\sigma, M_n^*}(i))^2} d\tau, \\ R_{n,3} &:= \sum_{i \in \mathcal{I}} \int_0^1 \frac{(1-\tau) r_n^{\frac{1}{2}} (P_{\rho_n, M_n^*}(i) - P_{\rho, M_n^*}(i)) r_n^{\frac{1}{2}} (P_{\sigma_n, M_n^*}(i) - P_{\sigma, M_n^*}(i))}{((1-\tau)P_{\sigma, M_n^*}(i) + \tau P_{\sigma_n, M_n^*}(i))^2} d\tau. \end{aligned}$$

Note that since $M_{n_{k_j}}^* \rightarrow M^*$ in operator norm a.s. and $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)) \rightarrow (L_1, L_2)$ in trace-norm a.s., we have $P_{\rho_{n_{k_j}}, M_{n_{k_j}}^*}(i) \rightarrow P_{\rho, M^*}(i)$, $P_{\sigma_{n_{k_j}}, M_{n_{k_j}}^*}(i) \rightarrow P_{\sigma, M^*}(i)$, and

$$\begin{aligned} r_{n_{k_j}} \left(P_{\rho_{n_{k_j}}, M_{n_{k_j}}^*}(i) - P_{\rho, M_{n_{k_j}}^*}(i) \right) &= \text{Tr} \left[M_{n_{k_j}}^*(i) r_{n_{k_j}} (\rho_{n_{k_j}} - \rho) \right] \rightarrow \text{Tr} [M^*(i) L_1], \\ r_{n_{k_j}} \left(P_{\sigma_{n_{k_j}}, M_{n_{k_j}}^*}(i) - P_{\sigma, M_{n_{k_j}}^*}(i) \right) &= \text{Tr} \left[M_{n_{k_j}}^*(i) r_{n_{k_j}} (\sigma_{n_{k_j}} - \sigma) \right] \rightarrow \text{Tr} [M^*(i) L_2], \\ r_{n_{k_j}}^{\frac{1}{2}} \left(P_{\rho_{n_{k_j}}, M_{n_{k_j}}^*}(i) - P_{\rho, M_{n_{k_j}}^*}(i) \right) &\rightarrow 0, \quad \text{and} \quad r_{n_{k_j}}^{\frac{1}{2}} \left(P_{\sigma_{n_{k_j}}, M_{n_{k_j}}^*}(i) - P_{\sigma, M_{n_{k_j}}^*}(i) \right) \rightarrow 0. \end{aligned}$$

Hence, we have $R_{n_{k_j}} \rightarrow 0$ and $f_{n_{k_j}} \rightarrow g(L_1, L_2)$. This implies that the RHS of (63a) converges to $g(L_1, L_2)$. Via analogous arguments, the RHS of (63b) also converges a.s. to $g(L_1, L_2)$ along the sequence $(n_{k_j})_{j \in \mathbb{N}}$, which implies that $g_{n_{k_j}} \rightarrow g(L_1, L_2)$ a.s. and hence also weakly as claimed. This completes the proof of the proposition. \square

⁵The conditions required for validity of Taylor's expansion requires $u, v, \bar{u}, \bar{v} > 0$, but as noted in the proof of [22, Proposition 1], this expansion is also valid for all u, v, \bar{u}, \bar{v} as mentioned above.

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Author's Response

Dear Dr. Mancini and Reviewers,

Thank you very much for the valuable feedback and for your time and diligence in reviewing our paper. Please find our detailed response to the reviewer's comments and suggestions below. We have tried our best to address the comments in the revision. In our response below, all references are according to the numbering in the revised version and revised parts of the paper are highlighted in blue.

To summarize briefly, the main changes from the previous version are as follows:

- 1) We have added further explanation to some of the steps in the proof that required further clarification, in particular, the points raised by the reviewers. We believe that this has improved the readability of the paper.
- 2) We have revised Lemma 13 (previously Lemma 1) as the proof of its first part had an issue, although not a critical one as already pointed out in the review. This lemma was only used in the proofs of our main results to extend from the case when the density operators had full support to the general case. Since some parts of the previous lemma were stronger than that required for our purposes, we have removed the erroneous Part (i) and rephrased Part (ii).
- 3) We recently noticed a bug in the application section of our paper. Specifically, the problem is that the density operator estimates constructed via Pauli tomography by normalizing the coefficients on the Pauli basis need not be positive semi-definite (this indeed holds for single qubit tomography but not necessarily for the multi-qubit case). In the revised version, we have rectified this issue by projecting the density estimates (in the sense of the Hilbert projection theorem) onto the convex set of positive semi-definite operators. Since the specific tomography scheme only appears as part of the application in constructing the density estimates, nothing else is affected. In particular, the limit distribution for the tomographic estimator (Proposition 10) and the performance guarantees of the hypothesis testing problem (Proposition 11) do not change.
- 4) We have addressed all the other comments raised by the reviewers.

