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 $\mathbb{E}[f(X_n)] \to \mathbb{E}[f(X)]$ for all bounded continuous functions $f : \mathfrak{S} \to \mathbb{R}$. 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 $f : \mathfrak{X} \to \mathfrak{B}$ is said to be integrable (in the sense of Bochner) if there exists a sequence of simple functions g_n such that $g_n \to f$, μ-a.e., and

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

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 $\left(r_{n_{k_j}}(\rho_{n_{k_j}} - \rho), r_{n_{k_j}}(\sigma_{n_{k_j}} - \sigma)\right) \xrightarrow{w} (L_1, L_2)$ that converges almost surely from a sequence $\left(r_{n_k}(\rho_{n_k} - \rho), r_{n_k}(\sigma_{n_k} - \sigma)\right) \xrightarrow{w} (L_1, L_2)$ 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, $\big((r_{n_k}(\rho_{n_k}-\rho), r_{n_k}(\sigma_{n_k}-\rho)\big) \xrightarrow{w} (L_1, L_2)$ 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 $\big((r_{n_{k_j}}(\rho_{n_{k_j}}-\rho), r_{n_{k_j}}(\sigma_{n_{k_j}}-\rho)\big) \to (L_1, L_2)$ 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

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

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

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

Since r_n is positive and the above equation has to hold for every M, taking limit $M \to \infty$ implies that $\left\|P_\rho^\perp L_1 P_\rho^\perp\right\|_1 = 0$. 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, $\mathrm{Tr}\,[AB] = \mathrm{Tr}\,[PAPBP]$.

(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 $\rho_n \ll \rho \ll \sigma$:

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

Here, P_ρ is the projector onto the support of ρ. We may now perform a Taylor's expansion by considering the operator function $f(A_1, A_2) = P_\rho\big(A_1(\log A_1 - \log A_2)\big)P_\rho$, 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 $\mathbb{1}_{\hat{\mathbf{s}}^{(n)}(\rho) \leq 1}$ 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 $L2$-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 interepreted 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.