Below, please find our point by point response to the reviewers comments.

Reviewer 1

We thank the reviewer for his/her feedback, which has helped improve our manuscript considerably.

Comment: *A large part of the paper is devoted to the derivatives and Taylor expansions of the divergences and the involved functions... I think such derivatives were already considered before and I am sure the authors can find the necessary computations in the literature. On the other hand, very small space is devoted to the random density operators which are the object of the study, the mode of their convergence and its properties and the techniques which are used in the proofs. Such techniques may be not so widespread in the quantum information community for which this paper surely would be interesting.*

Response: While it is plausible that these derivatives were computed elsewhere, we could not find a reference that computes all these derivatives in the form that we require. Also, we believe it is beneficial to state the expressions

for the derivatives here, as some of these expressions are lengthy and it may not be easy for the reader to find from multiple sources even if they exist. That said, if the referee is aware of a suitable reference, we would gladly add it and revise accordingly.

The technical concepts used such as weak convergence of random density operators and Bochner integrability were previously scattered within the *Notation* and *Proofs* section. We have now added a more detailed exposition of these concepts in the *Preliminaries* section (see Section II-B and II-D), which are repeated below:

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a sufficiently rich probability space on which all random elements are defined. A sequence of random elements $(X_n)_{n \in \mathbb{N}}$ taking values in a topological space \mathfrak{S} converges weakly to a random element X (taking values in \mathfrak{S}) if $\mathbb{E}[f(X_n)] \rightarrow \mathbb{E}[f(X)]$ for all bounded continuous functions $f : \mathfrak{S} \rightarrow \mathbb{R}$. This is denoted by $X_n \xrightarrow{w} X$. Here, the random element of interest is a random density operator (or operators), which is a Borel-measurable mapping from Ω to the space of density operators, \mathcal{S}_d . The weak limit of a random density operator is unique if it exists (see e.g. [83]). Since density operators have unit trace, the appropriate space \mathfrak{S} to consider weak convergence for our purposes is the space of trace-class operators, i.e., the space of operators with finite trace. In finite dimensions, we may take $\mathfrak{S} = \mathcal{L}(\mathbb{H}_d)$ equipped with any norm since all norms are equivalent.

We need the concept of Bochner-integrability [85] in the proofs of our main results, which we briefly mention. Let $(\mathfrak{X}, \Sigma, \mu)$ be a measure space and \mathfrak{B} be a Banach space. A function $f : \mathfrak{X} \rightarrow \mathfrak{B}$ is said to be integrable (in the sense of Bochner) if there exists a sequence of simple functions g_n such that $g_n \rightarrow f$, μ -a.e., and

$$\lim_{n \rightarrow \infty} \int_{\mathfrak{X}} \|f - g_n\|_{\mathfrak{B}} d\mu = 0,$$

where $\|\cdot\|_{\mathfrak{B}}$ denotes the Banach space norm. A Bochner-measurable function f is integrable iff $\int_{\mathfrak{X}} \|f\|_{\mathfrak{B}} d\mu < \infty$. Moreover, if f is integrable, then

$$\left\| \int_{\mathfrak{X}} f d\mu \right\|_{\mathfrak{B}} \leq \int_{\mathfrak{X}} \|f\|_{\mathfrak{B}} d\mu.$$

Comment: Although the authors briefly describe the main ideas of the proofs in the main body of the paper, which is a good thing, the proof themselves are quite unclear. The main techniques are only sparsely mentioned and it seems that many of the steps are just skipped. For example, I do not understand how the Skorohod representation theorem is applied in the subsequence argument in the proof of the theorems, the authors just write that "This is possible by Skorohods representation theorem (see e.g. [95])", as if a rabbit was just taken out of the hat. This seems to be the crucial argument in most of the proofs and should be better explained. There are also other points, for example the use of the portmanteau theorem at the beginning of p. 19 (and similarly also in other proofs).

Response: We have added a more detailed explanation for the points raised and also some others additionally. To answer the query regarding the usage of Skorokhod's representation theorem, we use it to extract a subsequence $(r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)) \xrightarrow{w} (L_1, L_2)$ that converges almost surely from a sequence $(r_{n_k}(\rho_{n_k} - \rho), r_{n_k}(\sigma_{n_k} - \sigma)) \xrightarrow{w} (L_1, L_2)$ that converges weakly. This is a useful technique which simplifies the arguments further downstream in the proof. The relevant text (see Page 18) is stated below for convenience:

To show the aforementioned claim of unique weak limit, consider any subsequence $(n_k)_{k \in \mathbb{N}}$. Then, $((r_{n_k}(\rho_{n_k} - \rho), r_{n_k}(\sigma_{n_k} - \rho)) \xrightarrow{w} (L_1, L_2)$ in $\|\cdot\|_1$ since every subsequence of weakly convergent sequence has the same weak limit. Hence, due to separability of $\mathcal{L}(\mathbb{H}_d)$ (for finite d), by Skorokhods representation theorem (see e.g. [83]), there exists a further subsequence $(n_{k_j})_{j \in \mathbb{N}}$ such that $((r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \rho)) \rightarrow (L_1, L_2)$ in $\|\cdot\|_1$ almost surely (a.s.).

Regarding the usage of Portmanteau Theorem, we have added further explanation (see Page 19) as detailed below:

Next, to see that the RHS of (10) is invariant to restricting to support of ρ , we first note that the support of L_1 and L_2 is contained in that of ρ . To show this, notice that for every $n \in \mathbb{N}$, $\rho_n - \rho \ll \rho$ and $\sigma_n - \rho \ll \rho$ because $\rho_n, \sigma_n \ll \rho$ by assumption. By Portmanteau's theorem [83, Theorem 1.3.4 (vii)], since $r_n(\rho_n - \rho) \xrightarrow{w} L_1$, we have

$$\liminf \mathbb{E}[f(r_n(\rho_n - \rho))] \geq f(L_1),$$

for every bounded Lipschitz continuous (w.r.t. to trace norm) non-negative f . Let P_ρ^\perp denote the projector onto the orthogonal complement of the support of ρ . Applying (37) to the bounded Lipschitz continuous function $f_M(L) = \|P_\rho^\perp L P_\rho^\perp\|_1 \wedge M$ on the space of trace-class operators, where $M > 0$, we obtain

$$0 = \liminf r_n \mathbb{E} \left[\|P_\rho^\perp (\rho_n - \rho) P_\rho^\perp\|_1 \right] \geq r_n \|P_\rho^\perp L_1 P_\rho^\perp\|_1 \wedge M \geq 0.$$

Since r_n is positive and the above equation has to hold for every M , taking limit $M \rightarrow \infty$ implies that $\|P_\rho^\perp L_1 P_\rho^\perp\|_1 = 0$. Hence, the support of L_1 is contained in that of ρ . Similar claim also holds for L_2 .

We want to emphasize that since many steps in the proof of Theorem 1 are also used in the proofs of the subsequent results, we only describe the arguments in detail in the first instance to reduce repetition. We would be happy to clarify any further questions by the referee.

Comment: *There are also mistakes, most notably, Lemma 1, part (i). This is quite obviously wrong, and its proof does not make any sense. This part is used also in the proof of part (ii), which, fortunately, is easy to see to be true in the case when $A \geq 0$, which is the only case when it was used in the paper.*

Response: Thank you for pointing out the bug in Lemma 1, Part (i) previously. As mentioned earlier, this part was not really required for our purposes, and the proof of Theorem 1 only relied on Part (ii) as stated in the revised form given below (see Page 14):

Lemma 13 (Properties of trace-class operators) *Let \mathbb{H} be a separable Hilbert space. Then, the following hold:*

- (i) *Let $A, B \in \mathcal{L}(\mathbb{H})$ be such that AB is trace-class. Let P be an orthogonal projection (i.e., Hermitian operator P satisfying $0 \leq P = P^2$) such that $A \ll P$. Then, $\text{Tr}[AB] = \text{Tr}[PAPBP]$.*
- (ii) *Let A, B, C be trace-class Hermitian operators such that $B \leq A \leq C$. Then, $\|A\|_1 \leq \|B\|_1 + \|C\|_1$.*

Note that this lemma is stated in a slightly more general form than before so that it is also applicable to the case of a separable Hilbert space.

Comment: *What is the meaning of Λ_j^+ and Λ_j^- ? I would say that measuring γ_j has outcomes just ± 1 .*

Response: In general, one may associate different outcomes to a measurement even if it corresponds to same eigenvalue (with multiplicities greater than one), resulting in a set of outcomes. However, we do not require this in our setting, and so we have now omitted the notation Λ_j^+ and Λ_j^- .

Comment: *Page 20, last set of displayed equations: in the last line, all the “tilded” terms are equal to their “untilded” versions, except for the last one, where it is not so automatic.*

Response: Thank you for pointing this out. The said step which had an issue was part of an argument used to extend Theorem 1 (ii) to the case when the density operators need not have full support. We now do this via a more direct approach; namely, the following holds by Lemma 13 when $\rho_n \ll \sigma_n \ll \sigma$ and $\rho_n \ll \rho \ll \sigma$:

$$\begin{aligned} D(\rho_n \| \sigma_n) - D(\rho \| \sigma) &= \text{Tr} [\rho_n (\log \rho_n - \log \sigma_n)] - \text{Tr} [\rho (\log \rho - \log \sigma)] \\ &= \text{Tr} [P_\rho (\rho_n (\log \rho_n - \log \sigma_n) P_\rho)] - \text{Tr} [P_\rho \rho (\log \rho - \log \sigma) P_\rho]. \end{aligned}$$

Here, P_ρ is the projector onto the support of ρ . We may now perform a Taylor’s expansion by considering the operator function $f(A_1, A_2) = P_\rho (A_1 (\log A_1 - \log A_2)) P_\rho$, i.e., the previously considered function sandwiched by P_ρ , and arrive at the desired result by ensuring uniform integrability of the remainder terms. The detailed arguments are given in Page 21.

Comment: *Eq. (19a): this is not a density operator in the case that $\|\hat{s}_n(\rho)\|_1 > 1$. The definition of $\hat{\rho}_n$ should be modified in an obvious way, which seems to be also used in the proof of Proposition 1. In Eq. (19a): also the notation $\mathbb{1}_{\hat{s}^{(n)}(\rho) \leq 1}$ etc, should better be explained.*

Response: Thank you for pointing out these typos, which have been fixed in the revised tomographic scheme mentioned earlier. We have also mentioned in the main text that $\mathbb{1}_{\mathcal{A}}$ denotes the indicator of set \mathcal{A} , which in our context is used as the indicator of a probabilistic event \mathcal{A} .

Comment: *Eqs. (30) (and elsewhere) it would really be better to use a notation that shows that these are also functions of t . P. 33, first equation: which norm is this? (maybe it should be $\|\cdot\|_1$?). P. 33, line 13 (displayed equation): the first term is not correct.*

Response: Corrected.

Comment: *Since the statements and their proofs are at different places in the paper, I would suggest to use one counter for all Lemmas, Propositions, Theorems, etc. Separate numbering makes them harder to find in the text.*

Response: Revised as suggested.

Reviewer 2

We thank the reviewer for the valuable feedback and comments. Below, please find a detailed response to each comment.

Comment: *The question is well motivated and a good fit with the chosen journal. The results are interesting, very much non-trivial, and will certainly find more applications in the future.*

Response: We thank the reviewer for the positive assessment of our article.

Comment: *I am wondering if the convergence results have further interpretations. E.g. (10) looks closely related to χ^2 divergences. In particular, (8) seems to include a weighted L^2 -norm, see e.g. (<https://arxiv.org/pdf/2102.04146>).*

Response: The reviewer is right that the expression in (10) resembles something like a χ^2 divergence. We have briefly noted this in Page 7 as stated below :

The RHS of (12) is reminiscent of the expression for χ^2 divergence and can be interpreted as a weighted L^2 norm between the limits L_1 and L_2 (see e.g., [89]).

One plausible interpretation could be attributed to the fact that KL divergence locally behaves (quadratically) like χ^2 divergence for small perturbations of the first argument around the second argument. Here, the perturbations are characterized by the limiting variable asymptotically and so it is not very surprising that the expression resembles χ^2 divergence with the densities replaced by the limiting variables. For the expression in (8), we may think of a similar interpretation since the generalization of χ^2 divergence to the non-commutative setting (see [94]) also involves a weighted L^2 norm similar to that defined in <https://arxiv.org/pdf/2102.04146>.

Comment: *A few derivations in the proof could use expanded explanations. E.g. Equations 24a ff. and top of page 29.*

Response: We have added more details to the derivations as suggested.

Comment: *Some inequalities should be equalities. E.g. (50a) and some others directly after.*

Response: Corrected. Thank you for pointing these out.

Comment: *The derivation of the continuity bound on page 37 seems similar to the relative entropy continuity bounds in (<https://arxiv.org/pdf/2102.04146>) ?*

Response: This is an interesting observation. While there is similarity, there are also some differences. The proof of Lemma 2.2. of the arxiv article and our continuity bound rely on different integral expressions for relative entropy in terms of weighted L^2 norm and trace norm between the density operators, respectively. Also, Lemma 2.2. focuses on continuity of relative entropy in terms of the weighted L^2 norm between its arguments while we bound the difference of two relative entropies in terms of trace distance.